INTERNATIONAL TABLES for CRYSTALLOGRAPHY

Volume

A

Space-group symmetry

Edited by Th. Hahn

Fifth edition

INTERNATIONAL TABLES
FOR
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Editor Theo Hahn
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Editors Hans Wondratschek and Ulrich Müller
First Edition 2004

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INTERNATIONAL TABLES
FOR
CRYSTALLOGRAPHY

Volume A
SPACE-GROUP SYMMETRY

Edited by
THEO HAHN

Fifth edition

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† Deceased.

Contents

Foreword to the First Edition

On behalf of the International Union of Crystallography the Editor of the present work wishes to express his sincere gratitude to the following organisations and institutions for their generous support, financial, in providing computer time, and otherwise, which has made possible the publication of this volume:

Centre d'études nucléaires de Saclay, Gif sur Yvette, France;

Lindgren fund of the Department of Earth and Planetary Sciences, Massachusetts Institute of Technology, Cambridge, MA, U.S.A.;

Ministère de l'Industrie et de la Recherche (DGRST), République de France, Paris, France;

Rekencentrum der Rijksuniversiteit, Groningen, The Netherlands, and its Director, Dr. D. W. Smits;

Rheinisch-Westfälische Technische Hochschule, Aachen, Federal Republic of Germany.

All members of the editorial team have contributed their time and talent to the whole work. The authors of the theoretical sections are given on the title page of each section. The contributors to the space-group tables are listed in the *Preface*.

The Editor wants to extend his particular appreciation to the following individuals: A. Vos (Groningen) has acted as secretary to the Commission since 1977; she has contributed greatly by coordinating and guiding the work and by 'keeping us down to earth' when the discussions tended to become too theoretical. D. S. Fokkema (Groningen) has carefully and patiently carried out all of the programming and computational work, both scientific and with respect to the computer typesetting of the space-group tables. The two senior members of the Commission, M. J. Buerger (Cambridge, MA) and J. D. H. Donnay (Montreal), deserve our respect for their constant and active participation. An unusual amount of help and consultation has been provided by H. Arnold (Aachen), W. Fischer (Marburg/Lahn) and H. Wondratschek (Karlsruhe). Mrs. D. Arnold has, where necessary, corrected and improved the space-group diagrams. The Union's Technical Editor, D. W. Penfold (Chester), very expertly has handled all problems of printing, lay-out and production. Various contributions by the following persons were of great benefit: D. W. J. Cruickshank (Manchester), E. Hellner (Marburg/Lahn), W. H. Holser (Eugene, OR), J. A. lbers (Evanston, IL), V. A. Koptsik (Moscow), J. Neubüser (Aachen), D. P. Shoemaker (Corvallis, OR).

The officers of the International Union of Crystallography who served during the preparation of these *Tables* have given their constant support and advice, in particular the two General Secretaries and Treasurers, S. E. Rasmussen (Aarhus) and K. V. J. Kurki-Suonio (Helsinki). The Union's Executive Secretary, J. N. King (Chester), has smoothed the administrative process throughout the work.

Last, but not least, the Editor is greatly indebted to his secretaries Ms E. David and Ms A. Puhl (Aachen) for their able and willing secretarial assistance.

Finally, the Editor wishes to state that the work on these *Tables*, even though at times controversial and frustrating, was always interesting and full of surprises. He hopes that all members of the editorial team will remember it as a stimulating and rewarding experience.

Aachen, January 1983 — Theo Hahn

Foreword to the Second, Revised Edition

The First Edition of this volume appeared in December 1983. In July 1984 a 'Reprint with Corrections' was undertaken. It contained about 30 corrections which were also published in *Acta Cryst.* (1984). A**40**, 485. In May 1985 a *Brief Teaching Edition* appeared. The present Second Edition of Volume A is considerably revised, and new material has been added; the major changes are:

(1) Corrections of all errors which have come to my attention; again, a list of these corrections will be published in *Acta Cryst.* Section A.

(2) In a number of places text portions or footnotes have been added or revised in order to incorporate new material or to enhance the clarity of the presentation. This applies especially to part (iv) of *Computer Production of Volume A* and to Sections 1, 2.1, 2.6, 2.11, 2.13, 2.16, 5.3, 8.2.2, 8.2.6, 9.1, 9.2, 9.3, 10.2, 10.4, and 14.3.

(3) References have been added, corrected or replaced by more recent ones, especially in Sections 2, 8, 9, 10, and 14.

(4) The *Subject Index* has been considerably revised.

(5) New diagrams have been prepared for the 17 plane groups (Section 6) and for the 25 trigonal space groups in Section 7. It is planned that in the next edition also the tetragonal and hexagonal space groups will receive new diagrams.* In order to conform to the triclinic, monoclinic, and orthorhombic space-group diagrams, in the new diagrams the symmetry elements are given on the left and the general position on the right.

(6) The major addition, however, is the incorporation of two new sections, 8.3.6 and 15, on normalizers of space groups. In Section 8.3.6 normalizers are treated within the framework of space-group symmetry, whereas Section 15 contains complete lists for affine and Euclidean normalizers of plane groups, space groups, and point groups. Both sections contain examples, applications, and suitable references. The incorporation of Section 8.3.6 has necessitated a repagination of all pages beyond Section 8.

I am indebted to all authors and readers who have supplied corrections and improvements. Particular thanks are due to E. Koch and W. Fischer (Marburg) and to H. Wondratschek (Karlsruhe) for writing the new Sections 15 and 8.3.6. I am grateful to R. A. Becker (Aachen) for the preparation of the new diagrams and to D. W. Penfold and M. H. Dacombe (Chester) for the technical editing of this volume.

Aachen, October 1986 — Theo Hahn

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* The 1989 Reprint of the Second, Revised Edition contains new diagrams for the hexagonal space groups and for the tetragonal space groups of crystal class 4/*mmm*.

Foreword to the Third, Revised Edition

The Second, Revised Edition of this volume appeared in 1987, a Reprint with Corrections followed in 1989. All corrections in the Second Edition were also published in *Acta Cryst.* (1987). A**43**, 836–838. The present Third Edition of Volume A contains corrections of all errors which have come to my attention, mainly in Sections 1 and 2. A list of these errors will be published again in *Acta Cryst.* Section A.

The main feature of the Third Edition is the incorporation of new diagrams for the tetragonal and, in particular, for the cubic space groups. With these additions the present volume contains new diagrams for the plane groups and for all tetragonal, trigonal, hexagonal, and cubic space groups. Revised diagrams for the triclinic, monoclinic, and orthorhombic space groups are planned for the next edition.

The cubic diagrams have been thoroughly re-designed. They contain, among others, new symbols for the 'inclined' two- and threefold axes, explicit graphical indication of the horizontal $\bar{4}$-axes (rather than their twofold 'subaxes'), complete sets of 'heights' (fractions) for the horizontal fourfold axes and for the $\bar{4}$-inversion points, as well as for the symmetries $4_2/m$ and $6_3/m$ in cubic, tetragonal, and hexagonal space groups. These changes have required also substantial modifications in Section 1.4. This section and its footnotes should be helpful towards a better understanding of the complexities of the cubic diagrams. Finally, Table 5.1 has been extended by one page (p. 80).

I am indebted to all authors and readers who have supplied corrections and improvements. I am grateful to R. A. Becker (Aachen) for the preparation of the new diagrams, to H. Arnold (Aachen), E. Koch and W. Fischer (Marburg) and to H. Wondratschek (Karlsruhe) for helpful discussions on and checking of the cubic diagrams, and to M. H. Dacombe (Chester) for the technical editing of this volume.

Aachen, January 1992 — THEO HAHN

Foreword to the Fourth, Revised Edition

Only two years ago, in 1992, the Third, Revised Edition of this volume appeared. A list of corrections in the Third Edition was published in *Acta Cryst.* (1993). A**49**, 592–593. The present Fourth Edition of Volume A contains corrections of all errors which have been brought to my attention, mainly in Section 2. A list of these errors will again be published in *Acta Cryst.* Section A.

There are four novel features in the Fourth Edition:

(i) The incorporation of new diagrams for the triclinic, monoclinic, and orthorhombic space groups. With these additions, the space-group-diagram project is completed, *i.e.* all 17 plane-group and 230 space-group descriptions now contain new diagrams. Also, the explanatory diagrams in Section 2.6 (Figs. 2.6.1 to 2.6.10) are newly done.

(ii) The new graphical symbol · · — · ·— for 'double' glide planes *e* oriented 'normal' and 'inclined' to the plane of projection has been incorporated in the following 17 space-group diagrams (*cf.* de Wolff *et al.*, *Acta Cryst.* (1992). A**48**, 727–732):

Orthorhombic:	*Abm*2 (No. 39), *Aba*2 (41), *Fmm*2 (42), *Cmca* (64), *Cmma* (67), *Ccca* (68) (both origins), *Fmmm* (69);
Tetragonal:	*I*4*mm* (107), *I*4*cm* (108), $I\bar{4}2m$ (121), *I*4/*mmm* (139), *I*4/*mcm* (140);
Cubic:	$Fm\bar{3}$ (202), $Fm\bar{3}m$ (225), $Fm\bar{3}c$ (226), $I\bar{4}3m$ (217), $Im\bar{3}m$ (229).

(iii) These changes and the publication of three *Nomenclature Reports* by the International Union of Crystallography in recent years have necessitated substantial additions to and revisions of Section 1, *Symbols and Terms*; in particular, printed and graphical symbols, as well as explanations, for the new 'double' glide plane *e* have been added, as have been references to the three nomenclature reports.

(iv) The introduction of the glide plane *e* leads to new space-group symbols for the following five space groups:

Space group No.	39	41	64	67	68
Present symbol:	*Abm*2	*Aba*2	*Cmca*	*Cmma*	*Ccca*
New symbol:	*Aem*2	*Aea*2	*Cmce*	*Cmme*	*Ccce*.

The new symbols have been added to the headlines of these space groups; they are also incorporated in the right-hand column of Table 12.5. It is intended that these new symbols will be given as the 'main' symbols in the next edition of Volume A.

It is a great pleasure to thank R. A. Becker (Aachen) for his year-long work of preparing the new space-group diagrams. I am again indebted to H. Arnold (Aachen), E. Koch and W. Fischer (Marburg), and to H. Wondratschek (Karlsruhe) for the patient and careful checking of the new diagrams. I am grateful to S. E. King (Chester) for the technical editing of this volume and to E. Nowack (Aachen) for help in the rearrangement of Section 1.

Aachen, January 1994 — THEO HAHN

Foreword to the Fifth, Revised Edition

Six years ago, in 1995, the Fourth Edition of Volume A appeared, followed by corrected reprints in 1996 and 1998. A list of corrections and innovations in the Fourth Edition was published in *Acta Cryst.* (1995). A**51**, 592–595.

The present Fifth Edition is much more extensively revised than any of its predecessors, even though the casual reader may not notice these changes. In keeping with the new millennium, the production of this edition has been completely computer-based. Although this involved an unusually large amount of effort at the start, it will permit easy and flexible modifications, additions and innovations in the future, including a possible electronic version of the volume. In the past, all corrections had to be done by 'cut-and-paste' work based on the printed version of the book.

The preparation of this new edition involved the following steps:

(i) The space-group tables (Parts 6 and 7) were reprogrammed and converted to LaTeX by M. I. Aroyo and P. B. Konstantinov in Sofia, Bulgaria, and printed from the LaTeX files. This work is described in the article '*Computer Production of Volume A*'.

(ii) The existing, recently prepared space-group diagrams were scanned and included in the LaTeX files.

(iii) The text sections of the volume were re-keyed in SGML format under the supervision of S. E. Barnes and N. J. Ashcroft (Chester) and printed from the resulting SGML files.

The following scientific innovations of the Fifth Edition are noteworthy, apart from corrections of known errors and flaws; these changes will again be published in *Acta Cryst.* Section A.

(1) The incorporation of the new symbol for the 'double' glide plane '*e*' into five space-group symbols, which was started in the Fourth Edition (*cf. Foreword to the Fourth Edition* and Chapter 1.3), has been completed:

In the headlines of space groups Nos. 39, 41, 64, 67 and 68, the new symbols containing the '*e*' glide are now the 'main' symbols and the old symbols are listed as 'Former space-group symbol'; the new symbols also appear in the diagrams.

The symbol '*e*' now also appears in the table in Section 1.3.1 and in Tables 3.1.4.1, 4.3.2.1, 12.3.4.1, 14.2.3.2 and 15.2.1.3.

(2) Several parts of the text have been substantially revised and reorganized, especially the article *Computer Production of Volume A*, Sections 2.2.13, 2.2.15 and 2.2.16, Parts 8, 9 and 10, Section 14.2.3, and Part 15.

(3) A few new topics have been added:

Section 9.1.8, with a description of the Delaunay reduction (H. Burzlaff & H. Zimmermann);

Chapter 9.3, *Further properties of lattices* (B. Gruber);

in Chapter 15.2, the affine normalizers of orthorhombic and monoclinic space groups are now replaced by Euclidean normalizers for special metrics (E. Koch, W. Fischer & U. Müller).

(4) The fonts for symbols for groups and for 'augmented' (4 × 4) matrices and (4 × 1) columns have been changed, *e.g.* $\mathcal{G}$ instead of $\mathfrak{G}$, $\mathbb{W}$ instead of $\mathscr{W}$ and $\mathbb{r}$ instead of $\mathscr{r}$; *cf.* Chapter 1.1.

It is my pleasure to thank all those authors who have contributed new programs or sections or who have substantially revised existing articles: M. I. Aroyo (Sofia), H. Burzlaff (Erlangen), B. Gruber (Praha), E. Koch (Marburg), P. B. Konstantinov (Sofia), U. Müller (Marburg), H. Wondratschek (Karlsruhe) and H. Zimmermann (Erlangen). I am indebted to S. E. Barnes and N. J. Ashcroft (Chester) for the careful and dedicated technical editing of this volume. Finally, I wish to express my sincere thanks to K. Stróż (Katowice) for his extensive checking of the data in the space-group tables using his program *SPACER* [*J. Appl. Cryst.* (1997), **30**, 178–181], which has led to several subtle improvements in the present edition.

Aachen, November 2001 — Theo Hahn

Preface

By Th. Hahn

History of the *International Tables*

The present work can be considered as the first volume of the third series of the *International Tables*. The first series was published in 1935 in two volumes under the title *Internationale Tabellen zur Bestimmung von Kristallstrukturen* with C. Hermann as editor. The publication of the second series under the title *International Tables for X-ray Crystallography* started with Volume I in 1952, with N. F. M. Henry and K. Lonsdale as editors. [Full references are given at the end of Part 2. Throughout this volume, the earlier editions are abbreviated as *IT* (1935) and *IT* (1952).] Three further volumes followed in 1959, 1962 and 1974. Comparison of the title of the present series, *International Tables for Crystallography*, with those of the earlier series reveals the progressively more general nature of the tables, away from the special topic of X-ray structure determination. Indeed, it is the aim of the present work to provide data and text which are useful for all aspects of crystallography.

The present volume is called A in order to distinguish it from the numbering of the previous series. It deals with crystallographic symmetry in 'direct space'. There are six other volumes in the present series: A1 (*Symmetry relations between space groups*), B (*Reciprocal space*), C (*Mathematical, physical and chemical tables*), D (*Physical properties of crystals*), E (*Subperiodic groups*) and F (*Crystallography of biological macromolecules*).

The work on this series started at the Rome Congress in 1963 when a new 'Commission on *International Tables*' was formed, with N. F. M. Henry as chairman. The main task of this commission was to prepare and publish a *Pilot Issue*, consisting of five parts as follows:

Year	Part	Editors
1972	Part 1: Direct Space	N. F. M. Henry
1972	Part 2: Reciprocal Space	Th. Hahn & H. Arnold
1969	Part 3: Patterson Data	M. J. Buerger
1973	Part 4: Synoptic Tables	J. D. H. Donnay, E. Hellner & N. F. M. Henry
1969	Part 5: Generalised Symmetry	V. A. Koptsik

The *Pilot Issue* was widely distributed with the aim of trying out the new ideas on the crystallographic community. Indeed, the responses to the *Pilot Issue* were a significant factor in determining the content and arrangement of the present volume.

Active preparation of Volume A started at the Kyoto Congress in 1972 with a revised Commission under the Chairmanship of Th. Hahn. The main decisions on the new volume were taken at a full Commission meeting in August 1973 at St. Nizier, France, and later at several smaller meetings at Amsterdam (1975), Warsaw (1978) and Aachen (1977/78/79). The manuscript of the volume was essentially completed by the time of the Ottawa Congress (1981), when the tenure of the Commission officially expired.

The major work of the preparation of the space-group tables in the First Edition of Volume A was carried out between 1972 and 1978 by D. S. Fokkema at the Rekencentrum of the Rijksuniversiteit Groningen as part of the *Computer trial project*, in close cooperation with A. Vos, D. W. Smits, the Editor and other Commission members. The work developed through various stages until at the end of 1978 the complete plane-group and space-group tables were available in printed form. The following years were spent with several rounds of proofreading of these tables by all members of the editorial team, with preparation and many critical readings of the various theoretical sections and with technical preparations for the actual production of the volume.

The First Edition of Volume A was published in 1983. With increasing numbers of later 'Revised Editions', however, it became apparent that corrections and modifications could not be done further by 'cut-and-paste' work based on the printed version of the volume. Hence, for this Fifth Edition, the plane- and space-group data have been reprogrammed and converted to an electronic form by M. I. Aroyo and P. B. Konstantinov (details are given in the following article *Computer Production of Volume A*) and the text sections have been re-keyed in SGML format. The production of the Fifth Edition was thus completely computer-based, which should allow for easier corrections and modifications in the future, as well as the possibility of an electronic version of the volume.

Scope and arrangement of Volume A

The present volume treats the symmetries of one-, two- and three-dimensional space groups and point groups in direct space. It thus corresponds to Volume 1 of *IT* (1935) and to Volume I of *IT* (1952). Not included in Volume A are 'partially periodic groups', like layer, rod and ribbon groups, or groups in dimensions higher than three. (Subperiodic groups are discussed in Volume E of this series.) The treatment is restricted to 'classical' crystallographic groups (groups of rigid motions); all extensions to 'generalized symmetry', like antisymmetric groups, colour groups, symmetries of defect crystals *etc.*, are beyond the scope of this volume.

Compared to its predecessors, the present volume is considerably increased in size. There are three reasons for this:

(i) Extensive additions and revisions of the data and diagrams in the *Space-group tables* (Parts 6 and 7), which lead to a standard layout of *two* pages per space group (see Section 2.2.1), as compared to *one* page in *IT* (1935) and *IT* (1952);

(ii) Replacement of the introductory text by a series of *theoretical sections*;

(iii) Extension of the *synoptic tables*.

The new features of the *description of each space group*, as compared to *IT* (1952), are as follows:

(1) Addition of Patterson symmetry;

(2) New types of diagrams for triclinic, monoclinic and orthorhombic space groups;

(3) Diagrams for cubic space groups, including stereodiagrams for the general positions;

(4) Extension of the origin description;

(5) Indication of the asymmetric unit;

(6) List of symmetry operations;

(7) List of generators;

(8) Coordinates of the general position ordered according to the list of generators selected;

(9) Inclusion of oriented site-symmetry symbols;

(10) Inclusion of projection symmetries for all space groups;

(11) Extensive listing of maximal subgroups and minimal supergroups;

(12) Special treatment (up to six descriptions) of monoclinic space groups;

(13) Symbols for the lattice complexes of each space group (given as separate tables in Part 14).

(14) Euclidean and affine normalizers of plane and space groups are listed in Part 15.

The volume falls into two parts which differ in content and, in particular, in the level of approach:

The first part, Parts 1–7, comprises the plane- and space-group tables themselves (Parts 6 and 7) and those parts of the volume which are directly useful in connection with their use (Parts 1–5). These include definitions of symbols and terms, a guide to the use of the tables, the determination of space groups, axes transformations, and synoptic tables of plane- and space-group symbols. Here, the emphasis is on the *practical* side. It is hoped that these parts with their many examples may be of help to a student or beginner of crystallography when they encounter problems during the investigation of a crystal.

In contrast, Parts 8–15 are of a much higher *theoretical* level and in some places correspond to an advanced textbook of crystallography. They should appeal to those readers who desire a deeper theoretical background to space-group symmetry. Part 8 describes an algebraic approach to crystallographic symmetry, followed by treatments of lattices (Part 9) and point groups (Part 10). The following three parts deal with more specialized topics which are important for the understanding of space-group symmetry: symmetry operations (Part 11), space-group symbols (Part 12) and isomorphic subgroups (Part 13). Parts 14 and 15 discuss lattice complexes and normalizers of space groups, respectively.

At the end of each part, references are given for further studies.

Contributors to the space-group tables

The crystallographic calculations and the computer typesetting procedures for the First Edition (1983) were performed by D. S. Fokkema. For the Fifth Edition, the space-group data were reprogrammed and converted to an electronic form by M. I. Aroyo and P. B. Konstantinov. Details are given in the following article *Computer Production of Volume A*.

The following authors supplied lists of data for the space-group tables in Parts 6 and 7:

Headline and Patterson symmetry: Th. Hahn & A. Vos.
Origin: J. D. H. Donnay, Th. Hahn & A. Vos.
Asymmetric unit: H. Arnold.
Names of symmetry operations: W. Fischer & E. Koch.
Generators: H. Wondratschek.
Oriented site-symmetry symbols: J. D. H. Donnay.
Maximal non-isomorphic subgroups: H. Wondratschek.
Maximal isomorphic subgroups of lowest index: E. F. Bertaut & Y. Billiet; W. Fischer & E. Koch.
Minimal non-isomorphic supergroups: H. Wondratschek, E. F. Bertaut & H. Arnold.

The *space-group diagrams* for the First Edition were prepared as follows:

Plane groups: Taken from *IT* (1952).

Triclinic, monoclinic & orthorhombic space groups: M. J. Buerger; amendments and diagrams for ‘synoptic’ descriptions of monoclinic space groups by H. Arnold. The diagrams for the space groups Nos. 47–74 (crystal class *mmm*) were taken, with some modifications, from the book: M. J. Buerger (1971), *Introduction to Crystal Geometry* (New York: McGraw-Hill) by kind permission of the publisher.

Tetragonal, trigonal & hexagonal space groups: Taken from *IT* (1952); amendments and diagrams for ‘origin choice 2’ by H. Arnold.

Cubic space groups, diagrams of symmetry elements: M. J. Buerger; amendments by H. Arnold & W. Fischer. The diagrams were taken from the book: M. J. Buerger (1956), *Elementary Crystallography* (New York: Wiley) by kind permission of the publisher.

Cubic space groups, stereodiagrams of general positions: G. A. Langlet.

New diagrams for all 17 plane groups and all 230 space groups were incorporated in stages in the Second, Third and Fourth Editions of this volume. This project was carried out at Aachen by R. A. Becker. All data and diagrams were checked by at least two further members of the editorial team until no more discrepancies were found.

At the conclusion of this *Preface*, it should be mentioned that during the preparation of this volume several problems led to long and sometimes controversial discussions. One such topic was the subdivision of the hexagonal crystal family into either hexagonal and trigonal or hexagonal and rhombohedral systems. This was resolved in favour of the hexagonal–trigonal treatment, in order to preserve continuity with *IT* (1952); the alternatives are laid out in Sections 2.1.2 and 8.2.8.

An even greater controversy evolved over the treatment of the monoclinic space groups and in particular over the question whether the *b* axis, the *c* axis, or both should be permitted as the ‘unique’ axis. This was resolved by the Union's Executive Committee in 1977 by taking recourse to the decision of the 1951 General Assembly at Stockholm [*cf. Acta Cryst.* (1951). **4**, 569]. It is hoped that the treatment of monoclinic space groups in this volume (*cf.* Section 2.2.16) represents a compromise acceptable to all parties concerned.

Computer Production of Volume A

First Edition, 1983

BY D. S. FOKKEMA

Starting from the 'Generators selected' for each space group, the following data were produced by computer on the so-called 'computer tape':

(i) The coordinate triplets of the general and special positions;
(ii) the locations of the symmetry elements;
(iii) the projection data;
(iv) the reflection conditions.

For some of these items minor interference by hand was necessary.

Further data, such as the headline and the sub- and supergroup entries, were supplied externally, in the form of punched cards. These data and their authors are listed in the *Preface*. The file containing these data is called the 'data file'. To ensure that the data file was free of errors, all its entries were punched and coded twice. The two resulting data files were compared by a computer program and corrected independently by hand until no more differences remained.

By means of a typesetting routine, which directs the different items to given positions on a page, the proper lay-out was obtained for the material on the computer tape and the data file. The resulting 'page file' also contained special instructions for the typesetting machine, for instance concerning the typeface to be used. The final typesetting in which the page file was read sequentially line by line was done without further human interference. After completion of the pages the space-group diagrams were added. Their authors are listed in the *Preface* too.

In the following a short description of the computer programs is given.

(i) *Positions*

In the computer program the coordinate triplets of the *general* position are considered as matrix representations of the symmetry operations (*cf.* Section 2.11) and are given by (4×4) matrices. The matrices of the general position are obtained by single-sided multiplication of the matrices representing the generators until no new matrices are found. Resulting matrices which differ only by a lattice translation are considered as equal. The matrices are translated into the coordinate-triplet form by a printing routine.

The coordinate triplets of the *special* positions describe points, lines, or planes, each of which is mapped onto itself by at least one symmetry operation of the space group (apart from the identity). This means that they can be found as a subspace of three-dimensional space which is invariant with respect to this symmetry operation. In practice, for a particular symmetry operation W the special coordinate triplet E representing the invariant subspace is computed. All triplets of the corresponding Wyckoff position are obtained by applying all symmetry operations of the space group to E. In the resulting list triplets which are identical to a previous one, or differ by a lattice translation from it, are omitted. To generate all special Wyckoff positions the complete procedure, mentioned above, is repeated for all symmetry operations W of the space group. Finally, it was decided to make the sequence of the Wyckoff positions and the first triplet of each position the same as in earlier editions of the *Tables*. Therefore, the Wyckoff letters and the first triplets were supplied by hand after which the necessary arrangements were carried out by the computer program.

(ii) *Symmetry operations*

Under the heading *Symmetry operations*, for each of the operations the name of the operation and the location of the corresponding symmetry element are given. To obtain these entries a list of all conceivable symmetry operations including their names was supplied to the computer. After decomposition of the translation part into a location part and a glide or screw part, each symmetry operation of a space group is identified with an operation in the list by comparing their rotation parts and their glide or screw parts. The location of the corresponding symmetry element is, for symmetry operations without glide or screw parts, calculated as the subspace of three-dimensional space that is invariant under the operation. For operations containing glide or screw components, this component is first subtracted from the (4×4) matrix representing the operation according to the procedure described in Section 11.3, and then the invariant subspace is calculated.

From the complete set of solutions of the equation describing the invariant subspace it must be decided whether this set constitutes a point, a line, or a plane. For rotoinversion axes the location of the inversion point is found from the operation itself, whereas the location and direction of the axis is calculated from the square of the operation.

(iii) *Symmetry of special projections*

The coordinate doublets of a projection are obtained by applying a suitable projection operator to the coordinate triplets of the general position. The coordinate doublets, *i.e.* the projected points, exhibit the symmetry of a plane group for which, however, the coordinate system may differ from the conventional coordinate system of that plane group. The program contains a list with all conceivable transformations and with the coordinate doublets of each plane group in standard notation. After transformation, where necessary, the coordinate doublets of the particular projection are identified with those of a standard plane group. In this way the symmetry group of the projection and the relations between the projected and the conventional coordinate systems are determined.

(iv) *Reflection conditions*

For each Wyckoff position the triplets h, k, l are divided into two sets,

(1) triplets for which the structure factors are systematically zero (extinctions), and

(2) triplets for which the structure factors are not systematically zero (reflections).

Conditions that define triplets of the second set are called reflection conditions.

The computer program contained a list of all conceivable reflection conditions. For each Wyckoff position the general and special reflection conditions were found as follows. A set of h, k, l triplets with h, k, and l varying from 0 to 12 was considered. For the Wyckoff position under consideration all structure factors were calculated for this set of h, k, l triplets for positions $x = 1/p$, $y = 1/q$, $z = 1/r$ with p, q, and r different prime numbers larger than 12.

In this way accidental zeros were avoided. The h, k, l triplets were divided into two groups: those with zero and those with non-zero structure factors. The reflection conditions for the Wyckoff position under consideration were selected from the stored list of all conceivable reflection conditions by the following procedure:

(1) All conditions which apply to at least one h, k, l triplet of the set with structure factor zero are deleted from the list of all conceivable reflection conditions,

(2) conditions which do not apply to at least one h, k, l triplet of the set with structure factor non-zero are deleted,

(3) redundant conditions are removed by ensuring that each h, k, l triplet with structure factor non-zero is described by one reflection condition only.

Finally the completeness of the resulting reflection conditions for the Wyckoff position was proved by verifying that for each h, k, l triplet with non-zero structure factor there is a reflection condition that describes it. If this turned out not to be the case the list of all conceivable reflection conditions stored in the program was evidently incomplete and had to be extended by the missing conditions, after which the procedure was repeated.

Fifth, Revised Edition, 2002

By M. I. Aroyo and P. B. Konstantinov

The computer production of the space-group tables in 1983 described above served well for the first and several subsequent editions of Volume A. With time, however, it became apparent that a modern, versatile and flexible computer version of the entire volume was needed (*cf. Preface* and *Foreword to the Fifth, Revised Edition*).

Hence, in October 1997, a new project for the electronic production of the Fifth Edition of Volume A was started. Part of this project concerned the computerization of the plane- and space-group tables (Part 6 and 7), excluding the space-group diagrams. The aim was to produce a PostScript file of the content of these tables which could be used for printing from and in which the layout of the tables had to follow exactly that of the previous editions of Volume A. Having the space-group tables in electronic form opens the way for easy corrections and modifications of later editions, as well as for a possible future electronic edition of Volume A.

The LaTeX document preparation system [Lamport, L. (1994). *A Document Preparation System*, 2nd ed. Reading, MA: Addison-Wesley], which is based on the TeX typesetting software, was used for the preparation of these tables. It was chosen because of its high versatility and general availability on almost any computer platform.

A separate file was created for each plane and space group and each setting. These 'data files' contain the information listed in the plane- and space-group tables and are encoded using standard LaTeX constructs. These specially designed commands and environments are defined in a separate 'package' file, which essentially contains programs responsible for the typographical layout of the data. Thus, the main principle of LaTeX – keeping content and presentation separate – was followed as closely as possible.

The final typesetting of all the plane- and space-group tables was done by a single computer job, taking 1 to 2 minutes on a modern workstation. References in the tables from one page to another were automatically computed. The result is a PostScript file which can be fed to a laser printer or other modern printing or typesetting equipment.

The different types of data in the LaTeX files were either keyed by hand or computer generated, and were additionally checked by specially written programs. The preparation of the data files can be summarized as follows:

Headline, *Origin*, *Asymmetric unit*: hand keyed.

Symmetry operations: partly created by a computer program. The algorithm for the derivation of symmetry operations from their matrix representation is similar to that described in the literature [*e.g.* Hahn, Th. & Wondratschek, H. (1994). *Symmetry of Crystals*. Sofia: Heron Press]. The data were additionally checked by automatic comparison with the output of the computer program *SPACER* [Stróż, K. (1997). *SPACER: a program to display space-group information for a conventional and nonconventional coordinate system. J. Appl. Cryst.* **30**, 178–181].

Generators: transferred automatically from the database of the forthcoming Volume A1 of *International Tables for Crystallography*, *Symmetry Relations between Space Groups* (edited by H. Wondratschek & U. Müller), hereafter referred to as *IT* A1.

General positions: created by a program. The algorithm uses the well known generating process for space groups based on their solvability property (H. Wondratschek, Part 8 of this volume).

Special positions: The first representatives of the Wyckoff positions were typed in by hand. The Wyckoff letters are assigned automatically by the TeX macros according to the order of appearance of the special positions in the data file. The multiplicity of the position, the oriented site-symmetry symbol and the rest of the representatives of the Wyckoff position were generated by a program. Again, the data were compared with the results of the program *SPACER*.

Reflection conditions: hand keyed. A program for automatic checking of the special-position coordinates and the corresponding reflection conditions with h, k, l ranging from -20 to 20 was developed.

Symmetry of special projections: hand keyed.

Maximal subgroups and minimal supergroups: most of the data were automatically transferred from the data files of *IT* A1. The macros for their typesetting were reimplemented to obtain exactly the layout of Volume A. The data of isomorphic subgroups (IIc) with indices greater than 4 were added by hand.

The contents of the LaTeX files and the arrangement of the data correspond exactly to that of previous editions of this volume with the following exceptions:

(i) Introduction of the glide-plane symbol 'e' [Wolff, P. M. de, Billiet, Y., Donnay, J. D. H., Fischer, W., Galiulin, R. B., Glazer, A. M., Hahn, Th., Senechal, M., Shoemaker, D. P., Wondratschek, H., Wilson, A. J. C. & Abrahams, S. C. (1992). *Symbols for symmetry elements and symmetry operations. Acta Cryst.* A**48**, 727–732] in the conventional Hermann–Mauguin symbols as described in Chapter 1.3, Note (x). The new notation was also introduced for some origin descriptions and in the nonconventional Hermann–Mauguin symbols of maximal subgroups.

(ii) Changes in the subgroup and supergroup data following the *IT* A1 conventions:

(1) Introduction of space-group numbers for subgroups and supergroups.

(2) Introduction of braces indicating the conjugation relations for maximal subgroups of types I and IIa.

(3) Rearrangement of the subgroup data: subgroups are listed according to rising index and falling space-group number within the same lattice-relation type.

(4) Analogous rearrangement of the supergroup data: the minimal supergroups are listed according to rising index and increasing space-group number. In a few cases of type-II minimal supergroups, however, the index rule is not followed.

(5) Nonconventional symbols of monoclinic subgroups: in the cases of differences between Volume A and *IT* A1 for these symbols, those used in *IT* A1 have been chosen.

(6) Isomorphic subgroups: in listing the isomorphic subgroups of lowest index (type IIc), preference was given to the index and not to the direction of the principal axis (as had been the case in previous editions of this volume).

(iii) Improvements to the data in Volume A proposed by K. Stróż:

(1) Changes of the translational part of the generators (2) and (3) of $Fd\bar{3}$ (203), origin choice 2;

(2) Changes in the geometrical description of the glide planes of type $x, 2x, z$ for the groups $R3m$ (160), $R3c$ (161), $R\bar{3}m$ (166), $R\bar{3}c$ (167), and the glide planes $\bar{x}, y, x$ for $Fm\bar{3}m$ (225), $Fd\bar{3}m$ (227);

(3) Changes in the sequence of the positions and symmetry operations for the 'rhombohedral axes' descriptions of space groups $R32$ (155), $R3m$ (160), $R3c$ (161), $R\bar{3}m$ (166) and $R\bar{3}c$ (167), *cf.* Sections 2.2.6 and 2.2.10.

The electronic preparation of the plane- and space-group tables was carried out on various Unix and Windows-based computers in Sofia, Bilbao and Karlsruhe. The development of the computer programs and the layout macros in the package file was done in parallel by different members of the team, which included Asen Kirov (Sofia), Eli Kroumova (Bilbao), Preslav Konstantinov and Mois Aroyo. Hans Wondratschek and Theo Hahn contributed to the final arrangement and checking of the data.

International Tables for Crystallography (2006). Vol. A, Chapter 1.1, pp. 2–3.

1.1. Printed symbols for crystallographic items

BY TH. HAHN

1.1.1. Vectors, coefficients and coordinates

Printed symbol	Explanation
$\mathbf{a}, \mathbf{b}, \mathbf{c}$; or $\mathbf{a}_i$	Basis vectors of the direct lattice
a, b, c	Lengths of basis vectors, lengths of cell edges (Lattice or cell parameters)
α, β, γ	Interaxial (lattice) angles $\mathbf{b} \wedge \mathbf{c}$, $\mathbf{c} \wedge \mathbf{a}$, $\mathbf{a} \wedge \mathbf{b}$ (Lattice or cell parameters)
V	Cell volume of the direct lattice
$\mathbf{G}$	Matrix of the geometrical coefficients (metric tensor) of the direct lattice
g_{ij}	Element of metric matrix (tensor) $\mathbf{G}$
$\mathbf{r}$; or $\mathbf{x}$	Position vector (of a point or an atom)
r	Length of the position vector $\mathbf{r}$
$x\mathbf{a}, y\mathbf{b}, z\mathbf{c}$	Components of the position vector $\mathbf{r}$
x, y, z; or x_i	Coordinates of a point (location of an atom) expressed in units of a, b, c; coordinates of end point of position vector $\mathbf{r}$; coefficients of position vector $\mathbf{r}$
$\boldsymbol{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$	Column of point coordinates or vector coefficients
$\mathbf{t}$	Translation vector
t	Length of the translation vector $\mathbf{t}$
t_1, t_2, t_3; or t_i	Coefficients of translation vector $\mathbf{t}$
$\boldsymbol{t} = \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix}$	Column of coefficients of translation vector $\mathbf{t}$
$\mathbf{u}$	Vector with integral coefficients
u, v, w; or u_i	Integers, coordinates of a (primitive) lattice point; coefficients of vector $\mathbf{u}$
$\boldsymbol{u} = \begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}$	Column of integral point coordinates or vector coefficients
$\mathbf{o}$	Zero vector
$\boldsymbol{o}$	Column of zero coefficients
$\mathbf{a}', \mathbf{b}', \mathbf{c}'$; or $\mathbf{a}'_i$	New basis vectors after a transformation of the coordinate system (basis transformation)
$\mathbf{r}'$; or $\mathbf{x}'$; x', y', z'; or x'_i	Position vector and point coordinates after a transformation of the coordinate system (basis transformation)
$\tilde{\mathbf{r}}$; or $\tilde{\mathbf{x}}$; $\tilde{x}, \tilde{y}, \tilde{z}$; or $\tilde{x}_i$	New position vector and point coordinates after a symmetry operation (motion)

1.1.2. Directions and planes

Printed symbol	Explanation
$[uvw]$	Indices of a lattice direction (zone axis)
$\langle uvw \rangle$	Indices of a set of all symmetrically equivalent lattice directions
(hkl)	Indices of a crystal face, or of a single net plane (Miller indices)
$(hkil)$	Indices of a crystal face, or of a single net plane, for the hexagonal axes $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, $\mathbf{c}$ (Bravais–Miller indices)
$\{hkl\}$	Indices of a set of all symmetrically equivalent crystal faces ('crystal form'), or net planes
$\{hkil\}$	Indices of a set of all symmetrically equivalent crystal faces ('crystal form'), or net planes, for the hexagonal axes $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, $\mathbf{c}$
hkl	Indices of the Bragg reflection (Laue indices) from the set of parallel equidistant net planes (hkl)
d_{hkl}	Interplanar distance, or spacing, of neighbouring net planes (hkl)

1.1.3. Reciprocal space

Printed symbol	Explanation
$\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$; or $\mathbf{a}^*_i$	Basis vectors of the reciprocal lattice
a^*, b^*, c^*	Lengths of basis vectors of the reciprocal lattice
$\alpha^*, \beta^*, \gamma^*$	Interaxial (lattice) angles of the reciprocal lattice $\mathbf{b}^* \wedge \mathbf{c}^*$, $\mathbf{c}^* \wedge \mathbf{a}^*$, $\mathbf{a}^* \wedge \mathbf{b}^*$
$\mathbf{r}^*$; or $\mathbf{h}$	Reciprocal-lattice vector
h, k, l; or h_i	Coordinates of a reciprocal-lattice point, expressed in units of a^*, b^*, c^*, coefficients of the reciprocal-lattice vector $\mathbf{r}^*$
V^*	Cell volume of the reciprocal lattice
$\mathbf{G}^*$	Matrix of the geometrical coefficients (metric tensor) of the reciprocal lattice

1.1.4. Functions

Printed symbol	Explanation
$\rho(xyz)$	Electron density at the point x, y, z
$P(xyz)$	Patterson function at the point x, y, z
$F(hkl)$; or F	Structure factor (of the unit cell), corresponding to the Bragg reflection hkl
$\lvert F(hkl) \rvert$; or $\lvert F \rvert$	Modulus of the structure factor $F(hkl)$
$\alpha(hkl)$; or α	Phase angle of the structure factor $F(hkl)$

1.1.5. Spaces

Printed symbol	Explanation
n	Dimension of a space
X	Point
$\tilde{X}$	Image of a point X after a symmetry operation (motion)
E^n	(Euclidean) point space of dimension n
$\mathbf{V}^n$	Vector space of dimension n
$\mathbf{L}$	Vector lattice
L	Point lattice

1.1.6. Motions and matrices

Printed symbol	Explanation
W; M	Symmetry operation; motion
$(\boldsymbol{W}, \boldsymbol{w})$	Symmetry operation W, described by an $(n \times n)$ matrix $\boldsymbol{W}$ and an $(n \times 1)$ column $\boldsymbol{w}$
$\mathbb{W}$	Symmetry operation W, described by an $(n+1) \times (n+1)$ 'augmented' matrix
$\boldsymbol{I}$	$(n \times n)$ unit matrix
T	Translation
$(\boldsymbol{I}, \boldsymbol{t})$	Translation T, described by the $(n \times n)$ unit matrix $\boldsymbol{I}$ and an $(n \times 1)$ column $\boldsymbol{t}$
$\mathbb{T}$	Translation T, described by an $(n+1) \times (n+1)$ 'augmented' matrix
I	Identity operation
$(\boldsymbol{I}, \boldsymbol{o})$	Identity operation I, described by the $(n \times n)$ unit matrix $\boldsymbol{I}$ and the $(n \times 1)$ column $\boldsymbol{o}$
$\mathbb{I}$	Identity operation I, described by the $(n+1) \times (n+1)$ 'augmented' unit matrix

Printed symbol	Explanation
$\mathbb{r}$, or $\mathbb{X}$	Position vector (of a point or an atom), described by an $(n+1) \times 1$ 'augmented' column
$(\boldsymbol{P}, \boldsymbol{p})$; or $(\boldsymbol{S}, \boldsymbol{s})$	Transformation of the coordinate system, described by an $(n \times n)$ matrix $\boldsymbol{P}$ or $\boldsymbol{S}$ and an $(n \times 1)$ column $\boldsymbol{p}$ or $\boldsymbol{s}$
$\mathbb{P}$; or $\mathbb{S}$	Transformation of the coordinate system, described by an $(n+1) \times (n+1)$ 'augmented' matrix
$(\boldsymbol{Q}, \boldsymbol{q})$	Inverse transformation of $(\boldsymbol{P}, \boldsymbol{p})$
$\mathbb{Q}$	Inverse transformation of $\mathbb{P}$

1.1.7. Groups

Printed symbol	Explanation
$\mathcal{G}$	Space group
$\mathcal{T}$	Group of all translations of $\mathcal{G}$
$\mathcal{S}$	Supergroup; also used for site-symmetry group
$\mathcal{H}$	Subgroup
$\mathcal{E}$	Group of all motions (Euclidean group)
$\mathcal{A}$	Group of all affine mappings (affine group)
$\mathcal{N}_{\mathcal{E}}(\mathcal{G})$; or $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$	Euclidean or affine normalizer of a space group $\mathcal{G}$
$\mathcal{P}$	Point group
$\mathcal{C}$	*Eigensymmetry* (inherent symmetry) group
$[i]$	Index i of sub- or supergroup
G	Element of a space group $\mathcal{G}$

references

1.2. Printed symbols for conventional centring types

BY TH. HAHN

1.2.1. Printed symbols for the conventional centring types of one-, two- and three-dimensional cells

For 'reflection conditions', see Tables 2.2.13.1 and 2.2.13.3. For the new centring symbol *S*, see Note (iii) below.

Printed symbol	Centring type of cell	Number of lattice points per cell	Coordinates of lattice points within cell
One dimension			
𝓅	Primitive	1	0
Two dimensions			
p	Primitive	1	0, 0
c	Centred	2	0, 0; $\frac{1}{2}, \frac{1}{2}$
*h**	Hexagonally centred	3	0, 0; $\frac{2}{3}, \frac{1}{3}$; $\frac{1}{3}, \frac{2}{3}$
Three dimensions			
P	Primitive	1	0, 0, 0
C	*C*-face centred	2	0, 0, 0; $\frac{1}{2}, \frac{1}{2}$, 0
A	*A*-face centred	2	0, 0, 0; 0, $\frac{1}{2}, \frac{1}{2}$
B	*B*-face centred	2	0, 0, 0; $\frac{1}{2}$, 0, $\frac{1}{2}$
I	Body centred	2	0, 0, 0; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
F	All-face centred	4	0, 0, 0; $\frac{1}{2}, \frac{1}{2}$, 0; 0, $\frac{1}{2}, \frac{1}{2}$; $\frac{1}{2}$, 0, $\frac{1}{2}$
R†	Rhombohedrally centred (description with 'hexagonal axes')	3	0, 0, 0; $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$; $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$ ('obverse setting') 0, 0, 0; $\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$; $\frac{2}{3}, \frac{1}{3}, \frac{2}{3}$ ('reverse setting')
	Primitive (description with 'rhombohedral axes')	1	0, 0, 0
H‡	Hexagonally centred	3	0, 0, 0; $\frac{2}{3}, \frac{1}{3}$, 0; $\frac{1}{3}, \frac{2}{3}$, 0

* The two-dimensional triple hexagonal cell *h* is an alternative description of the hexagonal plane net, as illustrated in Fig. 5.1.3.8. It is not used for systematic plane-group description in this volume; it is introduced, however, in the sub- and supergroup entries of the plane-group tables (Part 6). Plane-group symbols for the *h* cell are listed in Chapter 4.2. Transformation matrices are contained in Table 5.1.3.1.

† In the space-group tables (Part 7), as well as in *IT* (1935) and *IT* (1952) [for reference notation, see footnote on first page of Chapter 2.1], the seven rhombohedral *R* space groups are presented with two descriptions, one based on *hexagonal axes* (triple cell), one on *rhombohedral axes* (primitive cell). In the present volume, as well as in *IT* (1952), the *obverse* setting of the triple hexagonal cell *R* is used. Note that in *IT* (1935) the *reverse* setting was employed. The two settings are related by a rotation of the hexagonal cell with respect to the rhombohedral lattice around a threefold axis, involving a rotation angle of 60°, 180° or 300° (*cf.* Fig. 5.1.3.6). Further details may be found in Chapter 2.1, Section 4.3.5 and Chapter 9.1. Transformation matrices are contained in Table 5.1.3.1.

‡ The triple hexagonal cell *H* is an alternative description of the hexagonal Bravais lattice, as illustrated in Fig. 5.1.3.8. It was used for systematic space-group description in *IT* (1935), but replaced by *P* in *IT* (1952). In the space-group tables of this volume (Part 7), it is only used in the sub- and supergroup entries (*cf.* Section 2.2.15). Space-group symbols for the *H* cell are listed in Section 4.3.5. Transformation matrices are contained in Table 5.1.3.1.

1.2.2. Notes on centred cells

(i) The centring type of a cell may change with a change of the basis vectors; in particular, a primitive cell may become a centred cell and *vice versa.* Examples of relevant transformation matrices are contained in Table 5.1.3.1.

(ii) Section 1.2.1 contains only those conventional centring symbols which occur in the Hermann–Mauguin space-group symbols. There exist, of course, further kinds of centred cells which are unconventional; an interesting example is provided by the triple rhombohedral *D* cell, described in Section 4.3.5.3.

(iii) For the use of the letter *S* as a new general, setting-independent 'centring symbol' for monoclinic and orthorhombic Bravais lattices see Chapter 2.1, especially Table 2.1.2.1, and de Wolff *et al.* (1985).

(iv) Symbols for crystal families and Bravais lattices in one, two and three dimensions are listed in Table 2.1.2.1 and are explained in the *Nomenclature Report* by de Wolff *et al.* (1985).

International Tables for Crystallography (2006). Vol. A, Chapter 1.3, pp. 5–6.

1.3. Printed symbols for symmetry elements

BY TH. HAHN

1.3.1. Printed symbols for symmetry elements and for the corresponding symmetry operations in one, two and three dimensions

For 'reflection conditions', see Tables 2.2.13.2 and 2.2.13.3.

Printed symbol	Symmetry element and its orientation	Defining symmetry operation with glide or screw vector
m	Reflection plane, mirror plane	Reflection through the plane
	Reflection line, mirror line (two dimensions)	Reflection through the line
	Reflection point, mirror point (one dimension)	Reflection through the point
a, b or c	'Axial' glide plane	Glide reflection through the plane, with glide vector
a	$\perp$ [010] or $\perp$ [001]	$\frac{1}{2}\mathbf{a}$
b	$\perp$ [001] or $\perp$ [100]	$\frac{1}{2}\mathbf{b}$
c †	$\perp$ [100] or $\perp$ [010]	$\frac{1}{2}\mathbf{c}$
	$\perp$ [$1\bar{1}0$] or $\perp$ [110]	$\frac{1}{2}\mathbf{c}$
	$\perp$ [100] or $\perp$ [010] or $\perp$ [$\bar{1}\bar{1}0$]	$\frac{1}{2}\mathbf{c}$
	$\perp$ [$1\bar{1}0$] or $\perp$ [120] or $\perp$ [$\bar{2}\bar{1}0$]	$\frac{1}{2}\mathbf{c}$ hexagonal coordinate system
e ‡	'Double' glide plane (in centred cells only)	*Two* glide reflections through *one* plane, with perpendicular glide vectors
	$\perp$ [001]	$\frac{1}{2}\mathbf{a}$ *and* $\frac{1}{2}\mathbf{b}$
	$\perp$ [100]	$\frac{1}{2}\mathbf{b}$ *and* $\frac{1}{2}\mathbf{c}$
	$\perp$ [010]	$\frac{1}{2}\mathbf{a}$ *and* $\frac{1}{2}\mathbf{c}$
	$\perp$ [$1\bar{1}0$]; $\perp$ [110]	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$ *and* $\frac{1}{2}\mathbf{c}$; $\frac{1}{2}(\mathbf{a}-\mathbf{b})$ *and* $\frac{1}{2}\mathbf{c}$
	$\perp$ [$01\bar{1}$]; $\perp$ [011]	$\frac{1}{2}(\mathbf{b}+\mathbf{c})$ *and* $\frac{1}{2}\mathbf{a}$; $\frac{1}{2}(\mathbf{b}-\mathbf{c})$ *and* $\frac{1}{2}\mathbf{a}$
	$\perp$ [$\bar{1}01$]; $\perp$ [101]	$\frac{1}{2}(\mathbf{a}+\mathbf{c})$ *and* $\frac{1}{2}\mathbf{b}$; $\frac{1}{2}(\mathbf{a}-\mathbf{c})$ *and* $\frac{1}{2}\mathbf{b}$
n	'Diagonal' glide plane	Glide reflection through the plane, with glide vector
	$\perp$ [001]; $\perp$ [100]; $\perp$ [010]	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$; $\frac{1}{2}(\mathbf{b}+\mathbf{c})$; $\frac{1}{2}(\mathbf{a}+\mathbf{c})$
	$\perp$ [$1\bar{1}0$] or $\perp$ [$01\bar{1}$] or $\perp$ [$\bar{1}01$]	$\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
	$\perp$ [110]; $\perp$ [011]; $\perp$ [101]	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$; $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$; $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$
d §	'Diamond' glide plane	Glide reflection through the plane, with glide vector
	$\perp$ [001]; $\perp$ [100]; $\perp$ [010]	$\frac{1}{4}(\mathbf{a}\pm\mathbf{b})$; $\frac{1}{4}(\mathbf{b}\pm\mathbf{c})$; $\frac{1}{4}(\pm\mathbf{a}+\mathbf{c})$
	$\perp$ [$1\bar{1}0$]; $\perp$ [$01\bar{1}$]; $\perp$ [$\bar{1}01$]	$\frac{1}{4}(\mathbf{a}+\mathbf{b}\pm\mathbf{c})$; $\frac{1}{4}(\pm\mathbf{a}+\mathbf{b}+\mathbf{c})$; $\frac{1}{4}(\mathbf{a}\pm\mathbf{b}+\mathbf{c})$
	$\perp$ [110]; $\perp$ [011]; $\perp$ [101]	$\frac{1}{4}(-\mathbf{a}+\mathbf{b}\pm\mathbf{c})$; $\frac{1}{4}(\pm\mathbf{a}-\mathbf{b}+\mathbf{c})$; $\frac{1}{4}(\mathbf{a}\pm\mathbf{b}-\mathbf{c})$
g	Glide line (two dimensions)	Glide reflection through the line, with glide vector
	$\perp$ [01]; $\perp$ [10]	$\frac{1}{2}\mathbf{a}$; $\frac{1}{2}\mathbf{b}$
1	None	Identity
2, 3, 4, 6	n-fold rotation axis, n	Counter-clockwise rotation of $360/n$ degrees around the axis (see Note viii)
	n-fold rotation point, n (two dimensions)	Counter-clockwise rotation of $360/n$ degrees around the point
$\bar{1}$	Centre of symmetry, inversion centre	Inversion through the point
$\bar{2}=m$,¶ $\bar{3}, \bar{4}, \bar{6}$	Rotoinversion axis, $\bar{n}$, and inversion point on the axis††	Counter-clockwise rotation of $360/n$ degrees around the axis, followed by inversion through the point on the axis†† (see Note viii)
2_1 $3_1, 3_2$ $4_1, 4_2, 4_3$ $6_1, 6_2, 6_3, 6_4, 6_5$	n-fold screw axis, n_p	Right-handed screw rotation of $360/n$ degrees around the axis, with screw vector (pitch) (p/n) **t**; here **t** is the shortest lattice translation vector parallel to the axis in the direction of the screw

† In the rhombohedral space-group symbols $R3c$ (161) and $R\bar{3}c$ (167), the symbol c refers to the description with 'hexagonal axes'; *i.e.* the glide vector is $\frac{1}{2}\mathbf{c}$, along [001]. In the description with 'rhombohedral axes', this glide vector is $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$, along [111], *i.e.* the symbol of the glide plane would be *n*: *cf.* Section 4.3.5.
‡ For further explanations of the 'double' glide plane e, see Note (x) below.
§ Glide planes d occur only in orthorhombic F space groups, in tetragonal I space groups, and in cubic I and F space groups. They always occur in pairs with alternating glide vectors, for instance $\frac{1}{4}(\mathbf{a}+\mathbf{b})$ and $\frac{1}{4}(\mathbf{a}-\mathbf{b})$. The second power of a glide reflection d is a centring vector.
¶ Only the symbol m is used in the Hermann–Mauguin symbols, for both point groups and space groups.
†† The inversion point is a centre of symmetry if n is odd.

1.3.2. Notes on symmetry elements and symmetry operations

(i) Section 1.3.1 contains only those symmetry elements and symmetry operations which occur in the Hermann–Mauguin symbols of point groups and space groups. Further so-called 'additional symmetry elements' are described in Chapter 4.1 and listed in Tables 4.2.1.1 and 4.3.2.1 in the form of 'extended Hermann–Mauguin symbols'.

(ii) The printed symbols of symmetry elements (symmetry operations), except for glide planes (glide reflections), are independent of the choice and the labelling of the basis vectors and of the origin. The symbols of glide planes (glide reflections), however, may change with a change of the basis vectors. For this reason, the possible orientations of glide planes and the glide vectors of the corresponding operations are listed explicitly in columns 2 and 3.

(iii) In space groups, further kinds of glide planes and glide reflections (called g) occur which are not used in the Hermann–Mauguin symbols. They are listed in the space-group tables (Part 7) under *Symmetry operations* and in Table 4.3.2.1 for the tetragonal and cubic space groups; they are explained in Sections 2.2.9 and 11.1.2.

(iv) Whereas the term 'symmetry operation' is well defined (*cf.* Section 8.1.3), the word 'symmetry element' is used by crystallographers in a variety of often rather loose meanings. In 1989, the International Union of Crystallography published a *Nomenclature Report* which first defines a 'geometric element' as a geometric item that allows the fixed points of a symmetry operation (after removal of any intrinsic glide or screw translation) to be located and oriented in a coordinate system. A 'symmetry element' then is defined as a concept with a double meaning, namely the combination of a geometric element with the set of symmetry operations having this geometric element in common ('element set'). For further details and tables, see de Wolff *et al.* (1989) and Flack *et al.* (2000).

(v) To each glide plane, infinitely many different glide reflections belong, because to each glide vector listed in column 3 any lattice translation vector parallel to the glide plane may be added; this includes centring vectors of centred cells. Each resulting vector is a glide vector of a new glide reflection but with the same plane as the geometric element. Any of these glide operations can be used as a 'defining operation'.

Examples

(1) Glide plane $n \perp [001]$: All vectors $(u+\frac{1}{2})\mathbf{a}+(v+\frac{1}{2})\mathbf{b}$ are glide vectors (u, v any integers); this includes $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(-\mathbf{a}+\mathbf{b})$, $\frac{1}{2}(-\mathbf{a}-\mathbf{b})$.

(2) Glide plane $e \perp [001]$ in a C-centred cell: All vectors $(u+\frac{1}{2})\mathbf{a}+v\mathbf{b}$ and $u\mathbf{a}+(v+\frac{1}{2})\mathbf{b}$ are glide vectors, this includes $\frac{1}{2}\mathbf{a}$ and $\frac{1}{2}\mathbf{b}$ (which are related by the centring vector), *i.e.* the glide plane e is at the same time a glide plane a *and* a glide plane b; for this 'double' glide plane e see Note (x) below.

(3) Glide plane $c \perp [1\bar{1}0]$ in an F-centred cell: All vectors $\frac{1}{2}u(\mathbf{a}+\mathbf{b})+(v+\frac{1}{2})\mathbf{c}$ are glide vectors; this includes $\frac{1}{2}\mathbf{c}$ and $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$, *i.e.* the glide plane c is at the same time a glide plane n.

(vi) If among the infinitely many glide operations of the element set of a symmetry plane there exists *one* operation with glide vector zero, then this symmetry element is a mirror plane.

(vii) Similar considerations apply to screw axes; to the screw vector defined in column 3 any lattice translation vector parallel to the screw axis may be added. Again, this includes centring vectors of centred cells.

Example

Screw axis $3_1 \parallel [111]$ in a cubic primitive cell. For the first power (right-handed screw rotation of 120°), all vectors $(u+\frac{1}{3})(\mathbf{a}+\mathbf{b}+\mathbf{c})$ are screw vectors; this includes $\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{4}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$, $-\frac{2}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$. For the second power (right-handed screw rotation of 240°), all vectors $(u+\frac{2}{3})(\mathbf{a}+\mathbf{b}+\mathbf{c})$ are screw vectors; this includes $\frac{2}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{5}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$; $-\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$. The third power corresponds to all lattice vectors $u(\mathbf{a}+\mathbf{b}+\mathbf{c})$.

Again, if *one* of the screw vectors is zero, the symmetry element is a rotation axis.

(viii) In the space-group tables, under *Symmetry operations,* for rotations, screw rotations and roto-inversions, the 'sense of rotation' is indicated by symbols like 3^+, $\bar{4}^-$ *etc.*; this is explained in Section 11.1.2.

(ix) The members of the following pairs of screw axes are 'enantiomorphic', *i.e.* they can be considered as a right- and a left-handed screw, respectively, with the same screw vector: 3_1, 3_2; 4_1, 4_3; 6_1, 6_5; 6_2, 6_4. The following screw axes are 'neutral', *i.e.* they contain left- *and* right-handed screws with the same screw vector: 2_1; 4_2; 6_3.

(x) In the third *Nomenclature Report* of the IUCr (de Wolff *et al.*, 1992), two new printed symbols for glide planes were proposed: e for 'double' glide planes and k for 'transverse' glide planes.

For the e glide planes, new graphical symbols were introduced (*cf.* Sections 1.4.1, 1.4.2, 1.4.3 and Note iv in 1.4.4); they are applied to the diagrams of the relevant space groups: Seven orthorhombic A-, C- and F-space groups, five tetragonal I-space groups, and five cubic F- and I-space groups. The e glide plane occurs only in centred cells and is defined by *one* plane with *two* perpendicular glide vectors related by a centring translation; thus, in $Cmma$ (67), two glide operations a *and* b through the plane $xy0$ occur, their glide vectors being related by the centring vector $\frac{1}{2}(\mathbf{a}+\mathbf{b})$; the symbol e removes the ambiguity between the symbols a and b.

For five space groups, the Hermann–Mauguin symbol has been modified:

Space group No.	39	41	64	67	68
New symbol:	$Aem2$	$Aea2$	$Cmce$	$Cmme$	$Ccce$
Former symbol:	$Abm2$	$Aba2$	$Cmca$	$Cmma$	$Ccca$

The new symbol is now the standard one; it is indicated in the headline of these space groups, while the former symbol is given underneath.

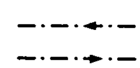
For the k glide planes, no new graphical symbol and no modification of a space-group symbol are proposed.

International Tables for Crystallography (2006). Vol. A, Chapter 1.4, pp. 7–11.

1.4. Graphical symbols for symmetry elements in one, two and three dimensions

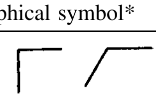
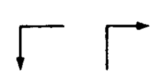
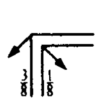
BY TH. HAHN

1.4.1. Symmetry planes normal to the plane of projection (three dimensions) and symmetry lines in the plane of the figure (two dimensions)

Symmetry plane or symmetry line	Graphical symbol	Glide vector in units of lattice translation vectors parallel and normal to the projection plane	Printed symbol
Reflection plane, mirror plane Reflection line, mirror line (two dimensions)		None	*m*
'Axial' glide plane Glide line (two dimensions)		$\frac{1}{2}$ lattice vector along line in projection plane $\frac{1}{2}$ lattice vector along line in figure plane	*a*, *b* or *c* *g*
'Axial' glide plane		$\frac{1}{2}$ lattice vector normal to projection plane	*a*, *b* or *c*
'Double' glide plane* (in centred cells only)		*Two* glide vectors: $\frac{1}{2}$ along line parallel to projection plane and $\frac{1}{2}$ normal to projection plane	*e*
'Diagonal' glide plane		*One* glide vector with *two* components: $\frac{1}{2}$ along line parallel to projection plane, $\frac{1}{2}$ normal to projection plane	*n*
'Diamond' glide plane† (pair of planes; in centred cells only)		$\frac{1}{4}$ along line parallel to projection plane, combined with $\frac{1}{4}$ normal to projection plane (arrow indicates direction parallel to the projection plane for which the normal component is positive)	*d*

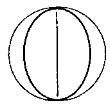
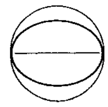
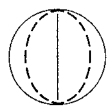
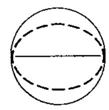
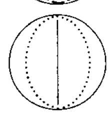
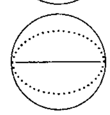
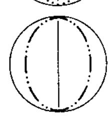
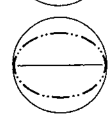
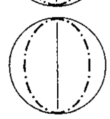
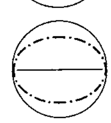
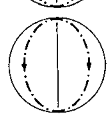
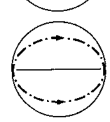
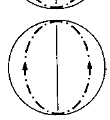
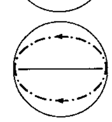
* For further explanations of the 'double' glide plane *e* see Note (iv) below and Note (x) in Section 1.3.2.
† See footnote § to Section 1.3.1.

1.4.2. Symmetry planes parallel to the plane of projection

Symmetry plane	Graphical symbol*	Glide vector in units of lattice translation vectors parallel to the projection plane	Printed symbol
Reflection plane, mirror plane		None	*m*
'Axial' glide plane		$\frac{1}{2}$ lattice vector in the direction of the arrow	*a*, *b* or *c*
'Double' glide plane† (in centred cells only)		*Two* glide vectors: $\frac{1}{2}$ in either of the directions of the two arrows	*e*
'Diagonal' glide plane		*One* glide vector with *two* components $\frac{1}{2}$ in the direction of the arrow	*n*
'Diamond' glide plane‡ (pair of planes; in centred cells only)	 	$\frac{1}{2}$ in the direction of the arrow; the glide vector is always half of a centring vector, *i.e.* one quarter of a diagonal of the conventional face-centred cell	*d*

* The symbols are given at the upper left corner of the space-group diagrams. A fraction h attached to a symbol indicates two symmetry planes with 'heights' h and $h + \frac{1}{2}$ above the plane of projection; *e.g.* $\frac{1}{8}$ stands for $h = \frac{1}{8}$ and $\frac{5}{8}$. No fraction means $h = 0$ and $\frac{1}{2}$ (*cf.* Section 2.2.6).
† For further explanations of the 'double' glide plane *e* see Note (iv) below and Note (x) in Section 1.3.2.
‡ See footnote § to Section 1.3.1.

1.4.3. Symmetry planes inclined to the plane of projection (in cubic space groups of classes $\bar{4}3m$ and $m\bar{3}m$ only)

Symmetry plane	Graphical symbol* for planes normal to $[011]$ and $[01\bar{1}]$	Graphical symbol* for planes normal to $[101]$ and $[10\bar{1}]$	Glide vector in units of lattice translation vectors for planes normal to $[011]$ and $[01\bar{1}]$	Glide vector in units of lattice translation vectors for planes normal to $[101]$ and $[10\bar{1}]$	Printed symbol
Reflection plane, mirror plane			None	None	*m*
'Axial' glide plane			$\frac{1}{2}$ lattice vector along $[100]$	$\frac{1}{2}$ lattice vector along $[010]$	*a* or *b*
'Axial' glide plane			$\frac{1}{2}$ lattice vector along $[01\bar{1}]$ or along $[011]$	$\frac{1}{2}$ lattice vector along $[10\bar{1}]$ or along $[101]$	
'Double' glide plane† [in space groups $I\bar{4}3m$ (217) and $Im\bar{3}m$ (229) only]			*Two* glide vectors: $\frac{1}{2}$ along $[100]$ *and* $\frac{1}{2}$ along $[01\bar{1}]$ or $\frac{1}{2}$ along $[011]$	*Two* glide vectors: $\frac{1}{2}$ along $[010]$ *and* $\frac{1}{2}$ along $[10\bar{1}]$ or $\frac{1}{2}$ along $[101]$	*e*
'Diagonal' glide plane			*One* glide vector: $\frac{1}{2}$ along $[11\bar{1}]$ or along $[111]$‡	*One* glide vector: $\frac{1}{2}$ along $[11\bar{1}]$ or along $[111]$‡	*n*
'Diamond' glide plane¶ (pair of planes; in centred cells only)			$\frac{1}{4}$ along $[1\bar{1}1]$ or along $[111]$§	$\frac{1}{4}$ along $[\bar{1}11]$ or along $[111]$§	*d*
			$\frac{1}{4}$ along $[\bar{1}\bar{1}1]$ or along $[\bar{1}11]$§	$\frac{1}{4}$ along $[\bar{1}\bar{1}1]$ or along $[1\bar{1}1]$§	

* The symbols represent orthographic projections. In the cubic space-group diagrams, complete orthographic projections of the symmetry elements around high-symmetry points, such as $0, 0, 0$; $\frac{1}{2}, 0, 0$; $\frac{1}{4}, \frac{1}{4}, 0$, are given as 'inserts'.

† For further explanations of the 'double' glide plane *e* see Note (iv) below and Note (x) in Section 1.3.2.

‡ In the space groups $F\bar{4}3m$ (216), $Fm\bar{3}m$ (225) and $Fd\bar{3}m$ (227), the shortest lattice translation vectors in the glide directions are $\mathbf{t}(1, \frac{1}{2}, \bar{\frac{1}{2}})$ or $\mathbf{t}(1, \frac{1}{2}, \frac{1}{2})$ and $\mathbf{t}(\frac{1}{2}, 1, \bar{\frac{1}{2}})$ or $\mathbf{t}(\frac{1}{2}, 1, \frac{1}{2})$, respectively.

§ The glide vector is half of a centring vector, *i.e.* one quarter of the diagonal of the conventional body-centred cell in space groups $I\bar{4}3d$ (220) and $Ia\bar{3}d$ (230).

¶ See footnote § to Section 1.3.1.

1.4.4. Notes on graphical symbols of symmetry planes

(i) The *graphical* symbols and their explanations (columns 2 and 3) are independent of the projection direction and the labelling of the basis vectors. They are, therefore, applicable to any projection diagram of a space group. The *printed* symbols of *glide planes* (column 4), however, may change with a change of the basis vectors, as shown by the following example.

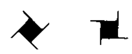
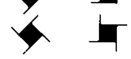
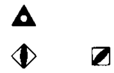
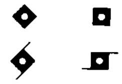
In the rhombohedral space groups $R3c$ (161) and $R\bar{3}c$ (167), the dotted line refers to a *c* glide when described with 'hexagonal axes' and projected along [001]; for a description with 'rhombohedral axes' and projection along [111], the same dotted glide plane would be called *n*. The dash-dotted *n* glide in the hexagonal description becomes an *a*, *b* or *c* glide in the rhombohedral description; *cf.* footnote † to Section 1.3.1.

(ii) The graphical symbols for glide planes in column 2 are not only used for the glide planes defined in Chapter 1.3, but also for the further glide planes *g* which are mentioned in Section 1.3.2 (Note x) and listed in Table 4.3.2.1; they are explained in Sections 2.2.9 and 11.1.2.

(iii) In monoclinic space groups, the 'parallel' glide vector of a glide plane may be along a lattice translation vector which is inclined to the projection plane.

(iv) In 1992, the International Union of Crystallography introduced the 'double' glide plane *e* and the graphical symbol ··–··– for *e* glide planes oriented 'normal' and 'inclined' to the plane of projection (de Wolff *et al.*, 1992); for details of *e* glide planes see Chapter 1.3. Note that the graphical symbol for *e* glide planes oriented 'parallel' to the projection plane has already been used in *IT* (1935) and *IT* (1952).

1.4.5. Symmetry axes normal to the plane of projection and symmetry points in the plane of the figure

Symmetry axis or symmetry point	Graphical symbol*	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symbol (partial elements in parentheses)
Identity	None	None	1
Twofold rotation axis Twofold rotation point (two dimensions)		None	2
Twofold screw axis: '2 sub 1'		$\frac{1}{2}$	2_1
Threefold rotation axis Threefold rotation point (two dimensions)		None	3
Threefold screw axis: '3 sub 1'		$\frac{1}{3}$	3_1
Threefold screw axis: '3 sub 2'		$\frac{2}{3}$	3_2
Fourfold rotation axis Fourfold rotation point (two dimensions)		None	4 (2)
Fourfold screw axis: '4 sub 1'		$\frac{1}{4}$	$4_1\ (2_1)$
Fourfold screw axis: '4 sub 2'		$\frac{1}{2}$	$4_2\ (2)$
Fourfold screw axis: '4 sub 3'		$\frac{3}{4}$	$4_3\ (2_1)$
Sixfold rotation axis Sixfold rotation point (two dimensions)		None	6 (3,2)
Sixfold screw axis: '6 sub 1'		$\frac{1}{6}$	$6_1\ (3_1, 2_1)$
Sixfold screw axis: '6 sub 2'		$\frac{1}{3}$	$6_2\ (3_2, 2)$
Sixfold screw axis: '6 sub 3'		$\frac{1}{2}$	$6_3\ (3, 2_1)$
Sixfold screw axis: '6 sub 4'		$\frac{2}{3}$	$6_4\ (3_1, 2)$
Sixfold screw axis: '6 sub 5'		$\frac{5}{6}$	$6_5\ (3_2, 2_1)$
Centre of symmetry, inversion centre: '1 bar' Reflection point, mirror point (one dimension)		None	$\bar{1}$
Inversion axis: '3 bar'		None	$\bar{3}\ (3, \bar{1})$
Inversion axis: '4 bar'		None	$\bar{4}\ (2)$
Inversion axis: '6 bar'		None	$\bar{6} \equiv 3/m$
Twofold rotation axis with centre of symmetry		None	$2/m\ (\bar{1})$
Twofold screw axis with centre of symmetry		$\frac{1}{2}$	$2_1/m\ (\bar{1})$
Fourfold rotation axis with centre of symmetry		None	$4/m\ (\bar{4}, 2, \bar{1})$
'4 sub 2' screw axis with centre of symmetry		$\frac{1}{2}$	$4_2/m\ (\bar{4}, 2, \bar{1})$
Sixfold rotation axis with centre of symmetry		None	$6/m\ (\bar{6}, \bar{3}, 3, 2, \bar{1})$
'6 sub 3' screw axis with centre of symmetry		$\frac{1}{2}$	$6_3/m\ (\bar{6}, \bar{3}, 3, 2_1, \bar{1})$

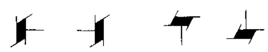
* Notes on the 'heights' h of symmetry points $\bar{1}$, $\bar{3}$, $\bar{4}$ and $\bar{6}$:

(1) Centres of symmetry $\bar{1}$ and $\bar{3}$, as well as inversion points $\bar{4}$ and $\bar{6}$ on $\bar{4}$ and $\bar{6}$ axes parallel to [001], occur in pairs at 'heights' h and $h + \frac{1}{2}$. In the space-group diagrams, only one fraction h is given, *e.g.* $\frac{1}{4}$ stands for $h = \frac{1}{4}$ and $\frac{3}{4}$. No fraction means $h = 0$ and $\frac{1}{2}$. In *cubic* space groups, however, because of their complexity, *both* fractions are given for vertical $\bar{4}$ axes, including $h = 0$ and $\frac{1}{2}$.

(2) Symmetries $4/m$ and $6/m$ contain vertical $\bar{4}$ and $\bar{6}$ axes; their $\bar{4}$ and $\bar{6}$ inversion points coincide with the centres of symmetry. This is not indicated in the space-group diagrams.

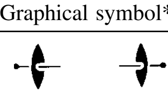
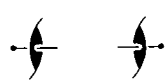
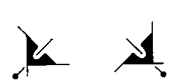
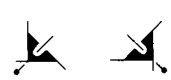
(3) Symmetries $4_2/m$ and $6_3/m$ also contain vertical $\bar{4}$ and $\bar{6}$ axes, but their $\bar{4}$ and $\bar{6}$ inversion points alternate with the centres of symmetry; *i.e.* $\bar{1}$ points at h and $h + \frac{1}{2}$ interleave with $\bar{4}$ or $\bar{6}$ points at $h + \frac{1}{4}$ and $h + \frac{3}{4}$. In the tetragonal and hexagonal space-group diagrams, only *one* fraction for $\bar{1}$ and one for $\bar{4}$ or $\bar{6}$ is given. In the cubic diagrams, *all four* fractions are listed for $4_2/m$; *e.g.* $Pm\bar{3}n$ (No. 223): $\bar{1}$: 0, $\frac{1}{2}$; $\bar{4}$: $\frac{1}{4}$, $\frac{3}{4}$.

1.4.6. Symmetry axes parallel to the plane of projection

Symmetry axis	Graphical symbol*	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symbol (partial elements in parentheses)
Twofold rotation axis		None	2
Twofold screw axis: ‘2 sub 1’		$\frac{1}{2}$	2_1
Fourfold rotation axis	 in cubic space groups only	None	4 (2)
Fourfold screw axis: ‘4 sub 1’		$\frac{1}{4}$	4_1 (2_1)
Fourfold screw axis: ‘4 sub 2’		$\frac{1}{2}$	4_2 (2)
Fourfold screw axis: ‘4 sub 3’		$\frac{3}{4}$	4_3 (2_1)
Inversion axis: ‘4 bar’		None	$\bar{4}$ (2)
Inversion point on ‘4 bar’-axis		–	$\bar{4}$ point

* The symbols for horizontal symmetry axes are given outside the unit cell of the space-group diagrams. *Twofold* axes always occur in pairs, at ‘heights’ h and $h + \frac{1}{2}$ above the plane of projection; here, a fraction h attached to such a symbol indicates two axes with heights h and $h + \frac{1}{2}$. No fraction stands for $h = 0$ and $\frac{1}{2}$. The rule of pairwise occurrence, however, is not valid for the horizontal *fourfold* axes in cubic space groups; here, *all* heights are given, including $h = 0$ and $\frac{1}{2}$. This applies also to the horizontal $\bar{4}$ axes and the $\bar{4}$ inversion points located on these axes.

1.4.7. Symmetry axes inclined to the plane of projection (in cubic space groups only)

Symmetry axis	Graphical symbol*	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symbol (partial elements in parentheses)
Twofold rotation axis	 Parallel to a face diagonal of the cube	None	2
Twofold screw axis: ‘2 sub 1’		$\frac{1}{2}$	2_1
Threefold rotation axis	 Parallel to a body diagonal of the cube	None	3
Threefold screw axis: ‘3 sub 1’		$\frac{1}{3}$	3_1
Threefold screw axis: ‘3 sub 2’		$\frac{2}{3}$	3_2
Inversion axis: ‘3 bar’		None	$\bar{3}$ $(3, \bar{1})$

* The dots mark the intersection points of axes with the plane at $h = 0$. In some cases, the intersection points are obscured by symbols of symmetry elements with height $h \geq 0$; examples: $Fd\bar{3}$ (203), origin choice 2; $Pn\bar{3}n$ (222), origin choice 2; $Pm\bar{3}n$ (223); $Im\bar{3}m$ (229); $Ia\bar{3}d$ (230).

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2.1. Classification and coordinate systems of space groups

BY TH. HAHN AND A. LOOIJENGA-VOS

2.1.1. Introduction

The present volume is a computer-based extension and complete revision of the symmetry tables of the two previous series of *International Tables,* the *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935) and the *International Tables for X-ray Crystallography* (1952).*

The main part of the volume consists of tables and diagrams for the 17 types of plane groups (Part 6) and the 230 types of space groups (Part 7). The two types of line groups are treated separately in Section 2.2.17, because of their simplicity. For the history of the *Tables* and a comparison of the various editions, reference is made to the *Preface* of this volume. Attention is drawn to Part 1 where the symbols and terms used in this volume are defined.

The present part forms a *guide* to the entries in the space-group tables with instructions for their practical use. Only a minimum of theory is provided, and the emphasis is on practical aspects. For the theoretical background the reader is referred to Parts 8–15, which include also suitable references. A textbook version of space-group symmetry and the use of these tables (with exercises) is provided by Hahn & Wondratschek (1994).

2.1.2. Space-group classification

In this volume, the plane groups and space groups are classified according to three criteria:

(i) According to *geometric crystal classes, i.e.* according to the crystallographic point group to which a particular space group belongs. There are 10 crystal classes in two dimensions and 32 in three dimensions. They are described and listed in Part 10 and in column 4 of Table 2.1.2.1. [For arithmetic crystal classes, see Section 8.2.3 in this volume and Chapter 1.4 of *International Tables for Crystallography*, Vol. C (2004).]

(ii) According to *crystal families*. The term crystal family designates the classification of the 17 plane groups into four categories and of the 230 space groups into *six* categories, as displayed in column 1 of Table 2.1.2.1. Here all 'hexagonal', 'trigonal' and 'rhombohedral' space groups are contained in one family, the hexagonal crystal family. The 'crystal family' thus corresponds to the term 'crystal system', as used frequently in the American and Russian literature.

The crystal families are symbolized by the lower-case letters *a*, *m*, *o*, *t*, *h*, *c*, as listed in column 2 of Table 2.1.2.1. If these letters are combined with the appropriate capital letters for the lattice-centring types (*cf.* Chapter 1.2), symbols for the 14 Bravais lattices result. These symbols and their occurrence in the crystal families are shown in column 8 of Table 2.1.2.1; *mS* and *oS* are the standard setting-independent symbols for the centred monoclinic and the one-face centred orthorhombic Bravais lattices, *cf.* de Wolff *et al.* (1985); symbols between parentheses represent alternative settings of these Bravais lattices.

(iii) According to *crystal systems*. This classification collects the plane groups into four categories and the space groups into *seven* categories. The classifications according to crystal families and crystal systems are the same for two dimensions.

For three dimensions, this applies to the triclinic, monoclinic, orthorhombic, tetragonal and cubic systems. The only complication exists in the hexagonal crystal family for which several subdivisions into systems have been proposed in the literature. In this volume, as well as in *IT* (1952), the space groups of the hexagonal crystal family are grouped into two 'crystal systems' as follows: all space groups belonging to the five crystal classes 3, $\bar{3}$, 32, 3*m* and $\bar{3}m$, *i.e.* having 3, 3_1, 3_2 or $\bar{3}$ as principal axis, form the *trigonal* crystal system, irrespective of whether the Bravais lattice is *hP* or *hR;* all space groups belonging to the seven crystal classes 6, $\bar{6}$, $6/m$, 622, 6*mm,* $\bar{6}2m$ and $6/mmm$, *i.e.* having 6, 6_1, 6_2, 6_3, 6_4, 6_5 or $\bar{6}$ as principal axis, form the *hexagonal* crystal system; here the lattice is always *hP* (*cf.* Section 8.2.8). The crystal systems, as defined above, are listed in column 3 of Table 2.1.2.1.

A different subdivision of the hexagonal crystal family is in use, mainly in the French literature. It consists of grouping all space groups based on the hexagonal Bravais lattice *hP* (lattice point symmetry $6/mmm$) into the 'hexagonal' system and all space groups based on the rhombohedral Bravais lattice *hR* (lattice point symmetry $\bar{3}m$) into the 'rhombohedral' system. In Section 8.2.8, these systems are called 'Lattice systems'. They were called 'Bravais systems' in earlier editions of this volume.

The theoretical background for the classification of space groups is provided in Chapter 8.2.

2.1.3. Conventional coordinate systems and cells

A plane group or space group usually is described by means of a *crystallographic coordinate system*, consisting of a *crystallographic basis* (basis vectors are lattice vectors) and a *crystallographic origin* (origin at a centre of symmetry or at a point of high site symmetry). The choice of such a coordinate system is not mandatory since in principle a crystal structure can be referred to any coordinate system; *cf.* Section 8.1.4.

The selection of a crystallographic coordinate system is not unique. Conventionally, a right-handed set of basis vectors is taken such that the symmetry of the plane or space group is displayed best. With this convention, which is followed in the present volume, the specific restrictions imposed on the cell parameters by each crystal family become particularly simple. They are listed in columns 6 and 7 of Table 2.1.2.1. If within these restrictions the smallest cell is chosen, a *conventional* (crystallographic) *basis* results. Together with the selection of an appropriate *conventional* (crystallographic) *origin* (*cf.* Sections 2.2.2 and 2.2.7), such a basis defines a *conventional* (crystallographic) *coordinate system* and a *conventional cell.* The conventional cell of a point lattice or a space group, obtained in this way, turns out to be either *primitive* or to exhibit one of the *centring types* listed in Chapter 1.2. The centring type of a conventional cell is transferred to the lattice which is described by this cell; hence, we speak of primitive, face-centred, body-centred *etc.* lattices. Similarly, the cell parameters are often called lattice parameters; *cf.* Section 8.3.1 and Chapter 9.1 for further details.

In the triclinic, monoclinic and orthorhombic crystal systems, additional conventions (for instance cell reduction or metrical conventions based on the lengths of the cell edges) are needed to determine the choice and the labelling of the axes. Reduced bases are treated in Chapters 9.1 and 9.2, orthorhombic settings in Section 2.2.6.4, and monoclinic settings and cell choices in Section 2.2.16.

In this volume, all space groups within a crystal family are referred to the same kind of conventional coordinate system with the exception of the hexagonal crystal family in three dimensions. Here, two kinds of coordinate systems are used, the hexagonal and the rhombohedral systems. In accordance with common crystallographic practice, all space groups based on the hexagonal Bravais lattice *hP* (18 trigonal and 27 hexagonal space groups) are described

* Throughout this volume, these editions are abbreviated as *IT* (1935) and *IT* (1952).

Table 2.1.2.1. *Crystal families, crystal systems, conventional coordinate systems and Bravais lattices in one, two and three dimensions*

Crystal family	Symbol*	Crystal system	Crystallographic point groups†	No. of space groups	Conventional coordinate system: Restrictions on cell parameters	Conventional coordinate system: Parameters to be determined	Bravais lattices*
One dimension							
–	–	–	1, $\boxed{m}$	2	None	a	*p*
Two dimensions							
Oblique (monoclinic)	*m*	Oblique	1, $\boxed{2}$	2	None	a, b γ‡	*mp*
Rectangular (orthorhombic)	*o*	Rectangular	m, $\boxed{2mm}$	7	$\gamma = 90°$	a, b	*op* *oc*
Square (tetragonal)	*t*	Square	4, $\boxed{4mm}$	3	$a = b$ $\gamma = 90°$	a	*tp*
Hexagonal	*h*	Hexagonal	3, 6 $3m$, $\boxed{6mm}$	5	$a = b$ $\gamma = 120°$	a	*hp*
Three dimensions							
Triclinic (anorthic)	*a*	Triclinic	1, $\boxed{\bar{1}}$	2	None	$a, b, c,$ α, β, γ	*aP*
Monoclinic	*m*	Monoclinic	$2, m, \boxed{2/m}$	13	b-unique setting $\alpha = \gamma = 90°$	a, b, c β‡	*mP* *mS* (*mC*, *mA*, *mI*)
					c-unique setting $\alpha = \beta = 90°$	$a, b, c,$ γ‡	*mP* *mS* (*mA*, *mB*, *mI*)
Orthorhombic	*o*	Orthorhombic	222, $mm2$, $\boxed{mmm}$	59	$\alpha = \beta = \gamma = 90°$	a, b, c	*oP* *oS* (*oC*, *oA*, *oB*) *oI* *oF*
Tetragonal	*t*	Tetragonal	$4, \bar{4}, 4/m$ $422, 4mm, \bar{4}2m,$ $\boxed{4/mmm}$	68	$a = b$ $\alpha = \beta = \gamma = 90°$	a, c	*tP* *tI*
Hexagonal	*h*	Trigonal	$3, \bar{3}$ $32, 3m, \boxed{\bar{3}m}$	18	$a = b$ $\alpha = \beta = 90°$, $\gamma = 120°$	a, c	*hP*
				7	$a = b = c$ $\alpha = \beta = \gamma$ (rhombohedral axes, primitive cell) $a = b$ $\alpha = \beta = 90°, \gamma = 120°$ (hexagonal axes, triple obverse cell)	a, α	*hR*
		Hexagonal	$6, \bar{6}, 6/m$ $622, 6mm, \bar{6}2m,$ $\boxed{6/mmm}$	27	$a = b$ $\alpha = \beta = 90°, \gamma = 120°$	a, c	*hP*
Cubic	*c*	Cubic	$23, m\bar{3}$ $432, \bar{4}3m, \boxed{m\bar{3}m}$	36	$a = b = c$ $\alpha = \beta = \gamma = 90°$	a	*cP* *cI* *cF*

* The symbols for crystal families (column 2) and Bravais lattices (column 8) were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985).
† Symbols surrounded by dashed or full lines indicate Laue groups; full lines indicate Laue groups which are also lattice point symmetries (holohedries).
‡ These angles are conventionally taken to be non-acute, *i.e.* $\geq 90°$.

only with a hexagonal coordinate system (primitive cell),* whereas the seven space groups based on the rhombohedral Bravais lattice *hR* are treated in two versions, one referred to 'hexagonal axes' (triple obverse cell) and one to 'rhombohedral axes' (primitive cell); *cf.* Chapter 1.2. In practice, hexagonal axes are preferred because they are easier to visualize.

Note: For convenience, the relations between the cell parameters a, c of the triple hexagonal cell and the cell parameters a', α' of the primitive rhombohedral cell (*cf.* Table 2.1.2.1) are listed:

$$a = a'\sqrt{2}\sqrt{1-\cos\alpha'} = 2a'\sin\frac{\alpha'}{2}$$

$$c = a'\sqrt{3}\sqrt{1+2\cos\alpha'}$$

$$\frac{c}{a} = \sqrt{\frac{3}{2}}\sqrt{\frac{1+2\cos\alpha'}{1-\cos\alpha'}} = \sqrt{\frac{9}{4\sin^2(\alpha'/2)} - 3}$$

$$a' = \tfrac{1}{3}\sqrt{3a^2 + c^2}$$

$$\sin\frac{\alpha'}{2} = \frac{3}{2\sqrt{3+(c^2/a^2)}} \quad \text{or} \quad \cos\alpha' = \frac{(c^2/a^2) - \frac{3}{2}}{(c^2/a^2)+3}.$$

* For a rhombohedral description (D cell) of the hexagonal Bravais lattice see Section 4.3.5.3.

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2.2. Contents and arrangement of the tables

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2.2.1. General layout

The presentation of the plane-group and space-group data in Parts 6 and 7 follows the style of the previous editions of *International Tables*. The entries for a space group are printed on two facing pages as shown below; an example (*Cmm*2, No. 35) is provided inside the front and back covers. Deviations from this standard sequence (mainly for cubic space groups) are indicated on the relevant pages.

Left-hand page:

(1) *Headline*

(2) *Diagrams* for the symmetry elements and the general position (for graphical symbols of symmetry elements see Chapter 1.4)

(3) *Origin*

(4) *Asymmetric unit*

(5) *Symmetry operations*

Right-hand page:

(6) *Headline* in abbreviated form

(7) *Generators selected*; this information is the basis for the order of the entries under *Symmetry operations* and *Positions*

(8) General and special *Positions*, with the following columns:

Multiplicity

Wyckoff letter

Site symmetry, given by the oriented site-symmetry symbol

Coordinates

Reflection conditions

Note: In a few space groups, two special positions with the same reflection conditions are printed on the same line

(9) *Symmetry of special projections* (not given for plane groups)

(10) *Maximal non-isomorphic subgroups*

(11) *Maximal isomorphic subgroups of lowest index*

(12) *Minimal non-isomorphic supergroups*

Note: Symbols for *Lattice complexes* of the plane groups and space groups are given in Tables 14.2.3.1 and 14.2.3.2. Normalizers of space groups are listed in Part 15.

2.2.2. Space groups with more than one description

For several space groups, more than one description is available. Three cases occur:

(i) *Two choices of origin (cf. Section 2.2.7)*

For all centrosymmetric space groups, the tables contain a description with a centre of symmetry as origin. Some centrosymmetric space groups, however, contain points of high site symmetry that do not coincide with a centre of symmetry. For these 24 cases, a further description (including diagrams) with a high-symmetry point as origin is provided. Neither of the two origin choices is considered standard. Noncentrosymmetric space groups and all plane groups are described with only one choice of origin.

Examples

(1) *Pnnn* (48)
Origin choice 1 at a point with site symmetry 222
Origin choice 2 at a centre with site symmetry $\bar{1}$.

(2) $Fd\bar{3}m$ (227)
Origin choice 1 at a point with site symmetry $\bar{4}3m$
Origin choice 2 at a centre with site symmetry $\bar{3}m$.

(ii) *Monoclinic space groups*

Two complete descriptions are given for each of the 13 monoclinic space groups, one for the setting with 'unique axis *b*', followed by one for the setting with 'unique axis *c*'.

Additional descriptions in synoptic form are provided for the following eight monoclinic space groups with centred lattices or glide planes:

$C2$ (5), Pc (7), Cm (8), Cc (9), $C2/m$ (12), $P2/c$ (13), $P2_1/c$ (14), $C2/c$ (15).

These synoptic descriptions consist of abbreviated treatments for three 'cell choices', here called 'cell choices 1, 2 and 3'. Cell choice 1 corresponds to the complete treatment, mentioned above; for comparative purposes, it is repeated among the synoptic descriptions which, for each setting, are printed on two facing pages. The cell choices and their relations are explained in Section 2.2.16.

(iii) *Rhombohedral space groups*

The seven rhombohedral space groups $R3$ (146), $R\bar{3}$ (148), $R32$ (155), $R3m$ (160), $R3c$ (161), $R\bar{3}m$ (166), and $R\bar{3}c$ (167) are described with two coordinate systems, first with *hexagonal axes* (triple hexagonal cell) and second with *rhombohedral axes* (primitive rhombohedral cell). For both descriptions, the same space-group symbol is used. The relations between the cell parameters of the two cells are listed in Chapter 2.1.

The hexagonal triple cell is given in the *obverse* setting (centring points $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$; $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$). In *IT* (1935), the *reverse* setting (centring points $\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$; $\frac{2}{3}, \frac{1}{3}, \frac{2}{3}$) was employed; *cf.* Chapter 1.2.

2.2.3. Headline

The description of each plane group or space group starts with a headline on a left-hand page, consisting of two (sometimes three) lines which contain the following information, when read from left to right.

First line

(1) The *short international* (Hermann–Mauguin) *symbol* for the plane or space group. These symbols will be further referred to as Hermann–Mauguin symbols. A detailed discussion of space-group symbols is given in Chapter 12.2, a brief summary in Section 2.2.4.

Note on standard monoclinic space-group symbols: In order to facilitate recognition of a monoclinic space-group type, the familiar short symbol for the *b*-axis setting (*e.g.* $P2_1/c$ for No. 14 or $C2/c$ for No. 15) has been adopted as the *standard symbol* for a space-group type. It appears in the headline of *every description of this space group* and thus does not carry any information about the setting or the cell choice of this particular description. No other short symbols for monoclinic space groups are used in this volume (*cf.* Section 2.2.16).

(2) The *Schoenflies symbol* for the space group.

Note: No Schoenflies symbols exist for the plane groups.

(3) The *short international* (Hermann–Mauguin) *symbol* for the point group to which the plane or space group belongs (*cf.* Chapter 12.1).
(4) The name of the *crystal system* (*cf.* Table 2.1.2.1).

Second line
(5) The sequential *number of the plane or space group*, as introduced in *IT* (1952).
(6) The *full international* (Hermann–Mauguin) *symbol* for the plane or space group.
For monoclinic space groups, the headline of every description contains the full symbol appropriate to that description.
(7) The *Patterson symmetry* (see Section 2.2.5).

Third line
This line is used, where appropriate, to indicate origin choices, settings, cell choices and coordinate axes (see Section 2.2.2). For five orthorhombic space groups, an entry ‘Former space-group symbol’ is given; *cf.* Chapter 1.3, Note (x).

2.2.4. International (Hermann–Mauguin) symbols for plane groups and space groups (*cf.* Chapter 12.2)

2.2.4.1. *Present symbols*

Both the short and the full Hermann–Mauguin symbols consist of two parts: (i) a letter indicating the centring type of the conventional cell, and (ii) a set of characters indicating symmetry elements of the space group (modified point-group symbol).

(i) The letters for the centring types of cells are listed in Chapter 1.2. Lower-case letters are used for two dimensions (nets), capital letters for three dimensions (lattices).

(ii) The one, two or three entries after the centring letter refer to the one, two or three kinds of *symmetry directions* of the lattice belonging to the space group. These symmetry directions were called *blickrichtungen* by Heesch (1929). Symmetry directions occur either as singular directions (as in the monoclinic and orthorhombic crystal systems) or as sets of symmetrically equivalent symmetry directions (as in the higher-symmetrical crystal systems). Only one representative of each set is required. The (sets of) symmetry directions and their sequence for the different lattices are summarized in Table 2.2.4.1. According to their position in this sequence, the symmetry directions are referred to as ‘primary’, ‘secondary’ and ‘tertiary’ directions.

This sequence of lattice symmetry directions is transferred to the sequence of positions in the corresponding Hermann–Mauguin space-group symbols. Each position contains one or two characters designating symmetry elements (axes and planes) of the space group (*cf.* Chapter 1.3) that occur for the corresponding lattice symmetry direction. Symmetry planes are represented by their normals; if a symmetry axis and a normal to a symmetry plane are parallel, the two characters (symmetry symbols) are separated by a slash, as in $P6_3/m$ or $P2/m$ (‘two over m’).

For the different crystal lattices, the Hermann–Mauguin space-group symbols have the following form:

(i) *Triclinic* lattices have no symmetry direction because they have, in addition to translations, only centres of symmetry, $\bar{1}$. Thus, only two triclinic space groups, $P1$ (1) and $P\bar{1}$ (2), exist.

(ii) *Monoclinic* lattices have one symmetry direction. Thus, for monoclinic space groups, only one position after the centring letter is needed. This is used in the *short* Hermann–Mauguin symbols, as in $P2_1$. Conventionally, the symmetry direction is labelled either b (‘unique axis b’) or c (‘unique axis c’).

In order to distinguish between the different settings, the *full* Hermann–Mauguin symbol contains two extra entries ‘1’. They indicate those two axial directions that are not symmetry directions

Table 2.2.4.1. *Lattice symmetry directions for two and three dimensions*

Directions that belong to the same set of equivalent symmetry directions are collected between braces. The first entry in each set is taken as the representative of that set.

Lattice	Symmetry direction (position in Hermann–Mauguin symbol)		
	Primary	Secondary	Tertiary
Two dimensions			
Oblique	Rotation point in plane		
Rectangular		[10]	[01]
Square		$\{[10], [01]\}$	$\{[1\bar{1}], [11]\}$
Hexagonal		$\{[10], [01], [\bar{1}\bar{1}]\}$	$\{[1\bar{1}], [12], [\bar{2}\bar{1}]\}$
Three dimensions			
Triclinic	None		
Monoclinic*	[010] (‘unique axis b’) [001] (‘unique axis c’)		
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	$\{[100], [010]\}$	$\{[1\bar{1}0], [110]\}$
Hexagonal	[001]	$\{[100], [010], [\bar{1}\bar{1}0]\}$	$\{[1\bar{1}0], [120], [\bar{2}\bar{1}0]\}$
Rhombohedral (hexagonal axes)	[001]	$\{[100], [010], [\bar{1}\bar{1}0]\}$	
Rhombohedral (rhombohedral axes)	[111]	$\{[1\bar{1}0], [01\bar{1}], [\bar{1}01]\}$	
Cubic	$\{[100], [010], [001]\}$	$\{[111], [1\bar{1}\bar{1}], [\bar{1}1\bar{1}], [\bar{1}\bar{1}1]\}$	$\{[1\bar{1}0], [110], [01\bar{1}], [011], [\bar{1}01], [101]\}$

* For the full Hermann–Mauguin symbols see Section 2.2.4.1.

of the lattice. Thus, the symbols $P121$, $P112$ and $P211$ show that the b axis, c axis and a axis, respectively, is the unique axis. Similar considerations apply to the three *rectangular* plane groups *pm, pg* and *cm* (*e.g.* plane group No. 5: short symbol *cm*, full symbol $c1m1$ or $c11m$).

(iii) *Rhombohedral* lattices have two kinds of symmetry directions. Thus, the symbols of the seven rhombohedral space groups contain only two entries after the letter R, as in $R3m$ or $R3c$.

(iv) *Orthorhombic*, *tetragonal*, *hexagonal* and *cubic* lattices have three kinds of symmetry directions. Hence, the corresponding space-group symbols have three entries after the centring letter, as in *Pmna*, $P3m1$, $P6cc$ or $Ia\bar{3}d$.
Lattice symmetry directions that carry no symmetry elements for the space group under consideration are represented by the symbol ‘1’, as in $P3m1$ and $P31m$. If no misinterpretation is possible, entries ‘1’ at the end of a space-group symbol are omitted, as in $P6$ (instead of $P611$), $R\bar{3}$ (instead of $R\bar{3}1$), $I4_1$ (instead of $I4_111$), $F23$ (instead of $F231$); similarly for the plane groups.

Short and *full* Hermann–Mauguin symbols differ only for the plane groups of class m, for the monoclinic space groups, and for the space groups of crystal classes mmm, $4/mmm$, $\bar{3}m$, $6/mmm$, $m\bar{3}$ and $m\bar{3}m$. In the full symbols, symmetry axes *and* symmetry planes for each symmetry direction are listed; in the short symbols, symmetry axes are suppressed as much as possible. Thus, for space group No. 62, the full symbol is $P2_1/n\,2_1/m\,2_1/a$ and the short symbol is $Pnma$. For No. 194, the full symbol is $P6_3/m\,2/m\,2/c$ and the short symbol is $P6_3/mmc$. For No. 230, the two symbols are $I4_1/a\,\bar{3}\,2/d$ and $Ia\bar{3}d$.

Many space groups contain more kinds of symmetry elements than are indicated in the full symbol ('additional symmetry elements', *cf.* Chapter 4.1). A complete listing of the symmetry elements is given in Tables 4.2.1.1 and 4.3.2.1 under the heading *Extended full symbols*. Note that a centre of symmetry is never explicitly indicated (except for space group $P\bar{1}$); its presence or absence, however, can be readily inferred from the space-group symbol.

2.2.4.2. *Changes in Hermann–Mauguin space-group symbols as compared with the 1952 and 1935 editions of International Tables*

Extensive changes in the space-group symbols were applied in *IT* (1952) as compared with the original Hermann–Mauguin symbols of *IT* (1935), especially in the tetragonal, trigonal and hexagonal crystal systems. Moreover, new symbols for the c-axis setting of monoclinic space groups were introduced. All these changes are recorded on pp. 51 and 543–544 of *IT* (1952). In the present edition, the symbols of the 1952 edition are retained, except for the following four cases (*cf.* Chapter 12.4).

(i) *Two-dimensional groups*

Short Hermann–Mauguin symbols differing from the corresponding full symbols in *IT* (1952) are replaced by the full symbols for the listed plane groups in Table 2.2.4.2.

For the two-dimensional point group with two mutually perpendicular mirror lines, the symbol mm is changed to $2mm$.

For plane group No. 2, the entries '1' at the end of the full symbol are omitted:

No. 2: Change from $p211$ to $p2$.

With these changes, the symbols of the two-dimensional groups follow the rules that were introduced in *IT* (1952) for the space groups.

(ii) *Monoclinic space groups*

Additional *full* Hermann–Mauguin symbols are introduced for the eight monoclinic space groups with centred lattices or glide planes (Nos. 5, 7–9, 12–15) to indicate the various settings and cell choices. A complete list of symbols, including also the a-axis setting, is contained in Table 4.3.2.1; further details are given in Section 2.2.16.

For standard *short* monoclinic space-group symbols see Sections 2.2.3 and 2.2.16.

(iii) *Cubic groups*

The short symbols for all space groups belonging to the two cubic crystal classes $m\bar{3}$ and $m\bar{3}m$ now contain the symbol $\bar{3}$ instead of 3. This applies to space groups Nos. 200–206 and 221–230, as well as to the two point groups $m\bar{3}$ and $m\bar{3}m$.

Examples

No. 205: Change from $Pa3$ to $Pa\bar{3}$

No. 230: Change from $Ia3d$ to $Ia\bar{3}d$.

With this change, the centrosymmetric nature of these groups is apparent also in the short symbols.

(iv) *Glide-plane symbol e*

For the recent introduction of the 'double glide plane' e into five space-group symbols, see Chapter 1.3, Note (x).

Table 2.2.4.2. *Changes in Hermann–Mauguin symbols for two-dimensional groups*

No.	*IT* (1952)	Present edition
6	pmm	$p2mm$
7	pmg	$p2mg$
8	pgg	$p2gg$
9	cmm	$c2mm$
11	$p4m$	$p4mm$
12	$p4g$	$p4gm$
17	$p6m$	$p6mm$

2.2.5. Patterson symmetry

The entry *Patterson symmetry* in the headline gives the space group of the *Patterson function* $P(x, y, z)$. With neglect of anomalous dispersion, this function is defined by the formula

$$P(x,y,z) = \frac{1}{V}\sum_h\sum_k\sum_l |F(hkl)|^2 \cos 2\pi(hx+ky+lz).$$

The Patterson function represents the convolution of a structure with its inverse or the pair-correlation function of a structure. A detailed discussion of its use for structure determination is given by Buerger (1959). The space group of the Patterson function is identical to that of the 'vector set' of the structure, and is thus always centrosymmetric and symmorphic.*

The symbol for the Patterson space group of a crystal structure can be deduced from that of its space group in two steps:

(i) Glide planes and screw axes have to be replaced by the corresponding mirror planes and rotation axes, resulting in a symmorphic space group.

(ii) If this symmorphic space group is not centrosymmetric, inversions have to be added.

There are 7 different Patterson symmetries in two dimensions and 24 in three dimensions. They are listed in Table 2.2.5.1. Account is taken of the fact that the Laue class $\bar{3}m$ combines in two ways with the hexagonal translation lattice, namely as $\bar{3}m1$ and as $\bar{3}1m$.

Note: For the four orthorhombic space groups with A cells (Nos. 38–41), the standard symbol for their Patterson symmetry, $Cmmm$, is added (between parentheses) after the actual symbol $Ammm$ in the space-group tables.

The 'point group part' of the symbol of the Patterson symmetry represents the *Laue class* to which the plane group or space group belongs (*cf.* Table 2.1.2.1). In the absence of anomalous dispersion, the Laue class of a crystal expresses the *point symmetry of its diffraction record, i.e.* the symmetry of the reciprocal lattice weighted with $I(hkl)$.

* A space group is called 'symmorphic' if, apart from the lattice translations, all *generating* symmetry operations leave one common point fixed. Permitted as generators are thus only the point-group operations: rotations, reflections, inversions and rotoinversions (*cf.* Section 8.1.6).

Table 2.2.5.1. *Patterson symmetries for two and three dimensions*

Laue class	Lattice type	Patterson symmetry (with space-group number)				
Two dimensions						
2	p	$p2$ (2)				
$2mm$	p c	$p2mm$ (6)	$c2mm$ (9)			
4	p	$p4$ (10)				
$4mm$	p	$p4mm$ (11)				
6	p	$p6$ (16)				
$6mm$	p	$p6mm$ (17)				
Three dimensions						
$\bar{1}$	P	$P\bar{1}$ (2)				
$2/m$	P C	$P2/m$ (10)	$C2/m$ (12)			
mmm	P C I F	$Pmmm$ (47)	$Cmmm$ (65)	$Immm$ (71)	$Fmmm$ (69)	
$4/m$	P I	$P4/m$ (83)		$I4/m$ (87)		
$4/mmm$	P I	$P4/mmm$ (123)		$I4/mmm$ (139)		
$\bar{3}$	P R	$P\bar{3}$ (147)				$R\bar{3}$ (148)
$\bar{3}m1$	P R	$P\bar{3}m1$ (164)				$R\bar{3}m$ (166)
$\bar{3}1m$	P	$P\bar{3}1m$ (162)				
$6/m$	P	$P6/m$ (175)				
$6/mmm$	P	$P6/mmm$ (191)				
$m\bar{3}$	P I F	$Pm\bar{3}$ (200)		$Im\bar{3}$ (204)	$Fm\bar{3}$ (202)	
$m\bar{3}m$	P I F	$Pm\bar{3}m$ (221)		$Im\bar{3}m$ (229)	$Fm\bar{3}m$ (225)	

2.2.6. Space-group diagrams

The space-group diagrams serve two purposes: (i) to show the relative locations and orientations of the symmetry elements and (ii) to illustrate the arrangement of a set of symmetrically equivalent points of the general position.

All diagrams are orthogonal projections, *i.e.* the projection direction is perpendicular to the plane of the figure. Apart from the descriptions of the rhombohedral space groups with 'rhombohedral axes' (*cf.* Section 2.2.6.6), the projection direction is always a cell axis. If other axes are not parallel to the plane of the figure, they are indicated by the subscript p, as a_p, b_p or c_p. This applies to one or two axes for triclinic and monoclinic space groups (*cf.* Figs. 2.2.6.1 to 2.2.6.3), as well as to the three rhombohedral axes in Fig. 2.2.6.9.

The graphical symbols for symmetry elements, as used in the drawings, are displayed in Chapter 1.4.

In the diagrams, 'heights' h above the projection plane are indicated for symmetry planes and symmetry axes *parallel* to the projection plane, as well as for centres of symmetry. The heights are given as fractions of the shortest lattice translation normal to the projection plane and, if different from 0, are printed next to the graphical symbols. Each symmetry element at height h is accompanied by another symmetry element of the same type at height $h + \frac{1}{2}$ (this does not apply to the horizontal fourfold axes in the cubic diagrams). In the space-group diagrams, only the symmetry element at height h is indicated (*cf.* Chapter 1.4).

Schematic representations of the diagrams, displaying the origin, the labels of the axes, and the projection direction [*uvw*], are given in Figs. 2.2.6.1 to 2.2.6.10 (except Fig. 2.2.6.6). The general-position diagrams are indicated by the letter G.

2.2.6.1. *Plane groups*

Each description of a plane group contains two diagrams, one for the symmetry elements (left) and one for the general position (right). The two axes are labelled a and b, with a pointing downwards and b running from left to right.

2.2.6.2. *Triclinic space groups*

For each of the two triclinic space groups, three elevations (along a, b and c) are given, in addition to the general-position diagram G (projected along c) at the lower right of the set, as illustrated in Fig. 2.2.6.1.

The diagrams represent a reduced cell of type II for which the three interaxial angles are non-acute, *i.e.* $\alpha, \beta, \gamma \geq 90°$. For a cell of type I, all angles are acute, *i.e.* $\alpha, \beta, \gamma < 90°$. For a discussion of the two types of reduced cells, reference is made to Section 9.2.2.

2.2.6.3. *Monoclinic space groups (cf. Sections 2.2.2 and 2.2.16)*

The 'complete treatment' of each of the two settings contains four diagrams (Figs. 2.2.6.2 and 2.2.6.3). Three of them are projections of the symmetry elements, taken along the unique axis (upper left) and along the other two axes (lower left and upper right). For the general position, only the projection along the unique axis is given (lower right).

The 'synoptic descriptions' of the three cell choices (for each setting) are headed by a pair of diagrams, as illustrated in Fig. 2.2.6.4. The drawings on the left display the symmetry elements and the ones on the right the general position (labelled G). Each diagram is a projection of four neighbouring unit cells along the unique axis. It contains the outlines of the three cell choices drawn as heavy lines. For the labelling of the axes, see Fig. 2.2.6.4. The headline of the description of each cell choice contains a small-scale drawing, indicating the basis vectors and the cell that apply to that description.

2.2.6.4. *Orthorhombic space groups and orthorhombic settings*

The space-group tables contain a set of four diagrams for each orthorhombic space group. The set consists of three projections of the symmetry elements [along the c axis (upper left), the a axis (lower left) and the b axis (upper right)] in addition to the general-position diagram, which is given only in the projection along c

Table 2.2.6.1. *Numbers of distinct projections and different Hermann–Mauguin symbols for the orthorhombic space groups (space-group number placed between parentheses), listed according to point group as indicated in the headline*

Number of distinct projections	222	$mm2$	$2/m2/m2/m$
6		$Pmc2_1$ (26)	$P\ 2_1/m\ 2/m\ 2/a$ (51)
(22 space groups)		$Pma2$ (28)	$P\ 2/n\ 2_1/n\ 2/a$ (52)
		$Pca2_1$ (29)	$P\ 2/m\ 2/n\ 2_1/a$ (53)
		$Pnc2$ (30)	$P\ 2_1/c\ 2/c\ 2/a$ (54)
		$Pmn2_1$ (31)	$P\ 2/b\ 2_1/c\ 2_1/m$ (57)
		$Pna2_1$ (33)	$P\ 2_1/b\ 2/c\ 2_1/n$ (60)
		$Cmc2_1$ (36)	$P\ 2_1/n\ 2_1/m\ 2_1/a$ (62)
		$Amm2$ (38)	$C\ 2/m\ 2/c\ 2_1/m$ (63)
		$Abm2$ (39)	$C\ 2/m\ 2/c\ 2_1/a$ (64)
		$Ama2$ (40)	$I\ 2_1/m\ 2_1/m\ 2_1/a$ (74)
		$Aba2$ (41)	
		$Ima2$ (46)	
3	$P222_1$ (17)	$Pmm2$ (25)	$P\ 2/c\ 2/c\ 2/m$ (49)
(25 space groups)	$P2_12_12$ (18)	$Pcc2$ (27)	$P\ 2/b\ 2/a\ 2/n$ (50)
	$C222_1$ (20)	$Pba2$ (32)	$P\ 2_1/b\ 2_1/a\ 2/m$ (55)
	$C222$ (21)	$Pnn2$ (34)	$P\ 2_1/c\ 2_1/c\ 2/n$ (56)
		$Cmm2$ (35)	$P\ 2_1/n\ 2_1/n\ 2/m$ (58)
		$Ccc2$ (37)	$P\ 2_1/m\ 2_1/m\ 2/n$ (59)
		$Fmm2$ (42)	$C\ 2/m\ 2/m\ 2/m$ (65)
		$Fdd2$ (43)	$C\ 2/c\ 2/c\ 2/m$ (66)
		$Imm2$ (44)	$C\ 2/m\ 2/m\ 2/a$ (67)
		$Iba2$ (45)	$C\ 2/c\ 2/c\ 2/a$ (68)
			$I\ 2/b\ 2/a\ 2/m$ (72)
2			$P\ 2_1/b\ 2_1/c\ 2_1/a$ (61)
(2 space groups)			$I\ 2_1/b\ 2_1/c\ 2_1/a$ (73)
1	$P222$ (16)		$P\ 2/m\ 2/m\ 2/m$ (47)
(10 space groups)	$P2_12_12_1$ (19)		$P\ 2/n\ 2/n\ 2/n$ (48)
	$F222$ (22)		$F\ 2/m\ 2/m\ 2/m$ (69)
	$I222$ (23)		$F\ 2/d\ 2/d\ 2/d$ (70)
	$I2_12_12_1$ (24)		$I\ 2/m\ 2/m\ 2/m$ (71)
Total: (59)	(9)	(22)	(28)

(lower right). The projected axes, the origins and the projection directions of these diagrams are illustrated in Fig. 2.2.6.5. They refer to the so-called 'standard setting' of the space group, *i.e.* the setting described in the space-group tables and indicated by the 'standard Hermann–Mauguin symbol' in the headline.

For each orthorhombic space group, *six settings* exist, *i.e.* six different ways of assigning the labels *a*, *b*, *c* to the three orthorhombic symmetry directions; thus the shape and orientation of the cell are the same for each setting. These settings correspond to the six permutations of the labels of the axes (including the identity permutation); *cf.* Section 2.2.16:

$$\mathbf{abc} \quad \mathbf{ba\bar{c}} \quad \mathbf{cab} \quad \mathbf{\bar{c}ba} \quad \mathbf{bca} \quad \mathbf{a\bar{c}b}.$$

The symbol for each setting, here called 'setting symbol', is a shorthand notation for the transformation of the basis vectors of the

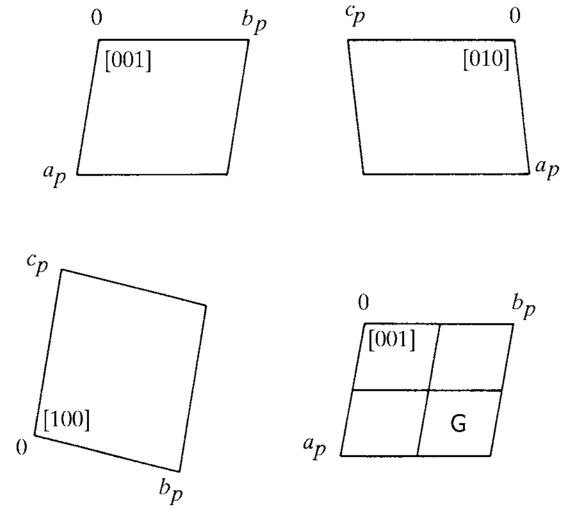


Fig. 2.2.6.1. Triclinic space groups (G = general-position diagram).

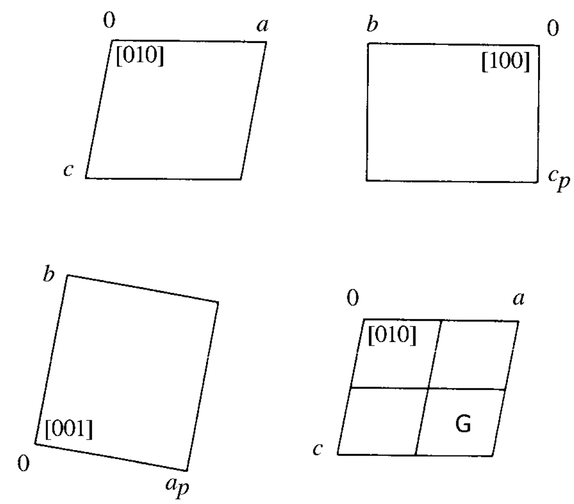


Fig. 2.2.6.2. Monoclinic space groups, setting with unique axis *b* (G = general-position diagram).

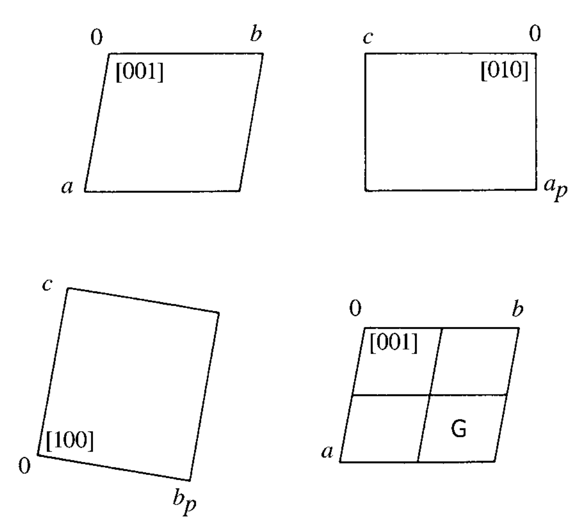


Fig. 2.2.6.3. Monoclinic space groups, setting with unique axis *c*.

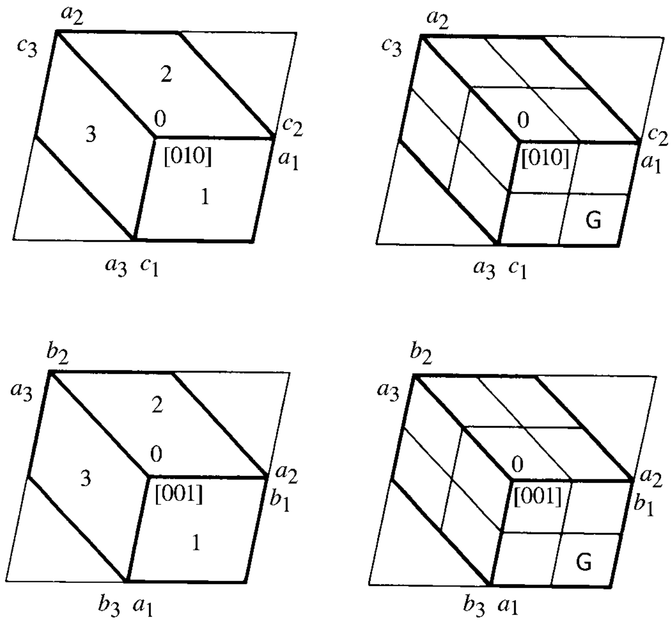


Fig. 2.2.6.4. Monoclinic space groups, cell choices 1, 2, 3. Upper pair of diagrams: setting with unique axis *b*. Lower pair of diagrams: setting with unique axis *c*. The numbers 1, 2, 3 within the cells and the subscripts of the labels of the axes indicate the cell choice (*cf.* Section 2.2.16). The unique axis points upwards from the page.

standard setting, **a**, **b**, **c**, into those of the setting considered. For instance, the setting symbol **cab** stands for the cyclic permutation

$$\mathbf{a}' = \mathbf{c}, \quad \mathbf{b}' = \mathbf{a}, \quad \mathbf{c}' = \mathbf{b}$$

or

$$(\mathbf{a}'\mathbf{b}'\mathbf{c}') = (\mathbf{abc})\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = (\mathbf{cab}),$$

where $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ is the new set of basis vectors. An interchange of two axes reverses the handedness of the coordinate system; in order to keep the system right-handed, each interchange is accompanied by the reversal of the sense of one axis, *i.e.* by an element $\bar{1}$ in the transformation matrix. Thus, $\mathbf{ba\bar{c}}$ denotes the transformation

$$(\mathbf{a}'\mathbf{b}'\mathbf{c}') = (\mathbf{abc})\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} = (\mathbf{ba\bar{c}}).$$

The six orthorhombic settings correspond to six Hermann–Mauguin symbols which, however, need not all be different; *cf.* Table 2.2.6.1.*

In the earlier (1935 and 1952) editions of *International Tables*, only one setting was illustrated, in a projection along *c*, so that it was usual to consider it as the 'standard setting' and to accept its cell edges as crystal axes and its space-group symbol as 'standard Hermann–Mauguin symbol'. In the present edition, however, *all six* orthorhombic settings are illustrated, as explained below.

The three projections of the symmetry elements can be interpreted in two ways. First, in the sense indicated above, that is, as different projections of a *single* (standard) setting of the space group, with the projected basis vectors **a**, **b**, **c** labelled as in Fig. 2.2.6.5. Second, each one of the three diagrams can be considered as the projection along $\mathbf{c}'$ of either one of *two different* settings: one setting in which $\mathbf{b}'$ is horizontal and one in which $\mathbf{b}'$ is vertical ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ refer to the setting under consideration). This second interpretation is used to illustrate in the same figure the space-group symbols corresponding to these two settings. In order to view these projections in conventional orientation ($\mathbf{b}'$ horizontal, $\mathbf{a}'$ vertical, origin in the upper left corner, projection down the positive $\mathbf{c}'$ axis), the setting with $\mathbf{b}'$ horizontal can be inspected directly with the figure upright; hence, the corresponding space-group symbol is printed above the projection. The other setting with $\mathbf{b}'$ vertical and $\mathbf{a}'$ horizontal, however, requires turning the figure over 90°, or looking at it from the side; thus, the space-group symbol is printed at the left, and it runs upwards.

The 'setting symbols' for the six settings are attached to the three diagrams of Fig. 2.2.6.6, which correspond to those of Fig. 2.2.6.5. In the orientation of the diagram where the setting symbol is read in the usual way, $\mathbf{a}'$ is vertical pointing downwards, $\mathbf{b}'$ is horizontal pointing to the right, and $\mathbf{c}'$ is pointing upwards from the page. Each setting symbol is printed in the position that in the space-group tables is actually occupied by the corresponding full Hermann–Mauguin symbol. The changes in the space-group symbol that are

* A space-group symbol is invariant under sign changes of the axes; *i.e.* the same symbol applies to the right-handed coordinate systems **abc**, $\mathbf{a\bar{b}\bar{c}}$, $\mathbf{\bar{a}b\bar{c}}$, $\mathbf{\bar{a}\bar{b}c}$ and the left-handed systems $\mathbf{\bar{a}bc}$, $\mathbf{a\bar{b}c}$, $\mathbf{ab\bar{c}}$, $\mathbf{\bar{a}\bar{b}\bar{c}}$.

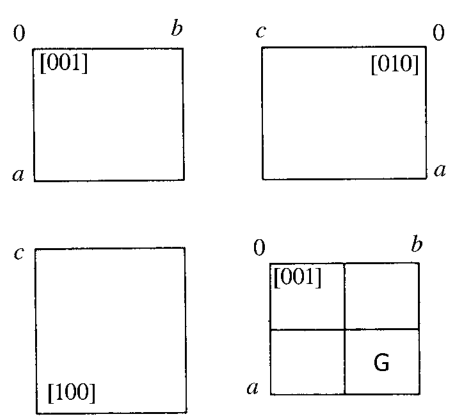


Fig. 2.2.6.5. Orthorhombic space groups. Diagrams for the 'standard setting' as described in the space-group tables (G = general-position diagram).

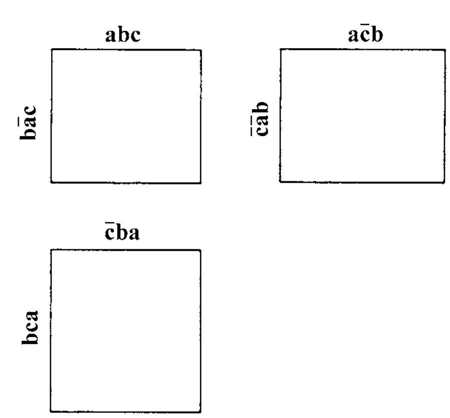


Fig. 2.2.6.6. Orthorhombic space groups. The three projections of the symmetry elements with the six setting symbols (see text). For setting symbols printed vertically, the page has to be turned clockwise by 90° or viewed from the side. Note that in the actual space-group tables instead of the setting symbols the corresponding full Hermann–Mauguin space-group symbols are printed.

associated with a particular setting symbol can easily be deduced by comparing Fig. 2.2.6.6 with the diagrams for the space group under consideration.

Not all of the 59 orthorhombic space groups have all six projections distinct, *i.e.* have different Hermann–Mauguin symbols for the six settings. This aspect is treated in Table 2.2.6.1. Only 22 space groups have six, 25 have three, 2 have two different symbols, while 10 have all symbols the same. This information can be of help in the early stages of a crystal-structure analysis.

The six setting symbols listed in the second paragraph of this section form the column headings of the orthorhombic entries in Table 4.3.2.1, which contains the extended Hermann–Mauguin symbols for the six settings of each orthorhombic space group. Note that some of these setting symbols exhibit different sign changes compared with those in Fig. 2.2.6.6.

2.2.6.5. *Tetragonal, trigonal P and hexagonal P space groups*

The pairs of diagrams for these space groups are similar to those in *IT* (1935) and *IT* (1952). Each pair consists of a general-position diagram (right) and a diagram of the symmetry elements (left), both projected along c, as illustrated in Figs. 2.2.6.7 and 2.2.6.8.

2.2.6.6. *Rhombohedral (trigonal R) space groups*

The seven rhombohedral R space groups are treated in two versions, the first based on 'hexagonal axes' (obverse setting), the second on 'rhombohedral axes' (*cf.* Sections 2.1.3 and 2.2.2). The pairs of diagrams are similar to those in *IT* (1952); the left or top one displays the symmetry elements, the right or bottom one the general position. This is illustrated in Fig. 2.2.6.9, which gives the axes a and b of the triple hexagonal cell and the projections of the axes of the primitive rhombohedral cell, labelled a_p, b_p and c_p. For convenience, all 'heights' in the space-group diagrams are fractions of the hexagonal c axis. For 'hexagonal axes', the projection direction is [001], for 'rhombohedral axes' it is [111]. In the general-position diagrams, the circles drawn in heavier lines represent atoms that lie within the primitive rhombohedral cell (provided the symbol '$-$' is read as $1 - z$ rather than as $-z$).

The pairs of drawings for the hexagonal and the rhombohedral descriptions of a space group are the same. In the rhombohedral descriptions of space groups Nos. 166 and 167, $R\bar{3}m$ and $R\bar{3}c$, the diagrams are omitted for reasons of space, and the reader is referred to the drawings in the hexagonal descriptions.

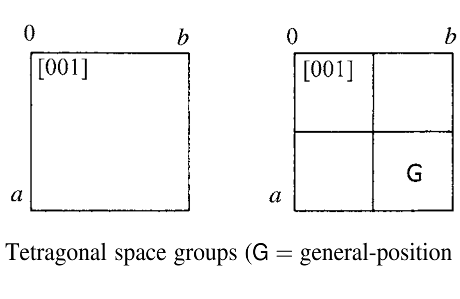


Fig. 2.2.6.7. Tetragonal space groups (G = general-position diagram).

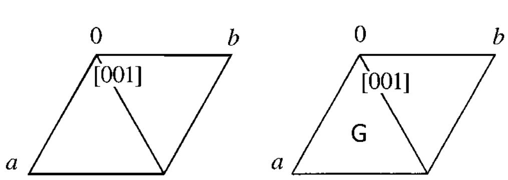


Fig. 2.2.6.8. Trigonal P and hexagonal P space groups (G = general-position diagram).

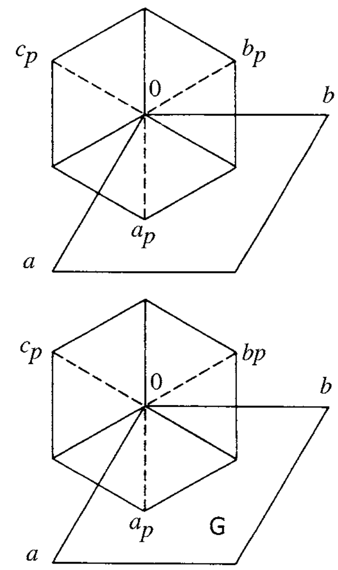


Fig. 2.2.6.9. Rhombohedral R space groups. Obverse triple hexagonal cell with 'hexagonal axes' a, b and primitive rhombohedral cell with projections of 'rhombohedral axes' a_p, b_p, c_p. Note: In the actual space-group diagrams only the upper edges (full lines), not the lower edges (dashed lines) of the primitive rhombohedral cell are shown (G = general-position diagram).

2.2.6.7. *Cubic space groups*

For each cubic space group, one projection of the symmetry elements along [001] is given, Fig. 2.2.6.10; for details of the diagrams, see Chapter 1.4 and Buerger (1956). For face-centred lattices F, only a quarter of the unit cell is shown; this is sufficient since the projected arrangement of the symmetry elements is translation-equivalent in the four quarters of an F cell. The three stereoscopic general-position diagrams in the lower part of the page are explained below.

The cubic diagrams given in *IT* (1935) were quite different from the ones used here. No drawings for cubic space groups were provided in *IT* (1952).

2.2.6.8. *Diagrams of the general position*

(i) *Non-cubic space groups*

In these diagrams, the 'heights' of the points are z coordinates, except for monoclinic space groups with unique axis b where they are y coordinates. For rhombohedral space groups, the heights are always fractions of the hexagonal c axis. The symbols $+$ and $-$ stand for $+z$ and $-z$ (or $+y$ and $-y$) in which z or y can assume any value. For points with symbols $+$ or $-$ preceded by a fraction, *e.g.*

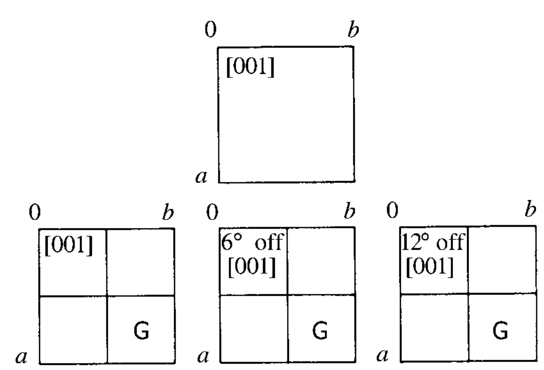


Fig. 2.2.6.10. Cubic space groups (G = general-position stereodiagrams).

$\frac{1}{2}+$ or $\frac{1}{3}-$, the relative z or y coordinate is $\frac{1}{2}$ *etc.* higher than that of the point with symbol $+$ or $-$.

Points represented by ○ and ⊙ are related by inversion, rotoinversion or mirror symmetry and are thus enantiomorphs of each other. If ○ were to be occupied by the centre of a right-handed molecule, the molecule at ⊙ would be left-handed.

Where a mirror plane exists parallel to the plane of projection, the two positions superimposed in projection are indicated by the use of a ring divided through the centre. The information given on each side refers to one of the two positions related by the mirror plane, as in $-$ ⦶ $+$.

(ii) *Stereodiagrams for cubic space groups (Fig. 2.2.6.10)*

For each cubic space group, three diagrams are given with the points of the general position as vertices of transparent polyhedra. (The spheres at the vertices are depicted as opaque, however.) For the 'starting point', the same coordinate values, $x = 0.048$, $y = 0.12$, $z = 0.08$, as in the cubic diagrams of *IT* (1935) have been used. The diagram on the left corresponds to that published in *IT* (1935); in this figure, the height h of the centre of each polyhedron is given, if different from zero. For space groups Nos. 198, 199 and 220, h refers to the special point to which the polyhedron (triangle) is connected by dotted lines. In all diagrams, polyhedra with height 1 are omitted. A grid of four squares is drawn to represent the four quarters of the basal plane of the cell.

Of the three diagrams, the image on the left and the central one form a stereopair, as well as the central image and that on the right (Langlet, 1972). The stereoscopic effect is obtained by a 6° tilt between each view. The separation of neighbouring images has the standard value of 55 mm. The presence of the two stereopairs has the advantage that difficulties in seeing the polyhedra due to overlap in one pair do not occur in the other. For space groups Nos. 219, 226 and 228, where the number of points was too large for one set, two sets of three drawings are provided, one for the upper and one for the lower half of the cell.

Notes:

(i) For space group $P4_132$ (213), the coordinates $\bar{x}, \bar{y}, \bar{z}$ have been chosen for the 'starting point' to bring out the enantiomorphism with $P4_332$ (212).

(ii) For the description of a space group with 'Origin choice 2', the coordinates x, y, z of all points have been shifted with the origin to retain the same polyhedra for both origin choices.

Readers who wish to compare other approaches to space-group diagrams and their history are referred to *IT* (1935), *IT* (1952) and the following publications: Astbury & Yardley (1924); Belov *et al.* (1980); Buerger (1956); Fedorov (1895; English translation, 1971); Friedel (1926); Hilton (1903); Niggli (1919); Schiebold (1929).

2.2.7. Origin

The determination and description of crystal structures and particularly the application of direct methods are greatly facilitated by the choice of a suitable origin and its proper identification. This is even more important if related structures are to be compared or if 'chains' of group–subgroup relations are to be constructed. In this volume, as well as in *IT* (1952), the origin of the unit cell has been chosen according to the following conventions (*cf.* Chapter 2.1 and Section 2.2.2):

(i) All centrosymmetric space groups are described with an inversion centre as origin. A further description is given if a centrosymmetric space group contains points of high site symmetry that do not coincide with a centre of symmetry.

Example: $I4_1/amd$ (141).

(ii) For noncentrosymmetric space groups, the origin is at a point of highest site symmetry, as in $P\bar{6}m2$ (187). If no site symmetry is higher than 1, except for the cases listed below under (iii), the origin is placed on a screw axis, or a glide plane, or at the intersection of several such symmetry elements.

Examples: $Pca2_1$ (29); $P6_1$ (169).

(iii) In space group $P2_12_12_1$ (19), the origin is chosen in such a way that it is surrounded symmetrically by three pairs of 2_1 axes. This principle is maintained in the following noncentrosymmetric cubic space groups of classes 23 and 432, which contain $P2_12_12_1$ as subgroup: $P2_13$ (198), $I2_13$ (199), $F4_132$ (210). It has been extended to other noncentrosymmetric orthorhombic and cubic space groups with $P2_12_12_1$ as subgroup, even though in these cases points of higher site symmetry *are* available: $I2_12_12_1$ (24), $P4_332$ (212), $P4_132$ (213), $I4_132$ (214).

There are several ways of determining the location and site symmetry of the origin. First, the origin can be inspected directly in the space-group diagrams (*cf.* Section 2.2.6). This method permits visualization of all symmetry elements that intersect the chosen origin.

Another procedure for finding the site symmetry at the origin is to look for a special position that contains the coordinate triplet 0, 0, 0 or that includes it for special values of the parameters, *e.g.* position 1*a*: 0, 0, z in space group $P4$ (75), or position 3*a* : $x, 0, \frac{1}{3}$; $0, x, \frac{2}{3}$; $\bar{x}, \bar{x}, 0$ in space group $P3_121$ (152). If such a special position occurs, the symmetry at the origin is given by the oriented site-symmetry symbol (see Section 2.2.12) of that special position; if it does not occur, the site symmetry at the origin is 1. For most practical purposes, these two methods are sufficient for the identification of the site symmetry at the origin.

2.2.7.1. *Origin statement*

In the line *Origin* immediately below the diagrams, the site symmetry of the origin is stated, if different from the identity. A further symbol indicates all symmetry elements (including glide planes and screw axes) that pass through the origin, if any. For space groups with two *origin choices*, for each of the two origins the location relative to the other origin is also given. An example is space group *Ccca* (68).

In order to keep the notation as simple as possible, no rigid rules have been applied in formulating the origin statements. Their meaning is demonstrated by the examples in Table 2.2.7.1, which should be studied together with the appropriate space-group diagrams.

These examples illustrate the following points:

(i) The site symmetry at the origin corresponds to the point group of the space group (examples *E*1–*E*3) or to a subgroup of this point group (*E*4–*E*11).

The presence of a symmetry centre at the origin is always stated explicitly, either by giving the symbol $\bar{1}$ (*E*1 and *E*4) or by the words 'at centre', followed by the full site symmetry between parentheses (*E*2 and *E*5). This completes the origin line, if no further glide planes or screw axes are present at the origin.

(ii) If glide planes or screw axes are present, as in examples *E*4–*E*11, they are given in the order of the symmetry directions listed in Table 2.2.4.1. Such a set of symmetry elements is described here in the form of a 'point-group-like' symbol (although it does not describe a group). With the help of the orthorhombic symmetry directions, the symbols in *E*4–*E*6 can be interpreted easily. The shortened notation of *E*6 and *E*7 is used for space groups of crystal classes $mm2$, $4mm$, $\bar{4}2m$, $3m$, $6mm$ and $\bar{6}2m$ if the site symmetry at the origin can be easily recognized from the shortened symbol.

Table 2.2.7.1. *Examples of origin statements*

Example number	Space group (No.)	Origin statement	Meaning of last symbol in $E4$–$E11$
$E1$	$P\bar{1}$ (2)	at $\bar{1}$	
$E2$	$P2/m$ (10)	at centre $(2/m)$	
$E3$	$P222$ (16)	at 222	
$E4$	$Pcca$ (54)	at $\bar{1}$ on $1ca$	$c \perp [010]$, $a \perp [001]$
$E5$	$Cmcm$ (63)	at centre $(2/m)$ at $2/mc2_1$	$2 \parallel [100]$, $m \perp [100]$, $c \perp [010]$, $2_1 \parallel [001]$
$E6$	$Pcc2$ (27)	on $cc2$; short for: on 2 on $cc2$	$c \perp [100]$, $c \perp [010]$, $2 \parallel [001]$
$E7$	$P4bm$ (100)	on $41g$; short for: on 4 on $41g$	$4 \parallel [001]$, $g \perp [1\bar{1}0]$ and $g \perp [110]$
$E8$	$P4_2mc$ (105)	on $2mm$ on 4_2mc	$4_2 \parallel [001]$, $m \perp [100]$ and $m \perp [010]$, $c \perp [1\bar{1}0]$ and $c \perp [110]$
$E9$	$P4_32_12$ (96)	on 2[110] at $2_11(1,2)$	$2_1 \parallel [001]$, 1 in $[1\bar{1}0]$ and $2 \parallel [110]$
$E10$	$P3_121$ (152)	on 2[110] at $3_1(1,1,2)1$	$3_1 \parallel [001]$, $2 \parallel [110]$
$E11$	$P3_112$ (151)	on 2[210] at $3_11(1,1,2)$	$3_1 \parallel [001]$, $2 \parallel [210]$

(iii) For the tetragonal, trigonal and hexagonal space groups, the situation is more complicated than for the orthorhombic groups. The tetragonal space groups have one primary, two secondary and two tertiary symmetry directions. For hexagonal groups, these numbers are one, three and three (Table 2.2.4.1). If the symmetry elements passing through the origin are the same for the two (three) secondary or the two (three) tertiary directions, only one entry is given at the relevant position of the origin statement [example $E7$: 'on $41g$' instead of 'on $41(g, g)$']. An exception occurs for the site-symmetry group $2mm$ (example $E8$), which is always written in full rather than as $2m1$.

If the symmetry elements are different, two (three) symbols are placed between parentheses, which stand for the two (three) secondary or tertiary directions. The order of these symbols corresponds to the order of the symmetry directions within the secondary or tertiary set, as listed in Table 2.2.4.1. Directions without symmetry are indicated by the symbol 1. With this rule, the last symbols in the examples $E9$–$E11$ can be interpreted.

Note that for some tetragonal space groups (Nos. 100, 113, 125, 127, 129, 134, 138, 141, 142) the glide-plane symbol g is used in the origin statement. This symbol occurs also in the block *Symmetry operations* of these space groups; it is explained in Sections 2.2.9 and 11.1.2.

(iv) To emphasize the orientation of the site-symmetry elements at the origin, examples $E9$ and $E10$ start with 'on 2[110]' and $E11$ with 'on 2[210]'. In $E8$, the site-symmetry group is $2mm$. Together with the space-group symbol this indicates that 2 is along the primary tetragonal direction, that the two symbols m refer to the two secondary symmetry directions [100] and [010], and that the tertiary set of directions does not contribute to the site symmetry.

For monoclinic space groups, an indication of the orientation of the symmetry elements is not necessary; hence, the site symmetry at the origin is given by non-oriented symbols. For orthorhombic space groups, the orientation is obvious from the symbol of the space group.

(v) The extensive description of the symmetry elements passing through the origin is not retained for the cubic space groups, as this would have led to very complicated notations for some of the groups.

2.2.8. Asymmetric unit

An asymmetric unit of a space group is a (simply connected) smallest closed part of space from which, by application of all symmetry operations of the space group, the whole of space is filled. This implies that mirror planes and rotation axes must form boundary planes and boundary edges of the asymmetric unit. A twofold rotation axis may bisect a boundary plane. Centres of inversion must either form vertices of the asymmetric unit or be located at the midpoints of boundary planes or boundary edges. For glide planes and screw axes, these simple restrictions do not hold. An asymmetric unit contains all the information necessary for the complete description of the crystal structure. In mathematics, an asymmetric unit is called 'fundamental region' or 'fundamental domain'.

Example

The boundary planes of the asymmetric unit in space group $Pmmm$ (47) are fixed by the six mirror planes $x, y, 0$; $x, y, \frac{1}{2}$; $x, 0, z$; $x, \frac{1}{2}, z$; $0, y, z$; and $\frac{1}{2}, y, z$. For space group $P2_12_12_1$ (19), on the other hand, a large number of connected regions, each with a volume of $\frac{1}{4}V(\text{cell})$, may be chosen as asymmetric unit.

In cases where the asymmetric unit is not uniquely determined by symmetry, its choice may depend on the purpose of its application. For the description of the structures of molecular crystals, for instance, it is advantageous to select asymmetric units that contain one or more complete molecules. In the space-group tables of this volume, the asymmetric units are chosen in such a way that Fourier summations can be performed conveniently.

For all triclinic, monoclinic and orthorhombic space groups, the asymmetric unit is chosen as a parallelepiped with one vertex at the origin of the cell and with boundary planes parallel to the faces of the cell. It is given by the notation

$$0 \le x_i \le \text{upper limit of } x_i,$$

where x_i stands for x, y or z.

For space groups with higher symmetry, cases occur where the origin does not coincide with a vertex of the asymmetric unit or where not all boundary planes of the asymmetric unit are parallel to those of the cell. In all these cases, parallelepipeds

$$\text{lower limit of } x_i \le x_i \le \text{upper limit of } x_i$$

are given that are equal to or larger than the asymmetric unit. Where necessary, the boundary planes lying within these parallelepipeds are given by additional inequalities, such as $x \le y$, $y \le \frac{1}{2} - x$ *etc.*

In the trigonal, hexagonal and especially the cubic crystal systems, the asymmetric units have complicated shapes. For this reason, they are also specified by the coordinates of their vertices. Drawings of asymmetric units for cubic space groups have been published by Koch & Fischer (1974). Fig. 2.2.8.1 shows the boundary planes occurring in the tetragonal, trigonal and hexagonal systems, together with their algebraic equations.

Examples

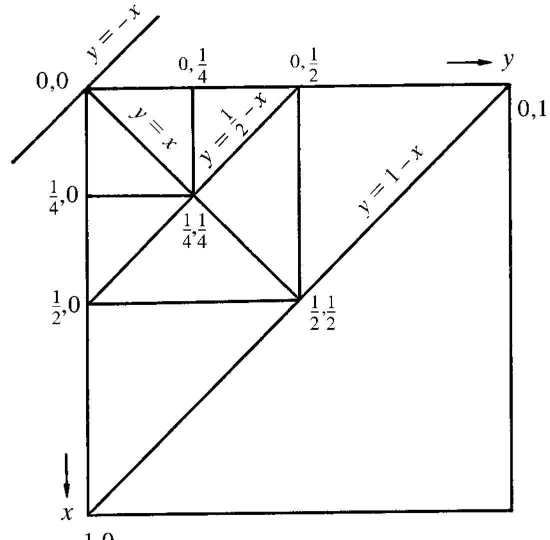
(1) In space group $P4mm$ (99), the boundary plane $y = x$ occurs in addition to planes parallel to the unit-cell faces; the asymmetric unit is given by

$$0 \le x \le \tfrac{1}{2};\quad 0 \le y \le \tfrac{1}{2};\quad 0 \le z \le 1;\quad x \le y.$$

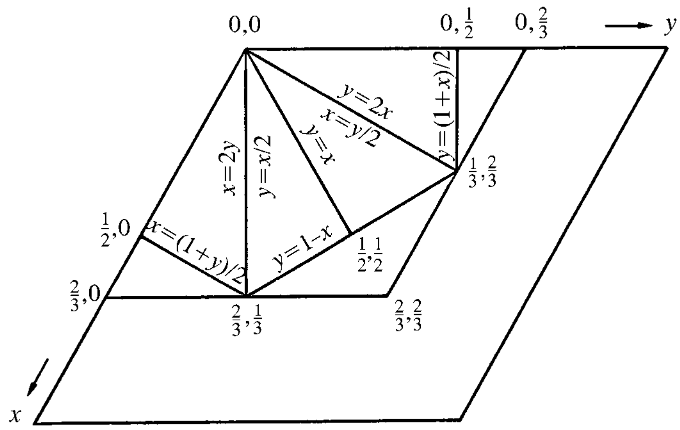
(2) In $P4bm$ (100), one of the boundary planes is $y = \frac{1}{2} - x$. The asymmetric unit is given by

$$0 \le x \le \tfrac{1}{2};\quad 0 \le y \le \tfrac{1}{2};\quad 0 \le z \le 1;\quad y \le \tfrac{1}{2} - x.$$

(3) In space group $R32$ (155; hexagonal axes), the boundary planes are, among others, $x = (1 + y)/2$, $y = 1 - x$, $y = (1 + x)/2$.



(*a*)



(*b*)

Fig. 2.2.8.1. Boundary planes of asymmetric units occurring in the space-group tables. (*a*) Tetragonal system. (*b*) Trigonal and hexagonal systems. The point coordinates refer to the vertices in the plane $z = 0$.

The asymmetric unit is defined by

$$0 \le x \le \tfrac{2}{3};\quad 0 \le y \le \tfrac{2}{3};\quad 0 \le z \le \tfrac{1}{6};$$
$$x \le (1+y)/2;\quad y \le \min(1-x, (1+x)/2)$$
$$\text{Vertices:}\quad 0,0,0 \quad \tfrac{1}{2},0,0 \quad \tfrac{2}{3},\tfrac{1}{3},0 \quad \tfrac{1}{3},\tfrac{2}{3},0 \quad 0,\tfrac{1}{2},0$$
$$0,0,\tfrac{1}{6} \quad \tfrac{1}{2},0,\tfrac{1}{6} \quad \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{6} \quad \tfrac{1}{3},\tfrac{2}{3},\tfrac{1}{6} \quad 0,\tfrac{1}{2},\tfrac{1}{6}.$$

It is obvious that the indication of the vertices is of great help in drawing the asymmetric unit.

Fourier syntheses

For complicated space groups, the easiest way to calculate Fourier syntheses is to consider the parallelepiped listed, without taking into account the additional boundary planes of the asymmetric unit. These planes should be drawn afterwards in the Fourier synthesis. For the computation of integrated properties from Fourier syntheses, such as the number of electrons for parts of the structure, the values at the boundaries of the asymmetric unit must be applied with a reduced weight if the property is to be obtained as the product of the content of the asymmetric unit and the multiplicity.

Example

In the parallelepiped of space group *Pmmm* (47), the weights for boundary planes, edges and vertices are $\frac{1}{2}$, $\frac{1}{4}$ and $\frac{1}{8}$, respectively.

Asymmetric units of the plane groups have been discussed by Buerger (1949, 1960) in connection with Fourier summations.

2.2.9. Symmetry operations

As explained in Sections 8.1.6 and 11.1.1, the coordinate triplets of the *General position* of a space group may be interpreted as a shorthand description of the symmetry operations in matrix notation. The geometric description of the symmetry operations is found in the space-group tables under the heading *Symmetry operations*.

2.2.9.1. *Numbering scheme*

The numbering $(1)\ldots(p)\ldots$ of the entries in the blocks *Symmetry operations* and *General position* (first block below *Positions*) is the same. Each listed coordinate triplet of the general position is preceded by a number between parentheses (p). The same number (p) precedes the corresponding symmetry operation. For space groups with *primitive* cells, both lists contain the same number of entries.

For space groups with *centred* cells, to the one block *General position* several (2, 3 or 4) blocks *Symmetry operations* correspond. The numbering scheme of the general position is applied to each one of these blocks. The number of blocks equals the multiplicity of the centred cell, *i.e.* the number of centring translations below the subheading *Coordinates*, such as $(0,0,0)+$, $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$, $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$.

Whereas for the *Positions* the reader is expected to add these centring translations to each printed coordinate triplet himself (in order to obtain the complete general position), for the *Symmetry operations* the corresponding data are listed explicitly. The different blocks have the subheadings 'For (0,0,0)+ set', 'For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set', *etc.* Thus, an obvious one-to-one correspondence exists between the analytical description of a symmetry operation in the form of its general-position coordinate triplet and the geometrical description under *Symmetry operations*. Note that the coordinates are reduced modulo 1, where applicable, as shown in the example below.

Example: Ibca (73)

The centring translation is $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. Accordingly, above the general position one finds $(0,0,0)+$ and $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$. In the block *Symmetry operations*, under the subheading 'For $(0,0,0)+$ set', entry (2) refers to the coordinate triplet $\bar{x}+\frac{1}{2},\ \bar{y},\ z+\frac{1}{2}$. Under the subheading 'For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set', however, entry (2) refers to $\bar{x},\ \bar{y}+\frac{1}{2},\ z$. The triplet $\bar{x},\ \bar{y}+\frac{1}{2},\ z$ is selected rather than $\bar{x}+1,\ \bar{y}+\frac{1}{2},\ z+1$, because the coordinates are reduced modulo 1.

In space groups with two origins where a 'symmetry element' and an 'additional symmetry element' are of different type (*e.g.* mirror *versus* glide plane, rotation *versus* screw axis, Tables 4.1.2.2 and 4.1.2.3), the origin shift may interchange the two *different* types in the *same* location (referred to the appropriate origin) under the same number (p). Thus, in $P4/nmm$ (129), (p) = (7) represents a $\bar{2}$ and a 2_1 axis, both in $x, x, 0$, whereas (p) = (16) represents a g and an m plane, both in x, x, z.

2.2.9.2. *Designation of symmetry operations*

An entry in the block *Symmetry operations* is characterized as follows.

(i) A symbol denoting the *type* of the symmetry operation (*cf.* Chapter 1.3), including its glide or screw part, if present. In most cases, the glide or screw part is given explicitly by fractional coordinates between parentheses. The sense of a rotation is indicated by the superscript + or −. Abbreviated notations are used for the glide reflections $a(\frac{1}{2},0,0) \equiv a$; $b(0,\frac{1}{2},0) \equiv b$; $c(0,0,\frac{1}{2}) \equiv c$. Glide reflections with complicated and unconventional glide parts are designated by the letter g, followed by the glide part between parentheses.

(ii) A coordinate triplet indicating the *location* and *orientation* of the symmetry element which corresponds to the symmetry operation. For rotoinversions, the location of the inversion point is given in addition.

Details of this symbolism are presented in Section 11.1.2.

Examples

(1) $a\ \ x,y,\frac{1}{4}$
Glide reflection with glide component $(\frac{1}{2},0,0)$ through the plane $x,y,\frac{1}{4}$, *i.e.* the plane parallel to (001) at $z=\frac{1}{4}$.

(2) $\bar{4}^{+}\ \ \frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
Fourfold rotoinversion, consisting of a counter clockwise rotation by 90° around the line $\frac{1}{4},\frac{1}{4},z$, followed by an inversion through the point $\frac{1}{4},\frac{1}{4},\frac{1}{4}$.

(3) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})\ \ x,x,z$
Glide reflection with glide component $(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ through the plane x,x,z, *i.e.* the plane parallel to $(1\bar{1}0)$ containing the point 0, 0, 0.

(4) $g(\frac{1}{3},\frac{1}{6},\frac{1}{6})\ \ 2x-\frac{1}{2},x,z$ (hexagonal axes)
Glide reflection with glide component $(\frac{1}{3},\frac{1}{6},\frac{1}{6})$ through the plane $2x-\frac{1}{2},x,z$, *i.e.* the plane parallel to $(1\bar{2}10)$, which intersects the a axis at $-\frac{1}{2}$ and the b axis at $\frac{1}{4}$; this operation occurs in $R\bar{3}c$ (167, hexagonal axes).

(5) Symmetry operations in *Ibca* (73)
Under the subheading 'For (0, 0, 0)+ set', the operation generating the coordinate triplet (2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ from (1) x, y, z is symbolized by $2(0,0,\frac{1}{2})\ \ \frac{1}{4},0,z$. This indicates a twofold screw rotation with screw part $(0,0,\frac{1}{2})$ for which the corresponding screw axis coincides with the line $\frac{1}{4},0,z$, *i.e.* runs parallel to [001] through the point $\frac{1}{4},0,0$. Under the subheading 'For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+ set', the operation generating the coordinate triplet (2) $\bar{x},\bar{y}+\frac{1}{2},z$ from (1) x,y,z is symbolized by $2\ \ 0,\frac{1}{4},z$. It is thus a twofold rotation (without screw part) around the line $0,\frac{1}{4},z$.

2.2.10. Generators

The line *Generators selected* states the symmetry operations and their sequence, selected to generate all symmetrically equivalent points of the *General position* from a point with coordinates x, y, z. Generating translations are listed as t(1, 0, 0), t(0, 1, 0), t(0, 0, 1); likewise for additional centring translations. The other symmetry operations are given as numbers (p) that refer to the corresponding coordinate triplets of the general position and the corresponding entries under *Symmetry operations*, as explained in Section 2.2.9 [for centred space groups the first block 'For (0, 0, 0)+ set' must be used].

For all space groups, the identity operation given by (1) is selected as the first generator. It is followed by the generators t(1, 0, 0), t(0, 1, 0), t(0, 0, 1) of the integral lattice translations and, if necessary, by those of the centring translations, *e.g.* $t(\frac{1}{2},\frac{1}{2},0)$ for a C lattice. In this way, point x, y, z and all its translationally equivalent points are generated. (The remark 'and its translationally equivalent points' will hereafter be omitted.) The sequence chosen for the generators following the translations depends on the crystal class of the space group and is set out in Table 8.3.5.1 of Section 8.3.5.

Example: $P12_1/c1$ (14, unique axis b, cell choice 1)
After the generation of (1) x, y, z, the operation (2) which stands for a twofold screw rotation around the axis $0,y,\frac{1}{4}$ generates point (2) of the general position with coordinate triplet $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$. Finally, the inversion (3) generates point (3) $\bar{x},\bar{y},\bar{z}$ from point (1), and point (4′) $x,\bar{y}-\frac{1}{2},z-\frac{1}{2}$ from point (2). Instead of (4′), however, the coordinate triplet (4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$ is listed, because the coordinates are reduced modulo 1.

The example shows that for the space group $P12_1/c1$ two operations, apart from the identity and the generating translations, are sufficient to generate all symmetrically equivalent points. Alternatively, the inversion (3) plus the glide reflection (4), or the glide reflection (4) plus the twofold screw rotation (2), might have been chosen as generators. The process of generation and the selection of the generators for the space-group tables, as well as the resulting sequence of the symmetry operations, are discussed in Section 8.3.5.

For different descriptions of the same space group (settings, cell choices, origin choices), the generating operations are the same. Thus, the transformation relating the two coordinate systems transforms also the generators of one description into those of the other.

From the Fifth Edition onwards, this applies also to the description of the seven rhombohedral (R) space groups by means of 'hexagonal' and 'rhombohedral' axes. In previous editions, there was a difference in the *sequence* (not the data) of the 'coordinate triplets' and the 'symmetry operations' in both descriptions (*cf.* Section 2.10 in the First to Fourth Editions).

2.2.11. Positions

The entries under *Positions** (more explicitly called *Wyckoff positions*) consist of the one *General position* (upper block) and the *Special positions* (blocks below). The columns in each block, from left to right, contain the following information for each Wyckoff position.

(i) *Multiplicity M of the Wyckoff position*. This is the number of equivalent points per unit cell. For primitive cells, the multiplicity *M* of the general position is equal to the order of the point group of the space group; for centred cells, *M* is the product of the order of the point group and the number (2, 3 or 4) of lattice points per cell. The multiplicity of a special position is always a divisor of the multiplicity of the general position.

(ii) *Wyckoff letter*. This letter is merely a coding scheme for the Wyckoff positions, starting with a at the bottom position and continuing upwards in alphabetical order (the theoretical background on Wyckoff positions is given in Section 8.3.2).

(iii) *Site symmetry*. This is explained in Section 2.2.12.

(iv) *Coordinates*. The sequence of the coordinate triplets is based on the *Generators* (*cf.* Section 2.2.10). For centred space groups, the centring translations, for instance $(0,0,0)+\ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$, are listed above the coordinate triplets. The symbol '+' indicates that, in order to obtain a complete Wyckoff position, the components of

* The term *Position* (singular) is defined as a *set* of symmetrically equivalent points, in agreement with *IT* (1935): Point position; *Punktlage* (German); *Position* (French). Note that in *IT* (1952) the plural, equivalent positions, was used.

these centring translations have to be added to the listed coordinate triplets. Note that not all points of a position always lie within the unit cell; some may be outside since the coordinates are formulated modulo 1; thus, for example, $\bar{x}, \bar{y}, \bar{z}$ is written rather than $\bar{x}+1, \bar{y}+1, \bar{z}+1$.

The *M* coordinate triplets of a position represent the coordinates of the *M* equivalent points (atoms) in the unit cell. A graphic representation of the points of the general position is provided by the general-position diagram; *cf.* Section 2.2.6.

(v) *Reflection conditions*. These are described in Section 2.2.13.

The two types of positions, general and special, are characterized as follows:

(i) *General position*

A set of symmetrically equivalent points, *i.e.* a 'crystallographic orbit', is said to be in 'general position' if each of its points is left invariant only by the identity operation but by no other symmetry operation of the space group. Each space group has only one general position.

The coordinate triplets of a general position (which always start with *x*, *y*, *z*) can also be interpreted as a short-hand form of the matrix representation of the symmetry operations of the space group; this viewpoint is further described in Sections 8.1.6 and 11.1.1.

(ii) *Special position(s)*

A set of symmetrically equivalent points is said to be in 'special position' if each of its points is mapped onto itself by the identity and at least one further symmetry operation of the space group. This implies that specific constraints are imposed on the coordinates of each point of a special position; *e.g.* $x = \frac{1}{4}, y = 0$, leading to the triplet $\frac{1}{4}, 0, z$; or $y = x + \frac{1}{2}$, leading to the triplet $x, x + \frac{1}{2}, z$. The number of special positions in a space group [up to 26 in *Pmmm* (No. 47)] depends on the number and types of symmetry operations that map a point onto itself.

The set of *all* symmetry operations that map a point onto itself forms a group, known as the 'site-symmetry group' of that point. It is given in the third column by the 'oriented site-symmetry symbol' which is explained in Section 2.2.12. General positions always have site symmetry 1, whereas special positions have higher site symmetries, which can differ from one special position to another.

If in a crystal structure the centres of finite objects, such as molecules, are placed at the points of a special position, each such object must display a point symmetry that is at least as high as the site symmetry of the special position. Geometrically, this means that the centres of these objects are located on symmetry elements without translations (centre of symmetry, mirror plane, rotation axis, rotoinversion axis) or at the intersection of several symmetry elements of this kind (*cf.* space-group diagrams).

Note that the location of an object on a screw axis or on a glide plane does *not* lead to an increase in the site symmetry and to a consequent reduction of the multiplicity for that object. Accordingly, a space group that contains only symmetry elements *with* translation components does not have any special position. Such a space group is called 'fixed-point-free'. The 13 space groups of this kind are listed in Section 8.3.2.

Example: Space group $C12/c1$ (15, unique axis *b*, cell choice 1)

The general position 8*f* of this space group contains eight equivalent points per cell, each with site symmetry 1. The coordinate triplets of four points, (1) to (4), are given explicitly, the coordinates of the other four points are obtained by adding the components $\frac{1}{2}, \frac{1}{2}, 0$ of the *C*-centring translation to the coordinate triplets (1) to (4).

The space group has five special positions with Wyckoff letters *a* to *e*. The positions 4*a* to 4*d* require inversion symmetry, $\bar{1}$, whereas Wyckoff position 4*e* requires twofold rotation symmetry, 2, for any object in such a position. For position 4*e*, for instance, the four equivalent points have the coordinates $0, y, \frac{1}{4};\ 0, \bar{y}, \frac{3}{4};\ \frac{1}{2}, y+\frac{1}{2}, \frac{1}{4};\ \frac{1}{2}, \bar{y}+\frac{1}{2}, \frac{3}{4}$. The values of *x* and *z* are specified, whereas *y* may take any value. Since each point of position 4*e* is mapped onto itself by a twofold rotation, the multiplicity of the position is reduced from 8 to 4, whereas the order of the site-symmetry group is increased from 1 to 2.

From the entries 'Symmetry operations', the locations of the four twofold axes can be deduced as $0, y, \frac{1}{4};\ 0, y, \frac{3}{4};\ \frac{1}{2}, y, \frac{1}{4};\ \frac{1}{2}, y, \frac{3}{4}$.

From this example, the general rule is apparent that the product of the position multiplicity and the order of the corresponding site-symmetry group is constant for all Wyckoff positions of a given space group; it is the multiplicity of the general position.

Attention is drawn to ambiguities in the description of crystal structures in a few space groups, depending on whether the coordinate triplets of *IT* (1952) or of this edition are taken. This problem is analysed by Parthé *et al.* (1988).

2.2.12. Oriented site-symmetry symbols

The third column of each Wyckoff position gives the *Site symmetry** of that position. The site-symmetry group is isomorphic to a (proper or improper) subgroup of the point group to which the space group under consideration belongs. The site-symmetry groups of the different points of the same special position are conjugate (symmetrically equivalent) subgroups of the space group. For this reason, all points of one special position are described by the same site-symmetry symbol.

Oriented site-symmetry symbols (*cf.* Fischer *et al.*, 1973) are employed to show how the symmetry elements at a site are related to the symmetry elements of the crystal lattice. The site-symmetry symbols display the same sequence of symmetry directions as the space-group symbol (*cf.* Table 2.2.4.1). Sets of equivalent symmetry directions that do not contribute any element to the site-symmetry group are represented by a dot. In this way, the orientation of the symmetry elements at the site is emphasized, as illustrated by the following examples.

Examples

(1) In the tetragonal space group $P4_22_12$ (94), Wyckoff position 4*f* has site symmetry ..2 and position 2*b* has site symmetry 2.22. The easiest way to interpret the symbols is to look at the dots first. For position 4*f*, the 2 is preceded by two dots and thus must belong to a tertiary symmetry direction. Only one tertiary direction is used. Consequently, the site symmetry is the monoclinic point group 2 with one of the two tetragonal tertiary directions as twofold axis.

Position *b* has one dot, with one symmetry symbol before and two symmetry symbols after it. The dot corresponds, therefore, to the secondary symmetry directions. The first symbol 2 indicates a twofold axis along the primary symmetry direction (*c* axis). The final symbols 22 indicate two twofold axes along the two mutually perpendicular tertiary directions $[1\bar{1}0]$ and [110]. The site symmetry is thus orthorhombic, 222.

(2) In the cubic space group *I*23 (197), position 6*b* has 222.. as its oriented site-symmetry symbol. The orthorhombic group 222 is completely related to the primary set of cubic symmetry

* Often called point symmetry: *Punktsymmetrie* or *Lagesymmetrie* (German): *symétrie ponctuelle* (French).

directions, with the three twofold axes parallel to the three equivalent primary directions [100], [010], [001].

(3) In the cubic space group $Pn\bar{3}n$ (222), position 6b has 42.2 as its site-symmetry symbol. This 'cubic' site-symmetry symbol displays a tetragonal site symmetry. The position of the dot indicates that there is no symmetry along the four secondary cubic directions. The fourfold axis is connected with one of the three primary cubic symmetry directions and two equivalent twofold axes occur along the remaining two primary directions. Moreover, the group contains two mutually perpendicular (equivalent) twofold axes along those two of the six tertiary cubic directions $\langle 110 \rangle$ that are normal to the fourfold axis. Each pair of equivalent twofold axes is given by just one symbol 2. (Note that at the six sites of position 6b the fourfold axes are twice oriented along a, twice along b and twice along c.)

(4) In the tetragonal space group $P4_2/nnm$ (134), position 2a has site symmetry $\bar{4}2m$. The site has symmetry for all symmetry directions. Because of the presence of the primary $\bar{4}$ axis, only one of the twofold axes along the two secondary directions need be given explicitly and similarly for the mirror planes m perpendicular to the two tertiary directions.

The above examples show:

(i) The oriented site-symmetry symbols become identical to Hermann–Mauguin point-group symbols if the dots are omitted.

(ii) Sets of symmetry directions having more than one equivalent direction may require more than one character if the site-symmetry group belongs to a lower crystal system than the space group under consideration.

To show, for the same type of site symmetry, how the oriented site-symmetry symbol depends on the space group under discussion, the site-symmetry group $mm2$ will be considered in orthorhombic and tetragonal space groups. Relevant crystal classes are $mm2$, mmm, $4mm$, $\bar{4}2m$ and $4/mmm$. The site symmetry $mm2$ contains two mutually perpendicular mirror planes intersecting in a twofold axis.

For space groups of crystal class $mm2$, the twofold axis at the site must be parallel to the one direction of the rotation axes of the space group. The site-symmetry group $mm2$, therefore, occurs only in the orientation $mm2$. For space groups of class mmm (full symbol $2/m\ 2/m\ 2/m$), the twofold axis at the site may be parallel to a, b or c and the possible orientations of the site symmetry are $2mm$, $m2m$ and $mm2$. For space groups of the tetragonal crystal class $4mm$, the twofold axis of the site-symmetry group $mm2$ must be parallel to the fourfold axis of the crystal. The two mirror planes must belong either to the two secondary or to the two tertiary tetragonal directions so that $2mm.$ and $2.mm$ are possible site-symmetry symbols. Similar considerations apply to class $\bar{4}2m$ which can occur in two settings, $\bar{4}2m$ and $\bar{4}m2$. Finally, for class $4/mmm$ (full symbol $4/m\ 2/m\ 2/m$), the twofold axis of $2mm$ may belong to any of the three kinds of symmetry directions and possible oriented site symmetries are $2mm.$, $2.mm$, $m2m.$ and $m.2m$. In the first two symbols, the twofold axis extends along the single primary direction and the mirror planes occupy either both secondary or both tertiary directions; in the last two cases, one mirror plane belongs to the primary direction and the second to either one secondary or one tertiary direction (the other equivalent direction in each case being occupied by the twofold axis).

* The reflection conditions were called *Auslöschungen* (German), missing spectra (English) and *extinctions* (French) in *IT* (1935) and 'Conditions limiting possible reflections' in *IT* (1952); they are often referred to as 'Systematic or space-group absences' (*cf.* Chapter 12.3).

Table 2.2.13.1. *Integral reflection conditions for centred cells (lattices)*

Reflection condition	Centring type of cell	Centring symbol
None	Primitive	P R*(rhombohedral axes)
$h + k = 2n$	C-face centred	C
$k + l = 2n$	A-face centred	A
$h + l = 2n$	B-face centred	B
$h + k + l = 2n$	Body centred	I
$h + k, h + l$ and $k + l = 2n$ or: h, k, l all odd or all even ('unmixed')	All-face centred	F
$-h + k + l = 3n$	Rhombohedrally centred, obverse setting (standard)	R* (hexagonal axes)
$h - k + l = 3n$	Rhombohedrally centred, reverse setting	
$h - k = 3n$	Hexagonally centred	H†

* For further explanations see Chapters 1.2 and 2.1.
† For the use of the unconventional H cell, see Chapter 1.2.

2.2.13. Reflection conditions

The *Reflection conditions** are listed in the right-hand column of each Wyckoff position.

These conditions are formulated here, in accordance with general practice, as 'conditions of occurrence' (structure factor not systematically zero) and not as 'extinctions' or 'systematic absences' (structure factor zero). Reflection conditions are listed for *all* those three-, two- and one-dimensional sets of reflections for which extinctions exist; hence, for those nets or rows that are *not* listed, no reflection conditions apply.

There are two types of systematic reflection conditions for diffraction of crystals by radiation:

(1) *General conditions*. They apply to *all* Wyckoff positions of a space group, *i.e.* they are always obeyed, irrespective of which Wyckoff positions are occupied by atoms in a particular crystal structure.

(2) *Special conditions* ('extra' conditions). They apply only to *special* Wyckoff positions and occur always in addition to the general conditions of the space group. Note that each extra condition is valid only for the scattering contribution of those atoms that are located in the relevant special Wyckoff position. If the special position is occupied by atoms whose scattering power is high, in comparison with the other atoms in the structure, reflections violating the extra condition will be weak.

2.2.13.1. *General reflection conditions*

These are due to one of three effects:

(i) *Centred cells*. The resulting conditions apply to the whole three-dimensional set of reflections *hkl*. Accordingly, they are called *integral reflection conditions*. They are given in Table 2.2.13.1. These conditions result from the centring vectors of centred cells. They disappear if a primitive cell is chosen instead of a centred cell. Note that the centring symbol and the corresponding integral reflection condition may change with a change of the basis vectors (*e.g.* monoclinic: $C \rightarrow A \rightarrow I$).

Table 2.2.13.2. *Zonal and serial reflection conditions for glide planes and screw axes (cf. Chapter 1.3)*

(*a*) Glide planes

Type of reflections	Reflection condition	Glide plane: Orientation of plane	Glide plane: Glide vector	Glide plane: Symbol	Crystallographic coordinate system to which condition applies
$0kl$	$k = 2n$	(100)	$\mathbf{b}/2$	b	Monoclinic (a unique), Tetragonal (rows b, c, n); Orthorhombic, Cubic (all rows)
	$l = 2n$		$\mathbf{c}/2$	c	
	$k + l = 2n$		$\mathbf{b}/2 + \mathbf{c}/2$	n	
	$k + l = 4n$ $(k, l = 2n)$*		$\mathbf{b}/4 \pm \mathbf{c}/4$	d	
$h0l$	$l = 2n$	(010)	$\mathbf{c}/2$	c	Monoclinic (b unique), Tetragonal (rows c, a, n); Orthorhombic, Cubic (all rows)
	$h = 2n$		$\mathbf{a}/2$	a	
	$l + h = 2n$		$\mathbf{c}/2 + \mathbf{a}/2$	n	
	$l + h = 4n$ $(l, h = 2n)$*		$\mathbf{c}/4 \pm \mathbf{a}/4$	d	
$hk0$	$h = 2n$	(001)	$\mathbf{a}/2$	a	Monoclinic (c unique), Tetragonal (rows a, b, n); Orthorhombic, Cubic (all rows)
	$k = 2n$		$\mathbf{b}/2$	b	
	$h + k = 2n$		$\mathbf{a}/2 + \mathbf{b}/2$	n	
	$h + k = 4n$ $(h, k = 2n)$*		$\mathbf{a}/4 \pm \mathbf{b}/4$	d	
$h\bar{h}0l$, $0k\bar{k}l$, $\bar{h}0hl$	$l = 2n$	$(11\bar{2}0)$, $(\bar{2}110)$, $(1\bar{2}10)$ } $\{11\bar{2}0\}$	$\mathbf{c}/2$	c	Hexagonal
$hh.\overline{2h}.l$, $\overline{2h}.hhl$, $h.\overline{2h}.hl$	$l = 2n$	$(1\bar{1}00)$, $(01\bar{1}0)$, $(\bar{1}010)$ } $\{1\bar{1}00\}$	$\mathbf{c}/2$	c	Hexagonal
hhl, hkk, hkh	$l = 2n$, $h = 2n$, $k = 2n$	$(1\bar{1}0)$, $(01\bar{1})$, $(\bar{1}01)$ } $\{1\bar{1}0\}$	$\mathbf{c}/2$, $\mathbf{a}/2$, $\mathbf{b}/2$	c, n; a, n; b, n	Rhombohedral†
$hhl, h\bar{h}l$	$l = 2n$	$(1\bar{1}0), (110)$	$\mathbf{c}/2$	c, n	Tetragonal‡ (these two rows); Cubic§ (rows to end of table)
	$2h + l = 4n$		$\mathbf{a}/4 \pm \mathbf{b}/4 \pm \mathbf{c}/4$	d	
$hkk, hk\bar{k}$	$h = 2n$	$(01\bar{1}), (011)$	$\mathbf{a}/2$	a, n	
	$2k + h = 4n$		$\pm\mathbf{a}/4 + \mathbf{b}/4 \pm \mathbf{c}/4$	d	
$hkh, \bar{h}kh$	$k = 2n$	$(\bar{1}01), (101)$	$\mathbf{b}/2$	b, n	
	$2h + k = 4n$		$\pm\mathbf{a}/4 \pm \mathbf{b}/4 + \mathbf{c}/4$	d	

* Glide planes d with orientations (100), (010) and (001) occur only in orthorhombic and cubic F space groups. Combination of the integral reflection condition (*hkl:* all odd or all even) with the zonal conditions for the d glide planes leads to the further conditions given between parentheses.

† For rhombohedral space groups described with 'rhombohedral axes' the three reflection conditions ($l = 2n, h = 2n, k = 2n$) imply interleaving of c and n glides, a and n glides, b and n glides, respectively. In the Hermann–Mauguin space-group symbols, c is always used, as in $R3c$ (161) and $R\bar{3}c$ (167), because c glides occur also in the hexagonal description of these space groups.

‡ For tetragonal P space groups, the two reflection conditions (hhl and $h\bar{h}l$ with $l = 2n$) imply interleaving of c and n glides. In the Hermann–Mauguin space-group symbols, c is always used, irrespective of which glide planes contain the origin: *cf.* $P4cc$ (103), $P\bar{4}2c$ (112) and $P4/nnc$ (126).

§ For cubic space groups, the three reflection conditions ($l = 2n, h = 2n, k = 2n$) imply interleaving of c and n glides, a and n glides, and b and n glides, respectively. In the Hermann–Mauguin space-group symbols, either c or n is used, depending upon which glide plane contains the origin, *cf.* $P\bar{4}3n$ (218), $Pn\bar{3}n$ (222), $Pm\bar{3}n$ (223) *vs* $F\bar{4}3c$ (219), $Fm\bar{3}c$ (226), $Fd\bar{3}c$ (228).

(ii) *Glide planes*. The resulting conditions apply only to two-dimensional sets of reflections, *i.e.* to reciprocal-lattice nets containing the origin (such as $hk0$, $h0l$, $0kl$, hhl). For this reason, they are called *zonal reflection conditions*. The indices hkl of these 'zonal reflections' obey the relation $hu + kv + lw = 0$, where $[uvw]$, the direction of the zone axis, is normal to the reciprocal-lattice net. Note that the symbol of a glide plane and the corresponding zonal reflection condition may change with a change of the basis vectors (*e.g.* monoclinic: $c \rightarrow n \rightarrow a$).

(iii) *Screw axes*. The resulting conditions apply only to one-dimensional sets of reflections, *i.e.* reciprocal-lattice rows contain-

Table 2.2.13.2. (*cont.*)

(*b*) Screw axes

Type of reflections	Reflection conditions	Screw axis			Crystallographic coordinate system to which condition applies
		Direction of axis	Screw vector	Symbol	
$h00$	$h = 2n$	[100]	$\mathbf{a}/2$	2_1	Monoclinic (*a* unique), Orthorhombic, Tetragonal; Cubic
				4_2	Cubic
	$h = 4n$		$\mathbf{a}/4$	$4_1, 4_3$	Cubic
$0k0$	$k = 2n$	[010]	$\mathbf{b}/2$	2_1	Monoclinic (*b* unique), Orthorhombic, Tetragonal; Cubic
				4_2	Cubic
	$k = 4n$		$\mathbf{b}/4$	$4_1, 4_3$	Cubic
$00l$	$l = 2n$	[001]	$\mathbf{c}/2$	2_1	Monoclinic (*c* unique), Orthorhombic; Cubic
				4_2	Tetragonal; Cubic
	$l = 4n$		$\mathbf{c}/4$	$4_1, 4_3$	Tetragonal; Cubic
$000l$	$l = 2n$	[001]	$\mathbf{c}/2$	6_3	Hexagonal
	$l = 3n$		$\mathbf{c}/3$	$3_1, 3_2, 6_2, 6_4$	Hexagonal
	$l = 6n$		$\mathbf{c}/6$	$6_1, 6_5$	Hexagonal

ing the origin (such as $h00$, $0k0$, $00l$). They are called *serial reflection conditions*.

Reflection conditions of types (ii) and (iii) are listed in Table 2.2.13.2. They can be understood as follows: Zonal and serial reflections form two- or one-dimensional sections through the origin of reciprocal space. In direct space, they correspond to projections of a crystal structure onto a plane or onto a line. Glide planes or screw axes may reduce the translation periods in these projections (*cf.* Section 2.2.14) and thus decrease the size of the projected cell. As a consequence, the cells in the corresponding reciprocal-lattice sections are increased, which means that systematic absences of reflections occur.

For the two-dimensional groups, the reasoning is analogous. The reflection conditions for the plane groups are assembled in Table 2.2.13.3.

Table 2.2.13.3. *Reflection conditions for the plane groups*

Type of reflections	Reflection condition	Centring type of plane cell; or glide line with glide vector	Coordinate system to which condition applies
hk	None	Primitive *p*	All systems
	$h + k = 2n$	Centred *c*	Rectangular
	$h - k = 3n$	Hexagonally centred *h**	Hexagonal
$h0$	$h = 2n$	Glide line *g* normal to *b* axis; glide vector $\frac{1}{2}\mathbf{a}$	Rectangular, Square
$0k$	$k = 2n$	Glide line *g* normal to *a* axis; glide vector $\frac{1}{2}\mathbf{b}$	Rectangular, Square

* For the use of the unconventional *h* cell see Chapter 1.2.

For the *interpretation of observed reflections*, the general reflection conditions must be studied in the order (i) to (iii), as conditions of type (ii) may be included in those of type (i), while conditions of type (iii) may be included in those of types (i) or (ii). This is shown in the example below.

In the *space-group tables*, the reflection conditions are given according to the following rules:

(i) for a given space group, *all* reflection conditions are listed; hence for those nets or rows that are *not* listed no conditions apply. No distinction is made between 'independent' and 'included' conditions, as was done in *IT* (1952), where 'included' conditions were placed in parentheses;

(ii) the integral condition, if present, is always listed first, followed by the zonal and serial conditions;

(iii) conditions that have to be satisified simultaneously are separated by a comma or by 'AND'. Thus, if two indices must be even, say *h* and *l*, the condition is written $h, l = 2n$ rather than $h = 2n$ and $l = 2n$. The same applies to sums of indices. Thus, there are several different ways to express the integral conditions for an *F*-centred lattice: '$h + k, h + l, k + l = 2n$' or '$h + k, h + l = 2n$ and $k + l = 2n$' or '$h + k = 2n$ and $h + l, k + l = 2n$' (*cf.* Table 2.2.13.1);

(iv) conditions separated by 'OR' are alternative conditions. For example, '$hkl : h = 2n + 1$ or $h + k + l = 4n$' means that hkl is 'present' if either the condition $h = 2n + 1$ *or* the alternative condition $h + k + l = 4n$ is fulfilled. Obviously, hkl is a 'present' reflection also if both conditions are satisfied. Note that 'or' conditions occur only for the *special conditions* described in Section 2.2.13.2;

(v) in crystal systems with two or more symmetrically equivalent nets or rows (tetragonal and higher), only *one* representative set (the first one in Table 2.2.13.2) is listed; *e.g.* tetragonal: only the first members of the equivalent sets $0kl$ and $h0l$ or $h00$ and $0k0$ are listed;

(vi) for cubic space groups, it is stated that the indices hkl are 'cyclically permutable' or 'permutable'. The cyclic permutability of

h, k and l in all rhombohedral space groups, described with 'rhombohedral axes', and of h and k in some tetragonal space groups are not stated;

(vii) in the 'hexagonal-axes' descriptions of trigonal and hexagonal space groups, Bravais–Miller indices *hkil* are used. They obey two conditions:

(*a*) $h+k+i=0$, *i.e.* $i=-(h+k)$;

(*b*) the indices h, k, i are cyclically permutable; this is not stated. Further details can be found in textbooks of crystallography.

Note that the integral reflection conditions for a rhombohedral lattice, described with 'hexagonal axes', permit the presence of only one member of the pair *hkil* and $\bar{h}\bar{k}\bar{i}l$ for $l \neq 3n$ (*cf.* Table 2.2.13.1). This applies also to the zonal reflections $h\bar{h}0l$ and $\bar{h}h0l$, which for the rhombohedral space groups must be considered separately.

Example

For a monoclinic crystal (b unique), the following reflection conditions have been observed:

(1) *hkl*: $h+k=2n$;

(2) $0kl$: $k=2n$; $h0l$: $h, l=2n$; $hk0$: $h+k=2n$;

(3) $h00$: $h=2n$; $0k0$: $k=2n$; $00l$: $l=2n$.

Line (1) states that the cell used for the description of the space group is C centred. In line (2), the conditions $0kl$ with $k=2n$, $h0l$ with $h=2n$ and $hk0$ with $h+k=2n$ are a consequence of the integral condition (1), leaving only $h0l$ with $l=2n$ as a new condition. This indicates a glide plane c. Line (3) presents no new condition, since $h00$ with $h=2n$ and $0k0$ with $k=2n$ follow from the integral condition (1), whereas $00l$ with $l=2n$ is a consequence of a zonal condition (2). Accordingly, there need not be a twofold screw axis along [010]. Space groups obeying the conditions are Cc (9, b unique, cell choice 1) and $C2/c$ (15, b unique, cell choice 1). On the basis of diffraction symmetry and reflection conditions, no choice between the two space groups can be made (*cf.* Part 3).

For a different choice of the basis vectors, the reflection conditions would appear in a different form owing to the transformation of the reflection indices (*cf.* cell choices 2 and 3 for space groups Cc and $C2/c$ in Part 7).

2.2.13.2. *Special or 'extra' reflection conditions*

These apply either to the integral reflections *hkl* or to particular sets of zonal or serial reflections. In the space-group tables, the minimal special conditions are listed that, on combination with the general conditions, are sufficient to generate the complete set of conditions. This will be apparent from the examples below.

Examples

(1) $P4_222$ (93)

General position $8p$: $00l$: $l=2n$, due to 4_2; the projection on [001] of any crystal structure with this space group has periodicity $\frac{1}{2}c$.

Special position $4i$: *hkl*: $h+k+l=2n$; any set of symmetrically equivalent atoms in this position displays additional I centring.

Special position $4n$: $0kl$: $l=2n$; any set of equivalent atoms in this position displays a glide plane $c \perp [100]$. Projection of this set along [100] results in a halving of the original c axis, whence the special condition. Analogously for $h0l$: $l=2n$.

(2) $C12/c1$ (15, unique axis b, cell choice 1)

General position $8f$: *hkl*: $h+k=2n$, due to the C-centred cell.

Special position $4d$: *hkl*: $k+l=2n$, due to additional A and B centring for atoms in this position. Combination with the general condition results in *hkl*: $h+k, h+l, k+l=2n$ or *hkl* all odd or all even; this corresponds to an F-centred arrangement of atoms in this position.

Special position $4b$: *hkl*: $l=2n$, due to additional halving of the c axis for atoms in this position. Combination with the general condition results in *hkl*: $h+k, l=2n$; this corresponds to a C-centred arrangement in a cell with half the original c axis. No further condition results from the combination.

(3) $I12/a1$ (15, unique axis b, cell choice 3)

For the description of space group No. 15 with cell choice 3 (see Section 2.2.16 and space-group tables), the reflection conditions appear as follows:

General position $8f$: *hkl*: $h+k+l=2n$, due to the I-centred cell.

Special position $4b$: *hkl*: $h=2n$, due to additional halving of the a axis. Combination gives *hkl*: $h, k+l=2n$, *i.e.* an A-centred arrangement of atoms in a cell with half the original a axis.

An analogous result is obtained for position $4d$.

(4) $Fmm2$ (42)

General position $16e$: *hkl*: $h+k, h+l, k+l=2n$, due to the F-centred cell.

Special position $8b$: *hkl*: $h=2n$, due to additional halving of the a axis. Combination results in *hkl*: $h, k, l=2n$, *i.e.* all indices even; the atoms in this position are arranged in a primitive lattice with axes $\frac{1}{2}a$, $\frac{1}{2}b$ and $\frac{1}{2}c$.

For the cases where the special reflection conditions are described by means of combinations of 'OR' and 'AND' instructions, the 'AND' condition always has to be evaluated with priority, as shown by the following example.

Example: $P\bar{4}3n$ (218)

Special position $6d$: *hkl*: $h+k+l=2n$ or $h=2n+1$, $k=4n$ and $l=4n+2$.

This expression contains the following two conditions:

(*a*) *hkl*: $h+k+l=2n$;

(*b*) $h=2n+1$ and $k=4n$ and $l=4n+2$.

A reflection is 'present' (occurring) if either condition (*a*) is satisfied or if a permutation of the three conditions in (*b*) are simultaneously fulfilled.

2.2.13.3. *Structural or non-space-group absences*

Note that in addition *non-space-group absences* may occur that are not due to the symmetry of the space group (*i.e.* centred cells, glide planes or screw axes). Atoms in general or special positions may cause additional systematic absences if their coordinates assume special values [*e.g.* 'noncharacteristic orbits' (Engel *et al.*, 1984)]. Non-space-group absences may also occur for special arrangements of atoms ('false symmetry') in a crystal structure (*cf.* Templeton, 1956; Sadanaga *et al.*, 1978). Non-space-group absences may occur also for polytypic structures; this is briefly discussed by Durovič in Section 9.2.2.2.5 of *International Tables for Crystallography* (2004), Vol. C. Even though all these 'structural absences' are fortuitous and due to the special arrangements of atoms in a particular crystal structure, they have the appearance of space-group absences. Occurrence of structural absences thus may lead to an *incorrect assignment of the space group*. Accordingly, the reflection conditions in the space-group tables must be considered as a minimal set of conditions.

The use of reflection conditions and of the symmetry of reflection intensities for space-group determination is described in Part 3.

Table 2.2.14.1. *Cell parameters a', b', γ' of the two-dimensional cell in terms of cell parameters a, b, c, α, β, γ of the three-dimensional cell for the projections listed in the space-group tables of Part 7*

Projection direction	Triclinic	Monoclinic		Orthorhombic	Projection direction	Tetragonal
		Unique axis b	Unique axis c			
[001]	$a' = a\sin\beta$ $b' = b\sin\alpha$ $\gamma' = 180° - \gamma^*$ †	$a' = a\sin\beta$ $b' = b$ $\gamma' = 90°$	$a' = a$ $b' = b$ $\gamma' = \gamma$	$a' = a$ $b' = b$ $\gamma' = 90°$	[001]	$a' = a$ $b' = a$ $\gamma' = 90°$
[100]	$a' = b\sin\gamma$ $b' = c\sin\beta$ $\gamma' = 180° - \alpha^*$ †	$a' = b$ $b' = c\sin\beta$ $\gamma' = 90°$	$a' = b\sin\gamma$ $b' = c$ $\gamma' = 90°$	$a' = b$ $b' = c$ $\gamma' = 90°$	[100]	$a' = a$ $b' = c$ $\gamma' = 90°$
[010]	$a' = c\sin\alpha$ $b' = \alpha\sin\gamma$ $\gamma' = 180° - \beta^*$ †	$a' = c$ $b' = a$ $\gamma' = \beta$	$a' = c$ $b' = a\sin\gamma$ $\gamma' = 90°$	$a' = c$ $b' = a$ $\gamma' = 90°$	[110]	$a' = (a/2)\sqrt{2}$ $b' = c$ $\gamma' = 90°$

Projection direction	Hexagonal	Projection direction	Rhombohedral ‡	Projection direction	Cubic
[001]	$a' = a$ $b' = a$ $\gamma' = 120°$	[111]	$a' = \frac{2}{\sqrt{3}} a\sin(\alpha/2)$ $b' = \frac{2}{\sqrt{3}} a\sin(\alpha/2)$ $\gamma' = 120°$	[001]	$a' = a$ $b' = a$ $\gamma' = 90°$
[100]	$a' = (a/2)\sqrt{3}$ $b' = c$ $\gamma' = 90°$	$[1\bar{1}0]$	$a' = a\cos(\alpha/2)$ $b' = a$ $\gamma' = \delta$ §	[111]	$a' = a\sqrt{2/3}$ $b' = a\sqrt{2/3}$ $\gamma' = 120°$
[210]	$a' = a/2$ $b' = c$ $\gamma' = 90°$	$[\bar{2}11]$	$a' = \frac{1}{\sqrt{3}} a\sqrt{1 + 2\cos\alpha}$ $b' = a\sin(\alpha/2)$ $\gamma' = 90°$	[110]	$a' = (a/2)\sqrt{2}$ $b' = a$ $\gamma' = 90°$

† $\cos\alpha^* = \frac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma}$; $\cos\beta^* = \frac{\cos\gamma\cos\alpha - \cos\beta}{\sin\gamma\sin\alpha}$; $\cos\gamma^* = \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}$.

‡ The entry 'Rhombohedral' refers to the primitive rhombohedral cell with $a = b = c, \alpha = \beta = \gamma$ (*cf.* Table 2.1.2.1).

§ $\cos\delta = \frac{\cos\alpha}{\cos\alpha/2}$.

2.2.14. Symmetry of special projections

Projections of crystal structures are used by crystallographers in special cases. Use of so-called 'two-dimensional data' (zero-layer intensities) results in the projection of a crystal structure along the normal to the reciprocal-lattice net.

Even though the projection of a finite object along *any* direction may be useful, the projection of a *periodic* object such as a crystal structure is only sensible along a rational lattice direction (lattice row). Projection along a nonrational direction results in a constant density in at least one direction.

2.2.14.1. *Data listed in the space-group tables*

Under the heading *Symmetry of special projections*, the following data are listed for three projections of each space group; no projection data are given for the plane groups.

(i) *The projection direction*. All projections are orthogonal, *i.e.* the projection is made onto a plane normal to the projection direction. This ensures that spherical atoms appear as circles in the projection. For each space group, three projections are listed. If a lattice has three kinds of symmetry directions, the three projection directions correspond to the primary, secondary and tertiary symmetry directions of the lattice (*cf.* Table 2.2.4.1). If a lattice contains less than three kinds of symmetry directions, as in the triclinic, monoclinic and rhombohedral cases, the additional projection direction(s) are taken along coordinate axes, *i.e.* lattice rows lacking symmetry.

The directions for which projection data are listed are as follows:

Triclinic Monoclinic (both settings) Orthorhombic	[001]	[100]	[010]
Tetragonal	[001]	[100]	[110]
Hexagonal	[001]	[100]	[210]
Rhombohedral	[111]	$[1\bar{1}0]$	$[2\bar{1}\bar{1}]$
Cubic	[001]	[111]	[110]

(ii) *The Hermann–Mauguin symbol of the plane group* resulting from the projection of the space group. If necessary, the symbols are given in oriented form; for example, plane group *pm* is expressed either as $p1m1$ or as $p11m$.

(iii) *Relations between the basis vectors* $\mathbf{a}'$, $\mathbf{b}'$ of the plane group and the basis vectors **a**, **b**, **c** of the space group. Each set of basis vectors refers to the conventional coordinate system of the plane group or space group, as employed in Parts 6 and 7. The basis vectors of the two-dimensional cell are always called $\mathbf{a}'$ and $\mathbf{b}'$ irrespective of which two of the basis vectors **a**, **b**, **c** of the three-dimensional cell are projected to form the plane cell. All relations between the basis vectors of the two cells are expressed as vector equations, *i.e.* $\mathbf{a}'$ and $\mathbf{b}'$ are given as linear combinations of **a**, **b** and **c**. For the triclinic or monoclinic space groups, basis vectors **a**, **b** or **c** inclined to the plane of projection are replaced by the projected vectors $\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p$.

For primitive three-dimensional cells, the *metrical* relations between the lattice parameters of the space group and the plane group are collected in Table 2.2.14.1. The additional relations for centred cells can be derived easily from the table.

(iv) *Location of the origin* of the plane group with respect to the unit cell of the space group. The same description is used as for the location of symmetry elements (*cf.* Section 2.2.9).

Example

'Origin at x, 0, 0' or 'Origin at $\frac{1}{4}, \frac{1}{4}, z$'.

2.2.14.2. *Projections of centred cells (lattices)*

For centred lattices, two different cases may occur:

(i) The projection direction is parallel to a lattice-centring vector. In this case, the projected plane cell is primitive for the centring types A, B, C, I and R. For F lattices, the multiplicity is reduced from 4 to 2 because c-centred plane cells result from projections along face diagonals of three-dimensional F cells.

Examples

(1) A body-centred lattice with centring vector $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ gives a primitive net, if projected along [111], $[\bar{1}1\bar{1}]$, $[1\bar{1}1]$ or $[11\bar{1}]$.

(2) A C-centred lattice projects to a primitive net along the directions [110] and $[1\bar{1}0]$.

(3) An R-centred lattice described with 'hexagonal axes' (triple cell) results in a primitive net, if projected along $[\bar{1}11]$, [211] or $[\bar{1}\bar{2}1]$ for the obverse setting. For the reverse setting, the corresponding directions are $[1\bar{1}1]$, $[\bar{2}\bar{1}1]$, [121]; *cf.* Chapter 1.2.

(ii) The projection direction is not parallel to a lattice-centring vector (general projection direction). In this case, the plane cell has the same multiplicity as the three-dimensional cell. Usually, however, this centred plane cell is unconventional and a transformation is required to obtain the conventional plane cell. This transformation has been carried out for the projection data in this volume.

Examples

(1) Projection along [010] of a cubic I-centred cell leads to an unconventional quadratic c-centred plane cell. A simple cell transformation leads to the conventional quadratic p cell.

(2) Projection along [010] of an orthorhombic I-centred cell leads to a rectangular c-centred plane cell, which is conventional.

(3) Projection along [001] of an R-centred cell (both in obverse and reverse setting) results in a triple hexagonal plane cell h (the two-dimensional analogue of the H cell, *cf.* Chapter 1.2). A simple cell transformation leads to the conventional hexagonal p cell.

2.2.14.3. *Projections of symmetry elements*

A symmetry element of a space group does not project as a symmetry element unless its orientation bears a special relation to the projection direction; all translation components of a symmetry operation along the projection direction vanish, whereas those perpendicular to the projection direction (*i.e.* parallel to the plane of projection) may be retained. This is summarized in Table 2.2.14.2 for the various crystallographic symmetry elements. From this table the following conclusions can be drawn:

Table 2.2.14.2. *Projections of crystallographic symmetry elements*

Symmetry element in three dimensions	Symmetry element in projection
Arbitrary orientation	
Symmetry centre $\bar{1}$ Rotoinversion axis $\bar{3} \equiv 3 \times \bar{1}$	Rotation point 2 (at projection of centre)
Parallel to projection direction	
Rotation axis 2; 3; 4; 6	Rotation point 2; 3; 4; 6
Screw axis 2_1	Rotation point 2
$3_1, 3_2$	3
$4_1, 4_2, 4_3$	4
$6_1, 6_2, 6_3, 6_4, 6_5$	6
Rotoinversion axis $\bar{4}$	Rotation point 4
$\bar{6} \equiv 3/m$	3, with overlap of atoms
$\bar{3} \equiv 3 \times \bar{1}$	6
Reflection plane m	Reflection line m
Glide plane with $\perp$ component*	Glide line g
Glide plane without $\perp$ component*	Reflection line m
Normal to projection direction	
Rotation axis 2; 4; 6	Reflection line m
3	None
Screw axis 4_2; $6_2, 6_4$	Reflection line m
2_1; $4_1, 4_3$; $6_1, 6_3, 6_5$	Glide line g
$3_1, 3_2$	None
Rotoinversion axis $\bar{4}$	Reflection line m parallel to axis
$\bar{6} \equiv 3/m$	Reflection line m perpendicular to axis (through projection of inversion point)
$\bar{3} \equiv 3 \times \bar{1}$	Rotation point 2 (at projection of centre)
Reflection plane m	None, but overlap of atoms
Glide plane with glide vector **t**	Translation with translation vector **t**

* The term 'with $\perp$ component' refers to the component of the glide vector normal to the projection direction.

(i) n-fold rotation axes and n-fold screw axes, as well as rotoinversion axes $\bar{4}$, *parallel to the projection direction* project as n-fold rotation points; a $\bar{3}$ axis projects as a sixfold, a $\bar{6}$ axis as a threefold rotation point. For the latter, a doubling of the projected electron density occurs owing to the mirror plane normal to the projection direction ($\bar{6} \equiv 3/m$).

(ii) n-fold rotation axes and n-fold screw axes *normal to the projection direction* (*i.e.* parallel to the plane of projection) do not project as symmetry elements if n is odd. If n is even, all rotation and rotoinversion axes project as mirror lines: the same applies to the screw axes $4_2, 6_2$ and 6_4 because they contain an axis 2. Screw axes 2_1, 4_1, 4_3, 6_1, 6_3 and 6_5 project as glide lines because they contain 2_1.

(iii) Reflection planes *normal* to the projection direction do not project as symmetry elements but lead to a doubling of the projected electron density owing to overlap of atoms. Projection of a glide plane results in an additional translation; the new translation vector is equal to the glide vector of the glide plane. Thus, a reduction of the translation period in that particular direction takes place.

(iv) Reflection planes *parallel* to the projection direction project as reflection lines. Glide planes project as glide lines or as reflection lines, depending upon whether the glide vector has or has not a component parallel to the projection plane.

(v) Centres of symmetry, as well as $\bar{3}$ axes in *arbitrary* orientation, project as twofold rotation points.

Example: $C12/c1$ (15, b unique, cell choice 1)

The C-centred cell has lattice points at 0, 0, 0 and $\frac{1}{2}, \frac{1}{2}, 0$. In all projections, the centre $\bar{1}$ projects as a twofold rotation point.

Projection along [001]: The plane cell is centred; $2 \parallel [010]$ projects as m; the glide component $(0, 0, \frac{1}{2})$ of glide plane c vanishes and thus c projects as m.

Result: Plane group $c2mm$ (9), $\mathbf{a}' = \mathbf{a}_p, \mathbf{b}' = \mathbf{b}$.

Projection along [100]: The periodicity along b is halved because of the C centring; $2 \parallel [010]$ projects as m; the glide component $(0, 0, \frac{1}{2})$ of glide plane c is retained and thus c projects as g.

Result: Plane group $p2gm$ (7), $\mathbf{a}' = \mathbf{b}/2,\ \mathbf{b}' = \mathbf{c}_p$.

Projection along [010]: The periodicity along a is halved because of the C centring; that along c is halved owing to the glide component $(0, 0, \frac{1}{2})$ of glide plane c; $2 \parallel [010]$ projects as 2.

Result: Plane group $p2$ (2), $\mathbf{a}' = \mathbf{c}/2, \mathbf{b}' = \mathbf{a}/2$.

Further details about the geometry of projections can be found in publications by Buerger (1965) and Biedl (1966).

2.2.15. Maximal subgroups and minimal supergroups

The present section gives a brief summary, without theoretical explanations, of the sub- and supergroup data in the space-group tables. The theoretical background is provided in Section 8.3.3 and Part 13. Detailed sub- and supergroup data are given in *International Tables for Crystallography* Volume A1 (2004).

2.2.15.1. *Maximal non-isomorphic subgroups**

The maximal non-isomorphic subgroups $\mathcal{H}$ of a space group $\mathcal{G}$ are divided into two types:

I *translationengleiche* or t subgroups

II *klassengleiche* or k subgroups.

For practical reasons, type **II** is subdivided again into two blocks:

IIa the conventional cells of $\mathcal{G}$ and $\mathcal{H}$ are the same

IIb the conventional cell of $\mathcal{H}$ is larger than that of $\mathcal{G}$. †

Block **IIa** has no entries for space groups $\mathcal{G}$ with a primitive cell. For space groups $\mathcal{G}$ with a centred cell, it contains those maximal subgroups $\mathcal{H}$ that have lost some or all centring translations of $\mathcal{G}$ but none of the integral translations ('decentring' of a centred cell).

Within each block, the subgroups are listed in order of increasing index [i] and in order of decreasing space-group number for each value of i.

(i) *Blocks* **I** *and* **IIa**

In blocks **I** and **IIa**, *every* maximal subgroup $\mathcal{H}$ of a space group $\mathcal{G}$ is listed with the following information:

[i] HMS1 (HMS2, No.) Sequence of numbers.

The symbols have the following meaning:

[i]: index of $\mathcal{H}$ in $\mathcal{G}$ (*cf.* Section 8.1.6, footnote);

HMS1: Hermann–Mauguin symbol of $\mathcal{H}$, referred to the coordinate system and setting of $\mathcal{G}$; this symbol may be unconventional;

(HMS2, No.): conventional short Hermann–Mauguin symbol of $\mathcal{H}$, given only if HMS1 is not in conventional short form, and the space-group number of $\mathcal{H}$.

Sequence of numbers: coordinate triplets of $\mathcal{G}$ retained in $\mathcal{H}$. The numbers refer to the numbering scheme of the coordinate triplets of the general position of $\mathcal{G}$ (*cf.* Section 2.2.9). The following abbreviations are used:

Block **I** (all translations retained):

Number +	Coordinate triplet given by *Number*, plus those obtained by adding all centring translations of $\mathcal{G}$.
(*Numbers*) +	The same, but applied to all *Numbers* between parentheses.

Block **IIa** (not all translations retained):

Number + (t_1, t_2, t_3)	Coordinate triplet obtained by adding the translation t_1, t_2, t_3 to the triplet given by *Number*.
(*Numbers*) + (t_1, t_2, t_3)	The same, but applied to all *Numbers* between parentheses.

In blocks **I** and **IIa**, sets of conjugate subgroups are linked by left-hand braces. For an example, see space group $R\bar{3}$ (148) below.

Examples

(1) $\mathcal{G}$: $C1m1$ (8)

I	[2] $C1$ ($P1$, 1)	1+
IIa	[2] $P1a1$ (Pc, 7)	1; 2 + (1/2, 1/2, 0)
	[2] $P1m1$ (Pm, 6)	1; 2

where the numbers have the following meaning:

1+	x, y, z; $x + 1/2, y + 1/2, z$
1; 2	x, y, z; $x, \bar{y}, z$
1; 2 + (1/2, 1/2, 0)	x, y, z; $x + 1/2, \bar{y} + 1/2, z$.

(2) $\mathcal{G}$: $Fdd2$ (43)

I [2] $F112$ ($C2$, 5) (1; 2)+

where the numbers have the following meaning:

(1; 2)+ x, y, z; $x + 1/2, y + 1/2, z$;
$x + 1/2, y, z + 1/2$; $x, y + 1/2, z + 1/2$;
$\bar{x}, \bar{y}, z$; $\bar{x} + 1/2, \bar{y} + 1/2, z$;
$\bar{x} + 1/2, \bar{y}, z + 1/2$; $\bar{x}, \bar{y} + 1/2, z + 1/2$.

(3) $\mathcal{G}$: $P4_2/nmc = P4_2/n2_1/m2/c$ (137)

I [2] $P2/n2_1/m1$ ($Pmmn$, 59) 1; 2; 5; 6; 9; 10; 13; 14.

Operations 4_2, 2 and c, occurring in the Hermann–Mauguin symbol of $\mathcal{G}$, are lacking in $\mathcal{H}$. In the unconventional 'tetragonal version' $P2/n2_1/m1$ of the symbol of $\mathcal{H}$, $2_1/m$ stands for two sets of $2_1/m$ (along the two orthogonal secondary symmetry directions), implying that $\mathcal{H}$ is orthorhombic. In the conventional 'orthorhombic version', the full symbol of $\mathcal{H}$ reads $P2_1/m2_1/m2/n$ and the short symbol $Pmmn$.

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* Space groups with different space-group numbers are non-isomorphic, except for the members of the 11 pairs of enantiomorphic space groups which are isomorphic.
† Subgroups belonging to the enantiomorphic space-group type of $\mathcal{G}$ are isomorphic to $\mathcal{G}$ and, therefore, are listed under **IIc** and not under **IIb**.

(ii) *Block* **IIb**

Whereas in blocks **I** and **IIa** *every* maximal subgroup $\mathcal{H}$ of $\mathcal{G}$ is listed, *this is no longer the case* for the entries of block **IIb**. The information given in this block is:

[*i*] HMS1 (Vectors) (HMS2, No.)

The symbols have the following meaning:

[*i*]: index of $\mathcal{H}$ in $\mathcal{G}$;

HMS1: Hermann–Mauguin symbol of $\mathcal{H}$, referred to the coordinate system and setting of $\mathcal{G}$; this symbol may be unconventional;*

(Vectors): basis vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ of $\mathcal{H}$ in terms of the basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ of $\mathcal{G}$. No relations are given for unchanged axes, *e.g.* $\mathbf{a}' = \mathbf{a}$ is not stated;

(HMS2, No.): conventional short Hermann–Mauguin symbol, given only if HMS1 is not in conventional short form, and the space-group number of $\mathcal{H}$.

In addition to the general rule of increasing index [*i*] and decreasing space-group number (No.), the sequence of the **IIb** subgroups also depends on the type of cell enlargement. Subgroups with the same index and the same kind of cell enlargement are listed together in decreasing order of space-group number (see example 1 below).

In contradistinction to blocks **I** and **IIa**, for block **IIb** the coordinate triplets retained in $\mathcal{H}$ are *not* given. This means that the entry is the same for all subgroups $\mathcal{H}$ that have the same Hermann–Mauguin symbol and the same basis-vector relations to $\mathcal{G}$, but contain different sets of coordinate triplets. Thus, in block **IIb**, one entry may correspond to more than one subgroup,† as illustrated by the following examples.

Examples

(1) $\mathcal{G}$: $Pmm2$ (25)

IIb $\ldots$[2] $Pbm2$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pma2, 28$); [2] $Pcc2$ ($\mathbf{c}' = 2\mathbf{c}$) (27);

$\ldots$[2] $Cmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (35); $\ldots$

Each of the subgroups is referred to its own distinct basis $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$, which is different in each case. Apart from the translations of the enlarged cell, the generators of the subgroups, referred to $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$, are as follows:

$Pbm2$	x, y, z;	$\bar{x}, \bar{y}, z$;	$x, \bar{y}+1/2, z$		or
	x, y, z;	$\bar{x}, \bar{y}+1/2, z$;	$x, \bar{y}, z$		
$Pcc2$	x, y, z;	$\bar{x}, \bar{y}, z$;	$x, \bar{y}, z+1/2$		
$Cmm2$	x, y, z;	$x+1/2, y+1/2, z$;	$\bar{x}, \bar{y}, z$;	$x, \bar{y}, z$	or
	x, y, z;	$x+1/2, y+1/2, z$;	$\bar{x}, \bar{y}, z$;	$x, \bar{y}+1/2, z$	or
	x, y, z;	$x+1/2, y+1/2, z$;	$\bar{x}, \bar{y}+1/2, z$;	$x, \bar{y}, z$	or
	x, y, z;	$x+1/2, y+1/2, z$;	$\bar{x}, \bar{y}+1/2, z$;	$x, \bar{y}+1/2, z$.	

There are thus 2, 1 or 4 actual subgroups that obey the same basis-vector relations. The difference between the several subgroups represented by one entry is due to the different sets of symmetry operations of $\mathcal{G}$ that are retained in $\mathcal{H}$. This can also be expressed as different conventional origins of $\mathcal{H}$ with respect to $\mathcal{G}$.

(2) $\mathcal{G}$: $P3m1$ (156)

IIb $\ldots$[3] $H3m1$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P31m, 157$)

The nine subgroups of type $P31m$ may be described in two ways:

(i) By partial 'decentring' of ninetuple cells ($\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = 3\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$) with the same orientations as the cell of the group $\mathcal{G}(\mathbf{a}, \mathbf{b}, \mathbf{c})$ in such a way that the centring points 0, 0, 0; $2/3, 1/3, 0$; $1/3, 2/3, 0$ (referred to $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$) are retained. The *conventional* space-group symbol $P31m$ of these nine subgroups is referred to the same basis vectors $\mathbf{a}'' = \mathbf{a} - \mathbf{b}$, $\mathbf{b}'' = \mathbf{a} + 2\mathbf{b}$, $\mathbf{c}'' = \mathbf{c}$, but to different origins; *cf.* Section 2.2.15.5. This kind of description is used in the space-group tables of this volume.

(ii) Alternatively, one can describe the group $\mathcal{G}$ with an unconventional H-centred cell ($\mathbf{a}' = \mathbf{a} - \mathbf{b}$, $\mathbf{b}' = \mathbf{a} + 2\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$) referred to which the space-group symbol is $H31m$. 'Decentring' of this cell results in the conventional space-group symbol $P31m$ for the subgroups, referred to the basis vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$. This description is used in Section 4.3.5.

(iii) *Subdivision of k subgroups into blocks* **IIa** *and* **IIb**

The subdivision of *k* subgroups into blocks **IIa** and **IIb** has no group-theoretical background and depends on the coordinate system chosen. The *conventional* coordinate system of the space group $\mathcal{G}$ (*cf.* Section 2.1.3) is taken as the basis for the subdivision. This results in a uniquely defined subdivision, except for the seven rhombohedral space groups for which in the space-group tables both 'rhombohedral axes' (primitive cell) and 'hexagonal axes' (triple cell) are given (*cf.* Section 2.2.2). Thus, some *k* subgroups of a rhombohedral space group are found under **IIa** (*klassengleich*, centring translations lost) in the *hexagonal* description, and under **IIb** (*klassengleich*, conventional cell enlarged) in the *rhombohedral* description.

Example: $\mathcal{G}$: $R\bar{3}$ (148) $\qquad \mathcal{H}$: $P\bar{3}$ (147)

Hexagonal axes

I	[2] $R3$ (146)	$(1; 2; 3)+$
	[3] $R\bar{1}$ ($P\bar{1}, 2$)	$(1; 4)+$
IIa	[3] $P\bar{3}$ (147)	$1; 2; 3; 4; 5; 6$
	[3] $P\bar{3}$ (147)	$1; 2; 3; (4; 5; 6) + (\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$
	[3] $P\bar{3}$ (147)	$1; 2; 3; (4; 5; 6) + (\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$
IIb	none	

Rhombohedral axes

I	[2] $R3$ (146)	$1; 2; 3$
	[3] $R\bar{1}$ ($P\bar{1}, 2$)	$1; 4$
IIa	none	
IIb	[3] $P\bar{3}$ ($\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}$) (147).	

Apart from the change from **IIa** to **IIb**, the above example demonstrates again the restricted character of the **IIb** listing, discussed above. The three conjugate subgroups $P\bar{3}$ of index [3] are listed under **IIb** by one entry only, because for all three subgroups the basis-vector relations between $\mathcal{G}$ and $\mathcal{H}$ are the same. Note the brace for the **IIa** subgroups, which unites *conjugate subgroups* into classes.

2.2.15.2. *Maximal isomorphic subgroups of lowest index (cf. Part 13)*

Another set of *klassengleiche* subgroups are the *isomorphic subgroups* listed under **IIc**, *i.e.* the subgroups $\mathcal{H}$ which are of the

* Unconventional Hermann–Mauguin symbols may include unconventional cells like *c* centring in quadratic plane groups, *F* centring in monoclinic, or *C* and *F* centring in tetragonal space groups. Furthermore, the triple hexagonal cells *h* and *H* are used for certain sub- and supergroups of the hexagonal plane groups and of the trigonal and hexagonal *P* space groups, respectively. The cells *h* and *H* are defined in Chapter 1.2. Examples are subgroups of plane groups *p*3 (13) and *p*6*mm* (17) and of space groups $P3$ (143) and $P6/mcc$ (192).

† Without this restriction, the amount of data would be excessive. For instance, space group *Pmmm* (47) has 63 maximal subgroups of index [2], of which seven are *t* subgroups and listed explicitly under **I**. The 16 entries under **IIb** refer to 50 actual subgroups and the one entry under **IIc** stands for the remaining 6 subgroups.

same or of the enantiomorphic space-group type as $\mathcal{G}$. The kind of listing is the same as for block **IIb**. Again, one entry may correspond to more than one isomorphic subgroup.

As the number of maximal isomorphic subgroups of a space group is always infinite, the data in block **IIc** are restricted to the subgroups of lowest index. Different kinds of cell enlargements are presented. For monoclinic, tetragonal, trigonal and hexagonal space groups, cell enlargements both parallel and perpendicular to the main rotation axis are listed; for orthorhombic space groups, this is the case for all three directions, *a*, *b* and *c*. Two isomorphic subgroups $\mathcal{H}_1$ and $\mathcal{H}_2$ of equal index but with cell enlargements in different directions may, nevertheless, play an analogous role with respect to $\mathcal{G}$. In terms of group theory, $\mathcal{H}_1$ and $\mathcal{H}_2$ then are conjugate subgroups in the affine normalizer of $\mathcal{G}$, *i.e.* they are mapped onto each other by automorphisms of $\mathcal{G}$.* Such subgroups are collected into one entry, with the different vector relationships separated by 'or' and placed within one pair of parentheses; *cf.* example (4).

Examples

(1) $\mathcal{G}$: $P\bar{3}1c$ (163)

IIc [3] $P\bar{3}1c$ ($\mathbf{c}' = 3\mathbf{c}$) (163); [4] $P\bar{3}1c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (163).

The first subgroup of index [3] entails an enlargement of the *c* axis, the second one of index [4] an enlargement of the mesh size in the *a*,*b* plane.

(2) $\mathcal{G}$: $P23$ (195)

IIc [27] $P23$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (195).

It seems surprising that [27] is the lowest index listed, even though another isomorphic subgroup of index [8] exists. The latter subgroup, however, is not maximal, as chains of maximal non-isomorphic subgroups can be constructed as follows:

$$P23 \to [4]\ I23\ (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) \to [2]\ P23\ (\mathbf{a}', \mathbf{b}', \mathbf{c}')$$

or

$$P23 \to [2]\ F23\ (\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}) \to [4]\ P23\ (\mathbf{a}', \mathbf{b}', \mathbf{c}').$$

(3) $\mathcal{G}$: $P3_112$ (151)

IIc [2] $P3_212$ ($\mathbf{c}' = 2\mathbf{c}$) (153); [4] $P3_112$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (151); [7] $P3_112$ ($\mathbf{c}' = 7\mathbf{c}$) (151).

Note that the isomorphic subgroup of index [4] with $\mathbf{c}' = 4\mathbf{c}$ is not listed, because it is not maximal. This is apparent from the chain

$$P3_112 \to [2]\ P3_212\ (\mathbf{c}' = 2\mathbf{c}) \to [2]\ P3_112\ (\mathbf{c}'' = 2\mathbf{c}' = 4\mathbf{c}).$$

(4) $\mathcal{G}_1$: *Pnnm* (58)

IIc [3] *Pnnm* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (58); [3] *Pnnm* ($\mathbf{c}' = 3\mathbf{c}$) (58);

but $\mathcal{G}_2$: *Pnna* (52)

IIc [3] *Pnna* ($\mathbf{a}' = 3\mathbf{a}$) (52); [3] *Pnna* ($\mathbf{b}' = 3\mathbf{b}$) (52); [3] *Pnna* ($\mathbf{c}' = 3\mathbf{c}$) (52).

For $\mathcal{G}_1 = Pnnm$, the *x* and *y* directions are analogous, *i.e.* they may be interchanged by automorphisms of $\mathcal{G}_1$. Such an automorphism does not exist for $\mathcal{G}_2 = Pnna$ because this space group contains glide reflections *a* but not *b*.

2.2.15.3. *Minimal non-isomorphic supergroups*

If $\mathcal{G}$ is a maximal subgroup of a group $\mathcal{S}$, then $\mathcal{S}$ is called a minimal supergroup of $\mathcal{G}$. Minimal non-isomorphic supergroups are again subdivided into two types, the *translationengleiche* or *t* supergroups **I** and the *klassengleiche* or *k* supergroups **II**. For the minimal *t* supergroups **I** of $\mathcal{G}$, the listing contains the index [*i*] of $\mathcal{G}$ in $\mathcal{S}$, the *conventional* Hermann–Mauguin symbol of $\mathcal{S}$ and its space-group number in parentheses.

There are two types of minimal *k* supergroups **II**: supergroups with additional centring translations (which would correspond to the **IIa** type) and supergroups with smaller conventional unit cells than that of $\mathcal{G}$ (type **IIb**). Although the subdivision between **IIa** and **IIb** supergroups is not indicated in the tables, the list of minimal supergroups with additional centring translations (**IIa**) always precedes the list of **IIb** supergroups. The information given is similar to that for the non-isomorphic subgroups **IIb**, *i.e.*, where applicable, the relations between the basis vectors of group and supergroup are given, in addition to the Hermann–Mauguin symbols of $\mathcal{S}$ and its space-group number. The supergroups are listed in order of increasing index and increasing space-group number.

The block of supergroups contains only the *types* of the non-isomorphic minimal supergroups $\mathcal{S}$ of $\mathcal{G}$, *i.e.* each entry may correspond to more than one supergroup $\mathcal{S}$. In fact, the list of minimal supergroups $\mathcal{S}$ of $\mathcal{G}$ should be considered as a backwards reference to those space groups $\mathcal{S}$ for which $\mathcal{G}$ appears as a maximal subgroup. Thus, the relation between $\mathcal{S}$ and $\mathcal{G}$ can be found in the subgroup entries of $\mathcal{S}$.

Example: $\mathcal{G}$: $Pna2_1$ (33)

Minimal non-isomorphic supergroups

I [2] *Pnna* (52); [2] *Pccn* (56); [2] *Pbcn* (60); [2] *Pnma* (62).

II ...[2] $Pnm2_1$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pmn2_1$, 31); ....

Block **I** lists, among others, the entry [2] *Pnma* (62). Looking up the *subgroup* data of *Pnma* (62), one finds in block **I** the entry [2] $Pn2_1a$ ($Pna2_1$). This shows that the setting of *Pnma* does not correspond to that of $Pna2_1$ but rather to that of $Pn2_1a$. To obtain the supergroup $\mathcal{S}$ referred to the basis of $Pna2_1$, the basis vectors **b** and **c** must be interchanged. This changes *Pnma* to *Pnam*, which is the correct symbol of the supergroup of $Pna2_1$.

Note on R supergroups of trigonal P space groups: The trigonal *P* space groups Nos. 143–145, 147, 150, 152, 154, 156, 158, 164 and 165 each have two rhombohedral supergroups of type **II**. They are distinguished by different additional centring translations which correspond to the 'obverse' and 'reverse' settings of a triple hexagonal *R* cell; *cf.* Chapter 1.2. In the supergroup tables of Part 7, these cases are described as [3] *R*3 (obverse) (146); [3] *R*3 (reverse) (146) *etc.*

2.2.15.4. *Minimal isomorphic supergroups of lowest index*

No data are listed for isomorphic *supergroups* **IIc** because they can be derived directly from the corresponding data of *subgroups* **IIc** (*cf.* Part 13).

2.2.15.5. *Note on basis vectors*

In the *subgroup* data, $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ are the basis vectors of the subgroup $\mathcal{H}$ of the space group $\mathcal{G}$. The latter has the basis vectors **a**, **b**, **c**. In the *supergroup* data, $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ are the basis vectors of the supergroup $\mathcal{S}$ and **a**, **b**, **c** are again the basis vectors of $\mathcal{G}$. Thus, **a**, **b**, **c** and $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ exchange their roles if one considers the same group–subgroup relation in the subgroup and the supergroup tables.

Examples

(1) $\mathcal{G}$: *Pba*2 (32)

Listed under *subgroups* **IIb**, one finds, among other entries, [2] $Pna2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (33); thus, $\mathbf{c}(Pna2_1) = 2\mathbf{c}(Pba2)$.

* For normalizers of space groups, see Section 8.3.6 and Part 15, where also references to automorphisms are given.

Under *supergroups* **II** of $Pna2_1$ (33), the corresponding entry reads [2] $Pba2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (32); thus $\mathbf{c}(Pba2) = \frac{1}{2}\mathbf{c}(Pna2_1)$.

(2) Tetragonal *k* space groups with *P* cells. For index [2], the relations between the *conventional* basis vectors of the group and the subgroup read (*cf.* Fig. 5.1.3.5)

$$\mathbf{a}' = \mathbf{a} + \mathbf{b}, \qquad \mathbf{b}' = -\mathbf{a} + \mathbf{b} \qquad (\mathbf{a}', \mathbf{b}' \text{ for the subgroup}).$$

Thus, the basis vectors of the supergroup are

$$\mathbf{a}' = \tfrac{1}{2}(\mathbf{a} - \mathbf{b}), \quad \mathbf{b}' = \tfrac{1}{2}(\mathbf{a} + \mathbf{b}) \qquad (\mathbf{a}', \mathbf{b}' \text{ for the supergroup}).$$

An alternative description is

$$\mathbf{a}' = \mathbf{a} - \mathbf{b}, \qquad \mathbf{b}' = \mathbf{a} + \mathbf{b} \qquad (\mathbf{a}', \mathbf{b}' \text{ for the subgroup})$$

$$\mathbf{a}' = \tfrac{1}{2}(\mathbf{a} + \mathbf{b}), \quad \mathbf{b}' = \tfrac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad (\mathbf{a}', \mathbf{b}' \text{ for the supergroup}).$$

(3) Hexagonal *k* space groups. For index [3], the relations between the *conventional* basis vectors of the sub- and supergroup read (*cf.* Fig 5.1.3.8)

$$\mathbf{a}' = \mathbf{a} - \mathbf{b}, \qquad \mathbf{b}' = \mathbf{a} + 2\mathbf{b} \qquad (\mathbf{a}', \mathbf{b}' \text{ for the subgroup}).$$

Thus, the basis vectors of the supergroup are

$$\mathbf{a}' = \tfrac{1}{3}(2\mathbf{a} + \mathbf{b}), \ \mathbf{b}' = \tfrac{1}{3}(-\mathbf{a} + \mathbf{b}) \quad (\mathbf{a}', \mathbf{b}' \text{ for the supergroup}).$$

An alternative description is

$$\mathbf{a}' = 2\mathbf{a} + \mathbf{b}, \qquad \mathbf{b}' = -\mathbf{a} + \mathbf{b} \qquad (\mathbf{a}', \mathbf{b}' \text{ for the subgroup})$$

$$\mathbf{a}' = \tfrac{1}{3}(\mathbf{a} - \mathbf{b}), \quad \mathbf{b}' = \tfrac{1}{3}(\mathbf{a} + 2\mathbf{b}) \quad (\mathbf{a}', \mathbf{b}' \text{ for the supergroup}).$$

2.2.16. Monoclinic space groups

In this volume, space groups are described by one (or at most two) conventional coordinate systems (*cf.* Sections 2.1.3 and 2.2.2). Eight monoclinic space groups, however, are treated more extensively. In order to provide descriptions for frequently encountered cases, they are given in six versions.

The description of a monoclinic crystal structure in this volume, including its Hermann–Mauguin space-group symbol, depends upon two choices:

(i) the unit cell chosen, here called 'cell choice';

(ii) the labelling of the edges of this cell, especially of the monoclinic symmetry direction ('unique axis'), here called 'setting'.

2.2.16.1. *Cell choices*

One edge of the cell, *i.e.* one crystal axis, is always chosen along the monoclinic symmetry direction. The other two edges are located in the plane perpendicular to this direction and coincide with translation vectors in this 'monoclinic plane'. It is sensible and common practice (see below) to choose these two basis vectors from the *shortest three* translation vectors in that plane. They are shown in Fig. 2.2.16.1 and labelled **e**, **f** and **g**, in order of increasing length.* The two shorter vectors span the 'reduced mesh', here **e** and **f**; for this mesh, the monoclinic angle is $\leq 120°$, whereas for the other two primitive meshes larger angles are possible.

Other choices of the basis vectors in the monoclinic plane are possible, provided they span a primitive mesh. It turns out, however, that the space-group symbol for any of these (non-reduced) meshes already occurs among the symbols for the three meshes formed by **e**, **f**, **g** in Fig. 2.2.16.1; hence only these cases need be considered. They are designated in this volume as 'cell choice 1, 2 or 3' and are depicted in Fig. 2.2.6.4. The transformation matrices for the three cell choices are listed in Table 5.1.3.1.

* These three vectors obey the 'closed-triangle' condition $\mathbf{e} + \mathbf{f} + \mathbf{g} = \mathbf{0}$; they can be considered as two-dimensional homogeneous axes.

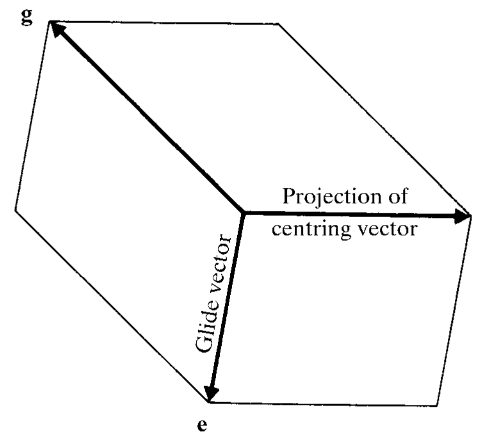

Fig. 2.2.16.1. The three primitive two-dimensional cells which are spanned by the shortest three translation vectors **e**, **f**, **g** in the monoclinic plane. For the present discussion, the glide vector is considered to be along **e** and the projection of the centring vector along **f**.

2.2.16.2. *Settings*

The term *setting* of a cell or of a space group refers to the assignment of labels (*a*, *b*, *c*) and directions to the edges of a given unit cell, resulting in a set of basis vectors **a**, **b**, **c**. (For orthorhombic space groups, the six settings are described and illustrated in Section 2.2.6.4.)

The symbol for each setting is a shorthand notation for the transformation of a given starting set **abc** into the setting considered. It is called here 'setting symbol'. For instance, the setting symbol **bca** stands for

$$\mathbf{a}' = \mathbf{b}, \quad \mathbf{b}' = \mathbf{c}, \quad \mathbf{c}' = \mathbf{a}$$

or

$$(\mathbf{a}'\mathbf{b}'\mathbf{c}') = (\mathbf{abc})\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = (\mathbf{bca}),$$

where $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ is the new set of basis vectors. (Note that the setting symbol **bca** does *not* mean that the old vector **a** changes its label to **b**, the old vector **b** changes to **c**, and the old **c** changes to **a**.) Transformation of one setting into another preserves the shape of the cell and its orientation relative to the lattice. The matrices of these transformations have *one* entry $+1$ or -1 in each row and column; all other entries are 0.

In monoclinic space groups, one axis, the monoclinic symmetry direction, is unique. Its label must be chosen first and, depending upon this choice, one speaks of 'unique axis *b*', 'unique axis *c*' or 'unique axis *a*'.† Conventionally, the positive directions of the two further ('oblique') axes are oriented so as to make the monoclinic angle non-acute, *i.e.* $\geq 90°$, and the coordinate system right-handed. For the three cell choices, settings obeying this condition and having the same label and direction of the unique axis are considered as one setting; this is illustrated in Fig. 2.2.6.4.

Note: These three cases of labelling the monoclinic axis are often called somewhat loosely *b*-axis, *c*-axis and *a*-axis 'settings'. It must be realized, however, that the choice of the 'unique axis' alone does *not* define a *single* setting but only a *pair*, as for each cell the labels of the two oblique axes can be interchanged.

† In *IT* (1952), the terms '1st setting' and '2nd setting' were used for 'unique axis *c*' and 'unique axis *b*'. In the present volume, these terms have been dropped in favour of the latter names, which are unambiguous.

Table 2.2.16.1 lists the setting symbols for the six monoclinic settings in three equivalent forms, starting with the symbols $\mathbf{a}\ \underline{\mathbf{b}}\ \mathbf{c}$ (first line), $\mathbf{a}\ \mathbf{b}\ \underline{\mathbf{c}}$ (second line) and $\underline{\mathbf{a}}\ \mathbf{b}\ \mathbf{c}$ (third line); the unique axis is underlined. These symbols are also found in the headline of the synoptic Table 4.3.2.1, which lists the space-group symbols for all monoclinic settings and cell choices. Again, the corresponding transformation matrices are listed in Table 5.1.3.1.

In the space-group tables, only the settings with b and c unique are treated and for these only the left-hand members of the double entries in Table 2.2.16.1. This implies, for instance, that the c-axis setting is obtained from the b-axis setting by cyclic permutation of the labels, *i.e.* by the transformation

$$(\mathbf{a}'\mathbf{b}'\underline{\mathbf{c}}') = (\mathbf{a}\underline{\mathbf{b}}\mathbf{c})\begin{pmatrix}0 & 1 & 0\\ 0 & 0 & 1\\ 1 & 0 & 0\end{pmatrix} = (\mathbf{c}\mathbf{a}\underline{\mathbf{b}}).$$

In the present discussion, also the setting with a unique is included, as this setting occurs in the subgroup entries of Part 7 and in Table 4.3.2.1. The a-axis setting $\underline{\mathbf{a}}'\mathbf{b}'\mathbf{c}' = \underline{\mathbf{c}}\mathbf{ab}$ is obtained from the c-axis setting also by cyclic permutation of the labels and from the b-axis setting by the reverse cyclic permutation: $\underline{\mathbf{a}}'\mathbf{b}'\mathbf{c}' = \underline{\mathbf{b}}\mathbf{ca}$.

By the conventions described above, the setting of each of the cell choices 1, 2 and 3 is determined once the label and the direction of the unique-axis vector have been selected. Six of the nine resulting possibilities are illustrated in Fig. 2.2.6.4.

2.2.16.3. *Cell choices and settings in the present tables*

There are five monoclinic space groups for which the Hermann–Mauguin symbols are independent of the cell choice, *viz* those space groups that do *not* contain centred lattices or glide planes:

$$P2 \text{ (No. 3)},\ P2_1 \text{ (4)},\ Pm \text{ (6)},\ P2/m \text{ (10)},\ P2_1/m \text{ (11)}.$$

In these cases, description of the space group by one cell choice is sufficient.

For the eight monoclinic space groups *with centred lattices or glide planes*, the Hermann–Mauguin symbol depends on the choice of the oblique axes with respect to the glide vector and/or the centring vector. These eight space groups are:

$$C2 \text{ (5)},\ Pc \text{ (7)},\ Cm \text{ (8)},\ Cc \text{ (9)},\ C2/m \text{ (12)},\ P2/c \text{ (13)},$$
$$P2_1/c \text{ (14)},\ C2/c \text{ (15)}.$$

Here, the glide vector or the projection of the centring vector onto the monoclinic plane are always directed along *one* of the vectors **e**, **f** or **g** in Fig. 2.2.16.1, *i.e.* are parallel to the shortest, the second-shortest or the third-shortest translation vector in the monoclinic plane (note that a glide vector and the projection of a centring vector cannot be parallel). This results in three possible orientations of the glide vector or the centring vector with respect to these crystal axes, and thus in three different full Hermann–Mauguin symbols (*cf.* Section 2.2.4) for each setting of a space group.

Table 2.2.16.2 lists the symbols for centring types and glide planes for the cell choices 1, 2, 3. The order of the three cell choices is defined as follows: The symbols occurring in the familiar 'standard short monoclinic space-group symbols' (see Section 2.2.3) define cell choice 1; for 'unique axis b', this applies to the centring type C and the glide plane c, as in Cm (8) and $P2_1/c$ (14). Cell choices 2 and 3 follow from the anticlockwise order 1–2–3 in Fig. 2.2.6.4 and their space-group symbols can be obtained from Table 2.2.16.2. The c-axis and the a-axis settings then are derived from the b-axis setting by cyclic permutations of the axial labels, as described in Section 2.2.16.2.

In the two space groups Cc (9) and $C2/c$ (15), glide planes occur in pairs, *i.e.* each vector **e**, **f**, **g** is associated either with a glide vector or with the centring vector of the cell. For Pc (7), $P2/c$ (13) and $P2_1/c$ (14), which contain only one type of glide plane, the left-hand member of each pair of glide planes in Table 2.2.16.2 applies.

In the space-group tables of this volume, the following treatments of monoclinic space groups are given:

(1) *Two complete descriptions* for each of the five monoclinic space groups with primitive lattices and without glide planes, one for 'unique axis b' and one for 'unique axis c', similar to the treatment in *IT* (1952).

(2) A total of *six descriptions* for each of the eight space groups with centred lattices or glide planes, as follows:

(*a*) *One complete* description for 'unique axis b' and 'cell choice' 1. This is considered the standard description of the space group, and its *short* Hermann–Mauguin symbol is used as the *standard* symbol of the space group.

This standard short symbol corresponds to the one symbol of *IT* (1935) and to that of the b-axis setting in *IT* (1952), *e.g.* $P2_1/c$ or $C2/c$. It serves only to identify the space-group type but carries no information about the setting or cell choice of a particular description. The *standard short symbol* is given in the headline of every description of a monoclinic space group; *cf.* Section 2.2.3.

(*b*) *Three condensed* (synoptic) descriptions for 'unique axis b' and the three 'cell choices' 1, 2, 3. Cell choice 1 is repeated to facilitate comparison with the other cell choices. Diagrams are provided to illustrate the three cell choices: *cf.* Section 2.2.6.

(*c*) *One complete* description for 'unique axis c' and 'cell choice' 1.

(*d*) *Three condensed* (synoptic) descriptions for 'unique axis c' and the three 'cell choices' 1, 2, 3. Again cell choice 1 is repeated and appropriate diagrams are provided.

All settings and cell choices are identified by the appropriate *full* Hermann–Mauguin symbols (*cf.* Section 2.2.4), *e.g.* $C12/c1$ or $I112/b$. For the two space groups Cc (9) and $C2/c$ (15) with pairs of different glide planes, the 'priority rule' (*cf.* Section 4.1.1) for

Table 2.2.16.1. *Monoclinic setting symbols (unique axis is underlined)*

Unique axis b		Unique axis c		Unique axis a		
$\boxed{\mathbf{a}\underline{\mathbf{b}}\mathbf{c}}$	$\mathbf{c}\underline{\bar{\mathbf{b}}}\mathbf{a}$	$\mathbf{ca}\underline{\mathbf{b}}$	$\mathbf{ac}\underline{\bar{\mathbf{b}}}$	$\underline{\mathbf{b}}\mathbf{ca}$	$\underline{\bar{\mathbf{b}}}\mathbf{ac}$	Starting set $\boxed{\mathbf{a}\underline{\mathbf{b}}\mathbf{c}}$
$\mathbf{b}\underline{\mathbf{c}}\mathbf{a}$	$\mathbf{a}\underline{\bar{\mathbf{c}}}\mathbf{b}$	$\boxed{\mathbf{ab}\underline{\mathbf{c}}}$	$\mathbf{ba}\underline{\bar{\mathbf{c}}}$	$\underline{\mathbf{c}}\mathbf{ab}$	$\underline{\bar{\mathbf{c}}}\mathbf{ba}$	Starting set $\boxed{\mathbf{ab}\underline{\mathbf{c}}}$
$\mathbf{c}\underline{\mathbf{a}}\mathbf{b}$	$\mathbf{b}\underline{\bar{\mathbf{a}}}\mathbf{c}$	$\mathbf{bc}\underline{\mathbf{a}}$	$\mathbf{cb}\underline{\bar{\mathbf{a}}}$	$\boxed{\underline{\mathbf{a}}\mathbf{bc}}$	$\underline{\bar{\mathbf{a}}}\mathbf{cb}$	Starting set $\boxed{\underline{\mathbf{a}}\mathbf{bc}}$

Note: An interchange of two axes involves a change of the handedness of the coordinate system. In order to keep the system right-handed, one sign reversal is necessary.

Table 2.2.16.2. *Symbols for centring types and glide planes of monoclinic space groups*

Setting		Cell choice 1	2	3
Unique axis b	Centring type	C	A	I
	Glide planes	c, n	n, a	a, c
Unique axis c	Centring type	A	B	I
	Glide planes	a, n	n, b	b, a
Unique axis a	Centring type	B	C	I
	Glide planes	b, n	n, c	c, b

glide planes (e before a before b before c before n) is *not* followed. Instead, in order to bring out the relations between the various settings and cell choices, the glide-plane symbol always refers to that glide plane which intersects the conventional origin.

Example: No. 15, standard short symbol $C2/c$

The full symbols for the three cell choices (rows) and the three unique axes (columns) read

$$\begin{array}{lll} C12/c1 & A12/n1 & I12/a1 \\ A112/a & B112/n & I112/b \\ B2/b11 & C2/n11 & I2/c11. \end{array}$$

Application of the priority rule would have resulted in the following symbols

$$\begin{array}{lll} C12/c1 & A12/a1 & I12/a1 \\ A112/a & B112/b & I112/a \\ B2/b11 & C2/c11 & I2/b11. \end{array}$$

Here, the transformation properties are obscured.

2.2.16.4. *Comparison with earlier editions of International Tables*

In *IT* (1935), each monoclinic space group was presented in one description only, with b as the unique axis. Hence, only one short Hermann–Mauguin symbol was needed.

In *IT* (1952), the c-axis setting (first setting) was newly introduced, in addition to the b-axis setting (second setting). This extension was based on a decision of the Stockholm General Assembly of the International Union of Crystallography in 1951 [*cf. Acta Cryst.* (1951), **4**, 569 and *Preface* to *IT* (1952)]. According to this decision, the b-axis setting should continue to be accepted as standard for morphological and structural studies. The two settings led to the introduction of *full* Hermann–Mauguin symbols for *all* 13 monoclinic space groups (*e.g.* $P12_1/c1$ and $P112_1/b$) and of two different *standard short* symbols (*e.g.* $P2_1/c$ and $P2_1/b$) for the *eight* space groups with centred lattices or glide planes [*cf.* p. 545 of *IT* (1952)]. In the present volume, only one of these standard short symbols is retained (see above and Section 2.2.3).

The c-axis setting (primed labels) was obtained from the b-axis setting (unprimed labels) by the following transformation

$$(\mathbf{a}'\mathbf{b}'\underline{\mathbf{c}}') = (\mathbf{a}\underline{\mathbf{b}}\mathbf{c})\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix} = (\mathbf{a}\mathbf{c}\underline{\bar{\mathbf{b}}}).$$

This corresponds to an interchange of two labels and not to the more logical cyclic permutation, as used in the present volume. The reason for this particular transformation was to obtain short space-group symbols that indicate the setting unambiguously; thus the lattice letters were chosen as C (b-axis setting) and B (c-axis setting). The use of A in either case would not have distinguished between the two settings [*cf.* pp. 7, 55 and 543 of *IT* (1952); see also Table 2.2.16.2].

As a consequence of the different transformations between b- and c-axis settings in *IT* (1952) and in this volume, some space-group symbols have changed. This is apparent from a comparison of pairs such as $P12_1/c1$ & $P112_1/b$ and $C12/c1$ & $B112/b$ in *IT* (1952) with the corresponding pairs in this volume, $P12_1/c1$ & $P112_1/a$ and $C12/c1$ & $A112/a$. The symbols with B-centred cells appear now for cell choice 2, as can be seen from Table 2.2.16.2.

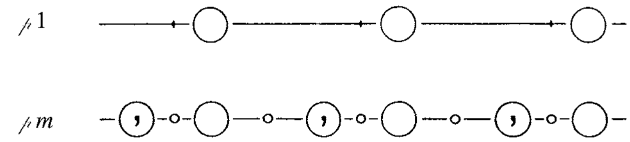

Fig. 2.2.17.1. The two line groups (one-dimensional space groups). Small circles are reflection points; large circles represent the general position; in line group $\mathscr{p}1$, the vertical bars are the origins of the unit cells.

2.2.16.5. *Selection of monoclinic cell*

In practice, the selection of the (right-handed) unit cell of a monoclinic crystal can be approached in three ways, whereby the axes refer to the b-unique setting; for c unique similar considerations apply:

(i) Irrespective of their lengths, the basis vectors are chosen such that, in Fig. 2.2.16.1, one obtains $\mathbf{c} = \mathbf{e}$, $\mathbf{a} = \mathbf{f}$ and $\mathbf{b}$ normal to $\mathbf{a}$ and $\mathbf{c}$ pointing upwards. This corresponds to a selection of cell choice 1. It ensures that the crystal structure can always be referred directly to the description and the space-group symbol in *IT* (1935) and *IT* (1952). However, this is at the expense of possibly using a non-reduced and, in many cases, even a very awkward cell.

(ii) Selection of the reduced mesh, *i.e.* the shortest two translation vectors in the monoclinic plane are taken as axes and labelled $\mathbf{a}$ and $\mathbf{c}$, with either $a < c$ or $c < a$. This results with equal probability in one of the three cell choices described in the present volume.

(iii) Selection of the cell on special grounds, *e.g.* to compare the structure under consideration with another related crystal structure. This may result again in a non-reduced cell and it may even necessitate use of the a-axis setting. In all these cases, the coordinate system chosen should be carefully explained in the description of the structure.

2.2.17. Crystallographic groups in one dimension

In one dimension, only one crystal family, one crystal system and one Bravais lattice exist. No name or common symbol is required for any of them. All one-dimensional lattices are primitive, which is symbolized by the script letter $\mathscr{p}$; *cf.* Chapter 1.2.

There occur two types of one-dimensional point groups, 1 and $m \equiv \bar{1}$. The latter contains reflections through a point (reflection point or mirror point). This operation can also be described as inversion through a point, thus $m \equiv \bar{1}$ for one dimension; *cf.* Chapters 1.3 and 1.4.

Two types of line groups (one-dimensional space groups) exist, with Hermann–Mauguin symbols $\mathscr{p}1$ and $\mathscr{p}m \equiv \mathscr{p}\bar{1}$, which are illustrated in Fig. 2.2.17.1. Line group $\mathscr{p}1$, which consists of one-dimensional translations only, has merely one (general) position with coordinate x. Line group $\mathscr{p}m$ consists of one-dimensional translations and reflections through points. It has one general and two special positions. The coordinates of the general position are x and $\bar{x}$; the coordinate of one special position is 0, that of the other $\frac{1}{2}$. The site symmetries of both special positions are $m \equiv \bar{1}$. For $\mathscr{p}1$, the origin is arbitrary, for $\mathscr{p}m$ it is at a reflection point.

The one-dimensional *point groups* are of interest as 'edge symmetries' of two-dimensional 'edge forms'; they are listed in Table 10.1.2.1. The one-dimensional *space groups* occur as projection and section symmetries of crystal structures.

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3.1. Space-group determination and diffraction symbols

By A. Looijenga-Vos and M. J. Buerger

3.1.1. Introduction

In this chapter, the determination of space groups from the Laue symmetry and the reflection conditions, as obtained from diffraction patterns, is discussed. Apart from Section 3.1.6.5, where differences between reflections *hkl* and $\bar{h}\bar{k}\bar{l}$ due to anomalous dispersion are discussed, it is assumed that Friedel's rule holds, *i.e.* that $|F(hkl)|^2 = |F(\bar{h}\bar{k}\bar{l})|^2$. This implies that the reciprocal lattice weighted by $|F(hkl)|^2$ has an inversion centre, even if this is not the case for the crystal under consideration. Accordingly, the symmetry of the weighted reciprocal lattice belongs, as was discovered by Friedel (1913), to one of the eleven Laue classes of Table 3.1.2.1. As described in Section 3.1.5, Laue class plus reflection conditions in most cases do not uniquely specify the space group. Methods that help to overcome these ambiguities, especially with respect to the presence or absence of an inversion centre in the crystal, are summarized in Section 3.1.6.

3.1.2. Laue class and cell

Space-group determination starts with the assignment of the *Laue class* to the weighted reciprocal lattice and the determination of the *cell geometry*. The conventional cell (except for the case of a primitive rhombohedral cell) is chosen such that the basis vectors coincide as much as possible with directions of highest symmetry (*cf.* Chapters 2.1 and 9.1).

The axial system should be taken right-handed. For the different crystal systems, the symmetry directions (*blickrichtungen*) are listed in Table 2.2.4.1. The symmetry directions and the convention that, within the above restrictions, the cell should be taken as small as possible determine the axes and their labels uniquely for crystal systems with symmetry higher than orthorhombic. For orthorhombic crystals, three directions are fixed by symmetry, but any of the three may be called *a*, *b* or *c*. For monoclinic crystals, there is one unique direction. It has to be decided whether this direction is called *b*, *c* or *a*. If there are no special reasons (physical properties, relations with other structures) to decide otherwise, the standard choice *b* is preferred. For triclinic crystals, usually the reduced cell is taken (*cf.* Chapter 9.2), but the labelling of the axes remains a matter of choice, as in the orthorhombic system.

If the lattice type turns out to be centred, which reveals itself by systematic absences in the general reflections *hkl* (Section 2.2.13), examination should be made to see whether the smallest cell has been selected, within the conventions appropriate to the crystal system. This is necessary since Table 3.1.4.1 for space-group determination is based on such a selection of the cell. Note, however, that for rhombohedral space groups two cells are considered, the triple hexagonal cell and the primitive rhombohedral cell.

The Laue class determines the crystal system. This is listed in Table 3.1.2.1. Note the conditions imposed on the lengths and the directions of the cell axes as well as the fact that there are crystal systems to which two Laue classes belong.

Table 3.1.2.1. *Laue classes and crystal systems*

Laue class	Crystal system	Conditions imposed on cell geometry
$\bar{1}$	Triclinic	None
$2/m$	Monoclinic	$\alpha = \gamma = 90°$ (*b* unique) $\alpha = \beta = 90°$ (*c* unique)
mmm	Orthorhombic	$\alpha = \beta = \gamma = 90°$
$4/m$ $4/mmm$	Tetragonal	$a = b; \alpha = \beta = \gamma = 90°$
$\bar{3}$ $\bar{3}m$	Trigonal	$a = b; \alpha = \beta = 90°; \gamma = 120°$ (hexagonal axes) $a = b = c; \alpha = \beta = \gamma$ (rhombohedral axes)
$6/m$ $6/mmm$	Hexagonal	$a = b; \alpha = \beta = 90°; \gamma = 120°$
$m\bar{3}$ $m\bar{3}m$	Cubic	$a = b = c; \alpha = \beta = \gamma = 90°$

3.1.3. Reflection conditions and diffraction symbol

In Section 2.2.13, it has been shown that 'extinctions' (sets of reflections that are systematically absent) point to the presence of a centred cell or the presence of symmetry elements with glide or screw components. Reflection conditions and Laue class together are expressed by the *Diffraction symbol*, introduced by Buerger (1935, 1942, 1969); it consists of the Laue-class symbol, followed by the extinction symbol representing the observed reflection conditions. Donnay & Harker (1940) have used the concept of extinctions under the name of 'morphological aspect' (or aspect for short) in their studies of crystal habit (*cf. Crystal Data*, 1972). Although the concept of aspect applies to diffraction as well as to morphology (Donnay & Kennard, 1964), for the present tables the expression 'extinction symbol' has been chosen because of the morphological connotation of the word aspect.

The *Extinction symbols* are arranged as follows. First, a capital letter is given representing the centring type of the cell (Section 1.2.1). Thereafter, the reflection conditions for the successive symmetry directions are symbolized. Symmetry directions not having reflection conditions are represented by a dash. A symmetry direction with reflection conditions is represented by the symbol for the corresponding glide plane and/or screw axis. The symbols applied are the same as those used in the Hermann–Mauguin space-group symbols (Section 1.3.1). If a symmetry direction has more than one kind of glide plane, for the diffraction symbol the same letter is used as in the corresponding space-group symbol. An exception is made for some centred orthorhombic space groups where *two* glide-plane symbols are given (between parentheses) for one of the symmetry directions, in order to stress the relation between the diffraction symbol and the symbols of the 'possible space groups'. For the various orthorhombic settings, treated in Table 3.1.4.1, the top lines of the two-line space-group symbols in Table 4.3.2.1 are used. In the monoclinic system, dummy numbers '1' are inserted for two directions even though they are not symmetry directions, to bring out the differences between the diffraction symbols for the *b*, *c* and *a* settings.

Example

Laue class: $12/m1$

Reflection conditions:

$$hkl : h + k = 2n;$$
$$h0l : h, l = 2n; \quad 0kl : k = 2n; \quad hk0 : h + k = 2n;$$
$$h00 : h = 2n; \quad 0k0 : k = 2n; \quad 00l : l = 2n.$$

As there are both c and n glide planes perpendicular to b, the diffraction symbol may be given as $1\,2/m\,1C1c1$ or as $1\,2/m\,1C1n1$. In analogy to the symbols of the possible space groups, $C1c1$ (9) and $C1\,2/c\,1$ (15), the diffraction symbol is called $1\,2/m\,1C1c1$.

For another cell choice, the reflection conditions are:

$$hkl : k + l = 2n;$$
$$h0l : h, l = 2n; \quad 0kl : k + l = 2n; \quad hk0 : k = 2n;$$
$$h00 : h = 2n; \quad 0k0 : k = 2n; \quad 00l : l = 2n.$$

For this second cell choice, the glide planes perpendicular to b are n and a. The diffraction symbol is given as $1\,2/m\,1A1n1$, in analogy to the symbols $A1n1$ (9) and $A1\,2/n\,1$ (15) adopted for the possible space groups.

3.1.4. Deduction of possible space groups

Reflection conditions, diffraction symbols, and possible space groups are listed in Table 3.1.4.1. For each crystal system, a different table is provided. The monoclinic system contains different entries for the settings with b, c and a unique. For monoclinic and orthorhombic crystals, all possible settings and cell choices are treated. In contradistinction to Table 4.3.2.1, which lists the space-group symbols for different settings and cell choices in a systematic way, the present table is designed with the aim to make space-group determination as easy as possible.

The left-hand side of the table contains the *Reflection conditions*. Conditions of the type $h = 2n$ or $h + k = 2n$ are abbreviated as h or $h + k$. Conditions like $h = 2n, k = 2n, h + k = 2n$ are quoted as h, k; in this case, the condition $h + k = 2n$ is not listed as it follows directly from $h = 2n, k = 2n$. Conditions with $l = 3n$, $l = 4n$, $l = 6n$ or more complicated expressions are listed explicitly.

From *left* to *right*, the table contains the integral, zonal and serial conditions. From *top* to *bottom*, the entries are ordered such that left columns are kept empty as long as possible. The leftmost column that contains an entry is considered as the 'leading column'. In this column, entries are listed according to increasing complexity. This also holds for the subsequent columns within the restrictions imposed by previous columns on the left. The make-up of the table is such that observed reflection conditions should be matched against the table by considering, within each crystal system, the columns from left to right.

The centre column contains the *Extinction symbol*. To obtain the complete diffraction symbol, the Laue-class symbol has to be added in front of it. Be sure that the correct Laue-class symbol is used if the crystal system contains two Laue classes. Particular care is needed for Laue class $\bar{3}m$ in the trigonal system, because there are two possible orientations of this Laue symmetry with respect to the crystal lattice, $\bar{3}m1$ and $\bar{3}1m$. The correct orientation can be obtained directly from the diffraction record.

The right-hand side of the table gives the *Possible space groups* which obey the reflection conditions. For crystal systems with two Laue classes, a subdivision is made according to the Laue symmetry. The entries in each Laue class are ordered according to their point groups. All space groups that match both the reflection conditions and the Laue symmetry, found in a diffraction experiment, are possible space groups of the crystal.

The space groups are given by their short Hermann–Mauguin symbols, followed by their number between parentheses, except for the monoclinic system, where full symbols are given (*cf.* Section 2.2.4). In the monoclinic and orthorhombic sections of Table 3.1.4.1, which contain entries for the different settings and cell choices, the 'standard' space-group symbols (*cf.* Table 4.3.2.1) are printed in bold face. Only these standard representations are treated in full in the space-group tables.

Example

The diffraction pattern of a compound has Laue class mmm. The crystal system is thus orthorhombic. The diffraction spots are indexed such that the reflection conditions are $0kl : l = 2n$; $h0l : h + l = 2n$; $h00 : h = 2n$; $00l : l = 2n$. Table 3.1.4.1 shows that the diffraction symbol is *mmmPcn–*. Possible space groups are $Pcn2$ (30) and $Pcnm$ (53). For neither space group does the axial choice correspond to that of the standard setting. For No. 30, the standard symbol is $Pnc2$, for No. 53 it is $Pmna$. The transformation from the basis vectors $\mathbf{a}_e, \mathbf{b}_e, \mathbf{c}_e$, used in the experiment, to the basis vectors $\mathbf{a}_s, \mathbf{b}_s, \mathbf{c}_s$ of the standard setting is given by $\mathbf{a}_s = \mathbf{b}_e, \mathbf{b}_s = -\mathbf{a}_e$ for No. 30 and by $\mathbf{a}_s = \mathbf{c}_e, \mathbf{c}_s = -\mathbf{a}_e$ for No. 53.

Possible pitfalls

Errors in the space-group determination may occur because of several reasons.

(1) *Twinning of the crystal*

Difficulties that may be encountered are shown by the following example. Say that a monoclinic crystal (b unique) with the angle β fortuitously equal to $\sim 90°$ is twinned according to (100). As this causes overlap of the reflections hkl and $\bar{h}kl$, the observed Laue symmetry is mmm rather than $2/m$. The same effect may occur within one crystal system. If, for instance, a crystal with Laue class $4/m$ is twinned according to (100) or (110), the Laue class $4/mmm$ is simulated (twinning by merohedry, *cf.* Catti & Ferraris, 1976, and Koch, 1999). Further examples are given by Buerger (1960). Errors due to twinning can often be detected from the fact that the observed reflection conditions do not match any of the diffraction symbols.

(2) *Incorrect determination of reflection conditions*

Either too many or too few conditions may be found. For serial reflections, the first case may arise if the structure is such that its projection on, say, the b direction shows pseudo-periodicity. If the pseudo-axis is b/p, with p an integer, the reflections $0k0$ with $k \neq p$ are very weak. If the exposure time is not long enough, they may be classified as unobserved which, incorrectly, would lead to the reflection condition $0k0 : k = p$. A similar situation may arise for zonal conditions, although in this case there is less danger of errors. Many more reflections are involved and the occurrence of pseudo-periodicity is less likely for two-dimensional than for one-dimensional projections.

For 'structural' or non-space-group absences, see Section 2.2.13.

The second case, too many observed reflections, may be due to multiple diffraction or to radiation impurity. A textbook description of multiple diffraction has been given by Lipson & Cochran (1966). A well known case of radiation impurity in X-ray diffraction is the contamination of a copper target with iron. On a photograph taken with the radiation from such a target, the iron radiation with $\lambda(\text{Fe}) \sim 5/4\lambda(\text{Cu})$ gives a reflection spot $4h_i4k_i4l$ at the position $5h_i5k_i5l$ for copper $[\lambda(\text{Cu}\ K\bar{\alpha}) = 1.5418\ \text{Å}, \lambda(\text{Fe}\ K\bar{\alpha}) = 1.9373\ \text{Å}]$. For reflections $0k0$, for instance, this may give rise to reflected intensity at the copper 050 position so that, incorrectly, the condition $0k0 : k = 2n$ may be excluded.

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups*

TRICLINIC. Laue class $\bar{1}$

Reflection conditions	Extinction symbol	Point group	
		1	$\bar{1}$
None	*P*–	*P*1(1)	$P\bar{1}$ (2)

MONOCLINIC, Laue class $2/m$

Unique axis *b*				Laue class 1 $2/m$ 1		
Reflection conditions				Point group		
hkl 0*kl* *hk*0	*h*0*l* *h*00 00*l*	0*k*0	Extinction symbol	2	*m*	$2/m$
			*P*1–1	***P*121** (3)	***P*1*m*1** (6)	***P*1 2/*m* 1** (10)
		k	$P12_11$	**$P12_11$** (4)		**$P1\ 2_1/m\ 1$** (11)
	h		*P*1*a*1		*P*1*a*1 (7)	*P*1 2/*a* 1 (13)
	h	*k*	$P1\ 2_1/a\ 1$			$P1\ 2_1/a\ 1$ (14)
	l		*P*1*c*1		***P*1*c*1** (7)	***P*1 2/*c* 1** (13)
	l	*k*	$P1\ 2_1/c\ 1$			**$P1\ 2_1/c\ 1$** (14)
	$h+l$		*P*1*n*1		*P*1*n*1 (7)	*P*1 2/*n* 1 (13)
	$h+l$	*k*	$P1\ 2_1/n\ 1$			$P1\ 2_1/n\ 1$ (14)
$h+k$	*h*	*k*	*C*1–1	***C*121** (5)	***C*1*m*1** (8)	***C*1 2/*m* 1** (12)
$h+k$	*h*, *l*	*k*	*C*1*c*1		***C*1*c*1** (9)	***C*1 2/*c* 1** (15)
$k+l$	*l*	*k*	*A*1–1	*A*121 (5)	*A*1*m*1 (8)	*A*1 2/*m* 1 (12)
$k+l$	*h*, *l*	*k*	*A*1*n*1		*A*1*n*1 (9)	*A*1 2/*n* 1 (15)
$h+k+l$	$h+l$	*k*	*I*1–1	*I*121 (5)	*I*1*m*1 (8)	*I*1 2/*m* 1 (12)
$h+k+l$	*h*, *l*	*k*	*I*1*a*1		*I*1*a*1 (9)	*I*1 2/*a* 1 (15)
Unique axis *c*				**Laue class 1 1 $2/m$**		
Reflection conditions				Point group		
hkl 0*kl* *h*0*l*	*hk*0 *h*00 0*k*0	00*l*	Extinction symbol	2	*m*	$2/m$
			*P*11–	*P*112 (3)	*P*11*m* (6)	*P*11 2/*m* (10)
		l	$P112_1$	$P112_1$ (4)		$P11\ 2_1/m$ (11)
	h		*P*11*a*		*P*11*a* (7)	*P*11 2/*a* (13)
	h	*l*	$P11\ 2_1/a$			$P11\ 2_1/a$ (14)
	k		*P*11*b*		*P*11*b* (7)	*P*11 2/*b* (13)
	k	*l*	$P11\ 2_1/b$			$P11\ 2_1/b$ (14)
	$h+k$		*P*11*n*		*P*11*n* (7)	*P*11 2/*n* (13)
	$h+k$	*l*	$P11\ 2_1/n$			$P11\ 2_1/n$ (14)
$h+l$	*h*	*l*	*B*11–	*B*112 (5)	*B*11*m* (8)	*B*11 2/*m* (12)
$h+l$	*h*, *k*	*l*	*B*11*n*		*B*11*n* (9)	*B*11 2/*n* (15)
$k+l$	*k*	*l*	*A*11–	*A*112 (5)	*A*11*m* (8)	*A*11 2/*m* (12)
$k+l$	*h*, *k*	*l*	*A*11*a*		*A*11*a* (9)	*A*11 2/*a* (15)
$h+k+l$	$h+k$	*l*	*I*11–	*I*112 (5)	*I*11*m* (8)	*I*11 2/*m* (12)
$h+k+l$	*h*, *k*	*l*	*I*11*b*		*I*11*b* (9)	*I*11 2/*b* (15)

(3) *Incorrect assignment of the Laue symmetry*

This may be caused by pseudo-symmetry or by 'diffraction enhancement'. A crystal with pseudo-symmetry shows small deviations from a certain symmetry, and careful inspection of the diffraction pattern is necessary to determine the correct Laue class. In the case of diffraction enhancement, the symmetry of the diffraction pattern is higher than the Laue symmetry of the crystal. Structure types showing this phenomenon are rare and have to fulfil specified conditions. For further discussions and references, see Perez-Mato & Iglesias (1977).

3.1.5. Diffraction symbols and possible space groups

Table 3.1.4.1 contains 219 extinction symbols which, when combined with the Laue classes, lead to 242 different diffraction symbols. If, however, for the monoclinic and orthorhombic systems

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

MONOCLINIC, Laue class $2/m$ (*cont.*)

Unique axis *a*				Laue class $2/m$ 1 1		
Reflection conditions				Point group		
hkl $h0l$ $hk0$	$0kl$ $0k0$ $00l$	$h00$	Extinction symbol	2	m	$2/m$
			P–11	$P211$ (3)	$Pm11$ (6)	$P2/m$ 11 (10)
		h	$P2_111$	$P2_111$ (4)		$P2_1/m$ 11 (11)
	k		$Pb11$		$Pb11$ (7)	$P2/b$ 11 (13)
	k	h	$P2_1/b$ 11			$P2_1/b$ 11 (14)
	l		$Pc11$		$Pc11$ (7)	$P2/c$ 11 (13)
	l	h	$P2_1/c$ 11			$P2_1/c$ 11 (14)
	$k+l$		$Pn11$		$Pn11$ (7)	$P2/n$ 11 (13)
	$k+l$	h	$P2_1/n$ 11			$P2_1/n$ 11 (14)
$h+k$	k	h	C–11	$C211$ (5)	$Cm11$ (8)	$C2/m$ 11 (12)
$h+k$	k, l	h	$Cn11$		$Cn11$ (9)	$C2/n$ 11 (15)
$h+l$	l	h	B–11	$B211$ (5)	$Bm11$ (8)	$B2/m$ 11 (12)
$h+l$	k, l	h	$Bb11$		$Bb11$ (9)	$B2/b$ 11 (15)
$h+k+l$	$k+l$	h	I–11	$I211$ (5)	$Im11$ (8)	$I2/m$ 11 (12)
$h+k+l$	k, l	h	$Ic11$		$Ic11$ (9)	$I2/c$ 11 (15)

ORTHORHOMBIC, Laue class mmm ($2/m$ $2/m$ $2/m$)

In this table, the symbol e in the space-group symbol represents the two glide planes given between parentheses in the corresponding extinction symbol. Only for one of the two cases does a bold printed symbol correspond with the standard symbol.

Reflection conditions								Laue class mmm ($2/m$ $2/m$ $2/m$)		
								Point group		
hkl	$0kl$	$h0l$	$hk0$	$h00$	$0k0$	$00l$	Extinction symbol	222	$mm2$ $m2m$ $2mm$	mmm
							$P---$	$\mathbf{P222}$ (16)	$\mathbf{Pmm2}$ (25)	$\mathbf{Pmmm}$ (47)
									$Pm2m$ (25)	
									$P2mm$ (25)	
						l	$P--2_1$	$\mathbf{P222_1}$ (17)		
					k		$P-2_1-$	$P22_12$ (17)		
					k	l	$P-2_12_1$	$P22_12_1$ (18)		
				h			$P2_1--$	$P2_122$ (17)		
				h		l	$P2_1-2_1$	$P2_122_1$ (18)		
				h	k		$P2_12_1-$	$\mathbf{P2_12_12}$ (18)		
				h	k	l	$P2_12_12_1$	$\mathbf{P2_12_12_1}$ (19)		
			h	h			$P--a$		$Pm2a$ (28)	
									$P2_1ma$ (26)	$\mathbf{Pmma}$ (51)
			k		k		$P--b$		$Pm2_1b$ (26)	
									$P2mb$ (28)	$Pmmb$ (51)
			$h+k$	h	k		$P--n$		$Pm2_1n$ (31)	
									$P2_1mn$ (31)	$\mathbf{Pmmn}$ (59)
		h		h			$P-a-$		$\mathbf{Pma2}$ (28)	$Pmam$ (51)
									$P2_1am$ (26)	
		h	h	h			$P-aa$		$P2aa$ (27)	$Pmaa$ (49)
		h	k	h	k		$P-ab$		$P2_1ab$ (29)	$Pmab$ (57)
		h	$h+k$	h	k		$P-an$		$P2an$ (30)	$Pman$ (53)
		l				l	$P-c-$		$\mathbf{Pmc2_1}$ (26)	
									$P2cm$ (28)	$Pmcm$ (51)
		l	h	h		l	$P-ca$		$P2_1ca$ (29)	$Pmca$ (57)
		l	k		k	l	$P-cb$		$P2cb$ (32)	$Pmcb$ (55)
		l	$h+k$	h	k	l	$P-cn$		$P2_1cn$ (33)	$Pmcn$ (62)

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

ORTHORHOMBIC, Laue class *mmm* (2/*m* 2/*m* 2/*m*) (*cont.*)

Reflection conditions								Laue class *mmm* (2/*m* 2/*m* 2/*m*)		
								Point group		
hkl	0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*	Extinction symbol	222	*mm*2 *m*2*m* 2*mm*	*mmm*
		$h+l$		h		l	*P–n–*		$\boldsymbol{Pmn2_1}$ (31)	
									$P2_1nm$ (31)	*Pmnm* (59)
		$h+l$	h	h		l	*P–na*		*P2na* (30)	***Pmna*** (53)
		$h+l$	k	h	k	l	*P–nb*		$P2_1nb$ (33)	*Pmnb* (62)
		$h+l$	$h+k$	h	k	l	*P–nn*		*P2nn* (34)	*Pmnn* (58)
	k				k		*Pb– –*		*Pbm2* (28)	
									$Pb2_1m$ (26)	*Pbmm* (51)
	k		h	h	k		*Pb–a*		$Pb2_1a$ (29)	*Pbma* (57)
	k		k		k		*Pb–b*		*Pb2b* (27)	*Pbmb* (49)
	k		$h+k$	h	k		*Pb–n*		*Pb2n* (30)	*Pbmn* (53)
	k	h		h	k		*Pba–*		***Pba2*** (32)	***Pbam*** (55)
	k	h	h	h	k		*Pbaa*			*Pbaa* (54)
	k	h	k	h	k		*Pbab*			*Pbab* (54)
	k	h	$h+k$	h	k		*Pban*			***Pban*** (50)
	k	l			k	l	*Pbc–*		$Pbc2_1$ (29)	***Pbcm*** (57)
	k	l	h	h	k	l	*Pbca*			***Pbca*** (61)
	k	l	k		k	l	*Pbcb*			*Pbcb* (54)
	k	l	$h+k$	h	k	l	*Pbcn*			***Pbcn*** (60)
	k	$h+l$		h	k	l	*Pbn–*		$Pbn2_1$ (33)	*Pbnm* (62)
	k	$h+l$	h	h	k	l	*Pbna*			*Pbna* (60)
	k	$h+l$	k	h	k	l	*Pbnb*			*Pbnb* (56)
	k	$h+l$	$h+k$	h	k	l	*Pbnn*			*Pbnn* (52)
	l					l	*Pc– –*		$Pcm2_1$ (26)	
									Pc2m (28)	*Pcmm* (51)
	l		h	h		l	*Pc–a*		*Pc2a* (32)	*Pcma* (55)
	l		k		k	l	*Pc–b*		$Pc2_1b$ (29)	*Pcmb* (57)
	l		$h+k$	h	k	l	*Pc–n*		$Pc2_1n$ (33)	*Pcmn* (62)
	l	h		h		l	*Pca–*		$\boldsymbol{Pca2_1}$ (29)	*Pcam* (57)
	l	h	h	h		l	*Pcaa*			*Pcaa* (54)
	l	h	k	h	k	l	*Pcab*			*Pcab* (61)
	l	h	$h+k$	h	k	l	*Pcan*			*Pcan* (60)
	l	l				l	*Pcc–*		***Pcc2*** (27)	***Pccm*** (49)
	l	l	h	h		l	*Pcca*			***Pcca*** (54)
	l	l	k		k	l	*Pccb*			*Pccb* (54)
	l	l	$h+k$	h	k	l	*Pccn*			***Pccn*** (56)
	l	$h+l$		h		l	*Pcn –*		*Pcn2* (30)	*Pcnm* (53)
	l	$h+l$	h	h		l	*Pcna*			*Pcna* (50)
	l	$h+l$	k	h	k	l	*Pcnb*			*Pcnb* (60)
	l	$h+l$	$h+k$	h	k	l	*Pcnn*			*Pcnn* (52)
	$k+l$				k	l	*Pn – –*		$Pnm2_1$ (31)	*Pnmm* (59)
									$Pn2_1m$ (31)	
	$k+l$		h	h	k	l	*Pn–a*		$Pn2_1a$ (33)	***Pnma*** (62)
	$k+l$		k		k	l	*Pn–b*		*Pn2b* (30)	*Pnmb* (53)
	$k+l$		$h+k$	h	k	l	*Pn–n*		*Pn2n* (34)	*Pnmn* (58)
	$k+l$	h		h	k	l	*Pna –*		$\boldsymbol{Pna2_1}$ (33)	*Pnam* (62)
	$k+l$	h	h	h	k	l	*Pnaa*			*Pnaa* (56)
	$k+l$	h	k	h	k	l	*Pnab*			*Pnab* (60)
	$k+l$	h	$h+k$	h	k	l	*Pnan*			*Pnan* (52)
	$k+l$	l			k	l	*Pnc –*		***Pnc2*** (30)	*Pncm* (53)
	$k+l$	l	h	h	k	l	*Pnca*			*Pnca* (60)

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

ORTHORHOMBIC, Laue class *mmm* (2/*m* 2/*m* 2/*m*) (*cont.*)

Reflection conditions								Laue class *mmm* (2/*m* 2/*m* 2/*m*)		
								Point group		
hkl	0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*	Extinction symbol	222	*mm*2 *m*2*m* 2*mm*	*mmm*
	k + *l*	*l*	*k*		*k*	*l*	*Pncb*			*Pncb* (50)
	k + *l*	*l*	*h* + *k*	*h*	*k*	*l*	*Pncn*			*Pncn* (52)
	k + *l*	*h* + *l*		*h*	*k*	*l*	*Pnn* −		***Pnn2*** (34)	***Pnnm*** (58)
	k + *l*	*h* + *l*	*h*	*h*	*k*	*l*	*Pnna*			***Pnna*** (52)
	k + *l*	*h* + *l*	*k*	*h*	*k*	*l*	*Pnnb*			*Pnnb* (52)
	k + *l*	*h* + *l*	*h* + *k*	*h*	*k*	*l*	*Pnnn*			***Pnnn*** (48)
h + *k*	*k*	*h*	*h* + *k*	*h*	*k*		*C* − − −	***C222*** (21)	***Cmm2*** (35)	***Cmmm*** (65)
									Cm2m (38)	
									C2mm (38)	
h + *k*	*k*	*h*	*h* + *k*	*h*	*k*	*l*	$C--2_1$	$\boldsymbol{C222_1}$ (20)		
h + *k*	*k*	*h*	*h*, *k*	*h*	*k*		*C*− −(*ab*)		*Cm2e* (39)	***Cmme*** (67)
									C2me (39)	
h + *k*	*k*	*h*, *l*	*h* + *k*	*h*	*k*	*l*	*C*−*c* −		$\boldsymbol{Cmc2_1}$ (36)	***Cmcm*** (63)
									C2cm (40)	
h + *k*	*k*	*h*, *l*	*h*, *k*	*h*	*k*	*l*	*C*−*c*(*ab*)		*C2ce* (41)	***Cmce*** (64)
h + *k*	*k*, *l*	*h*	*h* + *k*	*h*	*k*	*l*	*Cc* − −		$Ccm2_1$ (36)	*Ccmm* (63)
									Cc2m (40)	
h + *k*	*k*, *l*	*h*	*h*, *k*	*h*	*k*	*l*	*Cc* −(*ab*)		*Cc2e* (41)	*Ccme* (64)
h + *k*	*k*, *l*	*h*, *l*	*h* + *k*	*h*	*k*	*l*	*Ccc* −		***Ccc2*** (37)	***Cccm*** (66)
h + *k*	*k*, *l*	*h*, *l*	*h*, *k*	*h*	*k*	*l*	*Ccc*(*ab*)			***Ccce*** (68)
h + *l*	*l*	*h* + *l*	*h*	*h*		*l*	*B* − − −	*B*222 (21)	*Bmm*2 (38)	*Bmmm* (65)
									*Bm*2*m* (35)	
									*B*2*mm* (38)	
h + *l*	*l*	*h* + *l*	*h*	*h*	*k*	*l*	$B\!-\!2_1\!-$	$B22_12$ (20)		
h + *l*	*l*	*h* + *l*	*h*, *k*	*h*	*k*	*l*	*B*− −*b*		$Bm2_1b$ (36)	*Bmmb* (63)
									*B*2*mb* (40)	
h + *l*	*l*	*h*, *l*	*h*	*h*		*l*	*B* −(*ac*)−		*Bme*2 (39)	*Bmem* (67)
									*B*2*em* (39)	
h + *l*	*l*	*h*, *l*	*h*, *k*	*h*	*k*	*l*	*B* −(*ac*)*b*		*B*2*eb* (41)	*Bmeb* (64)
h + *l*	*k*, *l*	*h* + *l*	*h*	*h*	*k*	*l*	*Bb* − −		*Bbm*2 (40)	*Bbmm* (63)
									$Bb2_1m$ (36)	
h + *l*	*k*, *l*	*h* + *l*	*h*, *k*	*h*	*k*	*l*	*Bb*−*b*		*Bb*2*b* (37)	*Bbmb* (66)
h + *l*	*k*, *l*	*h*, *l*	*h*	*h*	*k*	*l*	*Bb*(*ac*)−		*Bbe*2 (41)	*Bbem* (64)
h + *l*	*k*, *l*	*h*, *l*	*h*, *k*	*h*	*k*	*l*	*Bb*(*ac*)*b*			*Bbeb* (68)
k + *l*	*k* + *l*	*l*	*k*		*k*	*l*	*A* − − −	*A*222 (21)	***Amm2*** (38)	*Ammm* (65)
									*Am*2*m* (38)	
									*A*2*mm* (35)	
k + *l*	*k* + *l*	*l*	*k*	*h*	*k*	*l*	$A2_1--$	$A2_122$ (20)		
k + *l*	*k* + *l*	*l*	*h*, *k*	*h*	*k*	*l*	*A*− −*a*		***Am2a*** (40)	*Amma* (63)
									$A2_1ma$ (36)	
k + *l*	*k* + *l*	*h*, *l*	*k*	*h*	*k*	*l*	*A*−*a* −		***Ama2*** (40)	*Amam* (63)
									$A2_1am$ (36)	
k + *l*	*k* + *l*	*h*, *l*	*h*, *k*	*h*	*k*	*l*	*A*−*aa*		*A*2*aa* (37)	*Amaa* (66)
k + *l*	*k*, *l*	*l*	*k*		*k*	*l*	*A*(*bc*)− −		***Aem2*** (39)	*Aemm* (67)
									*Ae*2*m* (39)	
k + *l*	*k*, *l*	*l*	*h*, *k*	*h*	*k*	*l*	*A*(*bc*)− *a*		*Ae*2*a* (41)	*Aema* (64)
k + *l*	*k*, *l*	*h*, *l*	*k*	*h*	*k*	*l*	*A*(*bc*)*a* −		***Aea2*** (41)	*Aeam* (64)
k + *l*	*k*, *l*	*h*, *l*	*h*, *k*	*h*	*k*	*l*	*A*(*bc*)*aa*			*Aeaa* (68)
h + *k* + *l*	*k* + *l*	*h* + *l*	*h* + *k*	*h*	*k*	*l*	*I* − − −	[***I222*** (23) $\boldsymbol{I2_12_12_1}$ (24)]*	***Imm2*** (44)	***Immm*** (71)
									*Im*2*m* (44)	

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

ORTHORHOMBIC, Laue class mmm ($2/m\ 2/m\ 2/m$) (*cont.*)

Reflection conditions								Laue class mmm ($2/m\ 2/m\ 2/m$)		
								Point group		
hkl	$0kl$	$h0l$	$hk0$	$h00$	$0k0$	$00l$	Extinction symbol	222	$mm2$ $m2m$ $2mm$	mmm
									$I2mm$ (44)	
$h+k+l$	$k+l$	$h+l$	h, k	h	k	l	$I--(ab)$		$Im2a$ (46)	***Imma*** (74)
									$I2mb$ (46)	$Immb$ (74)
$h+k+l$	$k+l$	h, l	$h+k$	h	k	l	$I-(ac)-$		***Ima2*** (46)	$Imam$ (74)
									$I2cm$ (46)	$Imcm$ (74)
$h+k+l$	$k+l$	h, l	h, k	h	k	l	$I-cb$		$I2cb$ (45)	$Imcb$ (72)
$h+k+l$	k, l	$h+l$	$h+k$	h	k	l	$I(bc)--$		$Iem2$ (46)	$Iemm$ (74)
									$Ie2m$ (46)	
$h+k+l$	k, l	$h+l$	h, k	h	k	l	$Ic-a$		$Ic2a$ (45)	$Icma$ (72)
$h+k+l$	k, l	h, l	$h+k$	h	k	l	$Iba-$		***Iba2*** (45)	***Ibam*** (72)
$h+k+l$	k, l	h, l	h, k	h	k	l	$Ibca$			***Ibca*** (73)
										$Icab$ (73)
$h+k, h+l, k+l$	k, l	h, l	h, k	h	k	l	$F---$	***F222*** (22)	***Fmm2*** (42)	***Fmmm*** (69)
									$Fm2m$ (42)	
									$F2mm$ (42)	
$h+k, h+l, k+l$	k, l	$h+l=4n$; h, l	$h+k=4n$; h, k	$h=4n$	$k=4n$	$l=4n$	$F-dd$		$F2dd$ (43)	
$h+k, h+l, k+l$	$k+l=4n$; k, l	h, l	$h+k=4n$; h, k	$h=4n$	$k=4n$	$l=4n$	$Fd-d$		$Fd2d$ (43)	
$h+k, h+l, k+l$	$k+l=4n$; k, l	$h+l=4n$; h, l	h, k	$h=4n$	$k=4n$	$l=4n$	$Fdd-$		***Fdd2*** (43)	
$h+k, h+l, k+l$	$k+l=4n$; k, l	$h+l=4n$; h, l	$h+k=4n$; h, k	$h=4n$	$k=4n$	$l=4n$	$Fddd$			***Fddd*** (70)

* Pair of space groups with common point group and symmetry elements but differing in the relative location of these elements.

TETRAGONAL, Laue classes $4/m$ and $4/mmm$

Reflection conditions							Extinction symbol	Laue class						
								$4/m$			$4/mmm$ ($4/m\ 2/m\ 2/m$)			
								Point group						
hkl	$hk0$	$0kl$	hhl	$00l$	$0k0$	$hh0$		4	$\bar{4}$	$4/m$	422	$4mm$	$\bar{4}2m$ $\bar{4}m2$	$4/mmm$
							$P---$	$P4$ (75)	$P\bar{4}$ (81)	$P4/m$ (83)	$P422$ (89)	$P4mm$ (99)	$P\bar{4}2m$ (111)	$P4/mmm$ (123)
													$P\bar{4}m2$ (115)	
					k		$P-2_1-$				$P42_12$ (90)		$P\bar{4}2_1m$ (113)	
				l			$P4_2--$	$P4_2$ (77)		$P4_2/m$ (84)	$P4_222$ (93)			
				l	k		$P4_22_1-$				$P4_22_12$ (94)			
				$l=4n$			$P4_1--$	$\left\{\begin{matrix} P4_1\ (76) \\ P4_3\ (78) \end{matrix}\right\}$†			$\left\{\begin{matrix} P4_122\ (91) \\ P4_322\ (95) \end{matrix}\right\}$†			
				$l=4n$	k		$P4_12_1-$				$\left\{\begin{matrix} P4_12_12\ (92) \\ P4_32_12\ (96) \end{matrix}\right\}$†			
			l	l			$P--c$					$P4_2mc$ (105)	$P\bar{4}2c$ (112)	$P4_2/mmc$ (131)
			l	l	k		$P-2_1c$						$P\bar{4}2_1c$ (114)	
		k			k		$P-b-$					$P4bm$ (100)	$P\bar{4}b2$ (117)	$P4/mbm$ (127)
		k	l	l	k		$P-bc$					$P4_2bc$ (106)		$P4_2/mbc$ (135)
		l		l			$P-c-$					$P4_2cm$ (101)	$P\bar{4}c2$ (116)	$P4_2/mcm$ (132)
		l	l	l			$P-cc$					$P4cc$ (103)		$P4/mcc$ (124)
		$k+l$		l	k		$P-n-$					$P4_2nm$ (102)	$P\bar{4}n2$ (118)	$P4_2/mnm$ (136)
		$k+l$	l	l	k		$P-nc$					$P4nc$ (104)		$P4/mnc$ (128)
	$h+k$				k		$Pn--$			$P4/n$ (85)				$P4/nmm$ (129)
	$h+k$			l	k		$P4_2/n--$			$P4_2/n$ (86)				
	$h+k$		l	l	k		$Pn-c$							$P4_2/nmc$ (137)

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

TETRAGONAL, Laue classes $4/m$ and $4/mmm$ (*cont.*)

Reflection conditions							Extinction symbol	Laue class						
								$4/m$			$4/mmm$ ($4/m\,2/m\,2/m$)			
								Point group						
hkl	$hk0$	$0kl$	hhl	$00l$	$0k0$	$hh0$		4	$\bar{4}$	$4/m$	422	$4mm$	$\bar{4}2m$ $\bar{4}m2$	$4/mmm$
	$h+k$	k			k		$Pnb-$							$P4/nbm$ (125)
	$h+k$	k	l	l	k		$Pnbc$							$P4_2/nbc$ (133)
	$h+k$	l		l	k		$Pnc-$							$P4_2/ncm$ (138)
	$h+k$	l	l	l	k		$Pncc$							$P4/ncc$ (130)
	$h+k$	$k+l$		l	k		$Pnn-$							$P4_2/nnm$ (134)
	$h+k$	$k+l$	l	l	k		$Pnnc$							$P4/nnc$ (126)
$h+k+l$	$h+k$	$k+l$	l	l	k		$I---$	$I4$ (79)	$I\bar{4}$ (82)	$I4/m$ (87)	$I422$ (97)	$I4mm$ (107)	$I\bar{4}2m$ (121) $I\bar{4}m2$ (119)	$I4/mmm$ (139)
$h+k+l$	$h+k$	$k+l$	l	$l=4n$	k		$I4_1--$	$I4_1$ (80)			$I4_122$ (98)			
$h+k+l$	$h+k$	$k+l$	‡	$l=4n$	k	h	$I--d$					$I4_1md$ (109)	$I\bar{4}2d$ (122)	
$h+k+l$	$h+k$	k, l	l	l	k		$I-c-$					$I4cm$ (108)	$I\bar{4}c2$ (120)	$I4/mcm$ (140)
$h+k+l$	$h+k$	k, l	‡	$l=4n$	k	h	$I-cd$					$I4_1cd$ (110)		
$h+k+l$	h, k	$k+l$	l	$l=4n$	k		$I4_1/a--$			$I4_1/a$ (88)				
$h+k+l$	h, k	$k+l$	‡	$l=4n$	k	h	$Ia-d$							$I4_1/amd$ (141)
$h+k+l$	h, k	k, l	‡	$l=4n$	k	h	$Iacd$							$I4_1/acd$ (142)

† Pair of enantiomorphic space groups, *cf.* Section 3.1.5.
‡ Condition: $2h+l=4n$; l.

(as well as for the R space groups of the trigonal system), the different cell choices and settings of one space group are disregarded, 101 extinction symbols* and 122 diffraction symbols for the 230 space-group types result.

Only in 50 cases does a diffraction symbol uniquely identify just one space group, thus leaving 72 diffraction symbols that correspond to more than one space group. The 50 unique cases can be easily recognized in Table 3.1.4.1 because the line for the possible space groups in the particular Laue class contains just one entry.

The non-uniqueness of the space-group determination has two reasons:

(i) Friedel's rule, *i.e.* the effect that, with neglect of anomalous dispersion, the diffraction pattern contains an inversion centre, even if such a centre is not present in the crystal.

Example

A monoclinic crystal (with unique axis b) has the diffraction symbol $1\,2/m\,1P1c1$. Possible space groups are $P1c1$ (7) without an inversion centre, and $P12/c1$ (13) with an inversion centre. In both cases, the diffraction pattern has the Laue symmetry $1\,2/m\,1$.

One aspect of Friedel's rule is that the diffraction patterns are the same for two enantiomorphic space groups. Eleven diffraction symbols each correspond to a pair of enantiomorphic space groups. In Table 3.1.4.1, such pairs are grouped between braces. Either of the two space groups may be chosen for structure solution. If due to anomalous scattering Friedel's rule does not hold, at the refinement stage of structure determination it may be possible to determine the absolute structure and consequently the correct space group from the enantiomorphic pair.

(ii) The occurrence of four space groups in two 'special' pairs, each pair belonging to the same point group: $I222$ (23) & $I2_12_12_1$ (24) and $I23$ (197) & $I2_13$ (199). The two space groups of each pair differ in the location of the symmetry elements with respect to each other. In Table 3.1.4.1, these two special pairs are given in square brackets.

3.1.6. Space-group determination by additional methods

3.1.6.1. *Chemical information*

In some cases, chemical information determines whether or not the space group is centrosymmetric. For instance, all proteins crystallize in noncentrosymmetric space groups as they are constituted of L-amino acids only. Less certain indications may be obtained by considering the number of molecules per cell and the possible space-group symmetry. For instance, if experiment shows that there are two molecules of formula $A_\alpha B_\beta$ per cell in either space group $P2_1$ or $P2_1/m$ and if the molecule $A_\alpha B_\beta$ cannot possibly have either a mirror plane or an inversion centre, then there is a strong indication that the correct space group is $P2_1$. Crystallization of $A_\alpha B_\beta$ in $P2_1/m$ with random disorder of the molecules cannot be excluded, however. In a similar way, multiplicities of Wyckoff positions and the number of formula units per cell may be used to distinguish between space groups.

* The increase from 97 (*IT*, 1952) to 101 extinction symbols is due to the separate treatment of the trigonal and hexagonal crystal systems in Table 3.1.4.1, in contradistinction to *IT* (1952), Table 4.4.3, where they were treated together. In *IT* (1969), diffraction symbols were listed by Laue classes and thus the number of extinction symbols is the same as that of diffraction symbols, namely 122.

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

TRIGONAL, Laue classes $\bar{3}$ and $\bar{3}m$

Reflection conditions				Extinction symbol	Laue class							
					$\bar{3}$		$\bar{3}m1$ ($\bar{3}$ $2/m$ 1) $\bar{3}m$			$\bar{3}1m$ ($\bar{3}$ 1 $2/m$)		
Hexagonal axes					Point group							
$hkil$	$h\bar{h}0l$	$hh\overline{2h}l$	$000l$		3	$\bar{3}$	321 32	$3m1$ $3m$	$\bar{3}m1$ $\bar{3}m$	312	$31m$	$\bar{3}1m$
				$P---$	$P3$ (143)	$P\bar{3}$ (147)	$P321$ (150)	$P3m1$ (156)	$P\bar{3}m1$ (164)	$P312$ (149)	$P31m$ (157)	$P\bar{3}1m$ (162)
			$l=3n$	$P3_1--$	$\left\{\begin{matrix} P3_1(144) \\ P3_2(145) \end{matrix}\right\}$§		$\left\{\begin{matrix} P3_121\ (152) \\ P3_221\ (154) \end{matrix}\right\}$§			$\left\{\begin{matrix} P3_112\ (151) \\ P3_212\ (153) \end{matrix}\right\}$§		
		l	l	$P--c$							$P31c$ (159)	$P\bar{3}1c$ (163)
	l		l	$P-c-$				$P3cl$ (158)	$P\bar{3}c1$ (165)			
$-h+k+l=3n$	$h+l=3n$	$l=3n$	$l=3n$	R(obv)$--$ ¶	$R3$ (146)	$R\bar{3}$ (148)	$R32$ (155)	$R3m$ (160)	$R\bar{3}m$ (166)			
$-h+k+l=3n$	$h+l=3n$; l	$l=3n$	$l=6n$	R(obv)$-$ c				$R3c$ (161)	$R\bar{3}c$ (167)			
$h-k+l=3n$	$-h+l=3n$	$l=3n$	$l=3n$	R(rev)$--$	$R3$ (146)	$R\bar{3}$ (148)	$R32$ (155)	$R3m$ (160)	$R\bar{3}m$ (166)			
$h-k+l=3n$	$-h+l=3n$; l	$l=3n$	$l=6n$	R(rev)$-$ c				$R3c$ (161)	$R\bar{3}c$ (167)			
Rhombohedral axes				Extinction symbol	Point group							
hkl		hhl	hhh		3	$\bar{3}$	32	$3m$	$\bar{3}m$			
				$R--$	$R3$(146)	$R\bar{3}$ (148)	$R32$ (155)	$R3m$ (160)	$R\bar{3}m$ (166)			
		l	h	$R-c$				$R3c$ (161)	$R\bar{3}c$ (167)			

§ Pair of enantiomorphic space groups; *cf.* Section 3.1.5.
¶ For obverse and reverse settings *cf.* Section 1.2.1. The obverse setting is standard in these tables.
The transformation reverse → obverse is given by **a**(obv.) = −**a**(rev.), **b**(obv.) = −**b**(rev.), **c**(obv.) = **c**(rev.).

HEXAGONAL, Laue classes $6/m$ and $6/mmm$

Reflection conditions			Extinction symbol	Laue class						
				$6/m$			$6/mmm$ ($6/m$ $2/m$ $2/m$)			
				Point group						
$h\bar{h}0l$	$hh\overline{2h}l$	$000l$		6	$\bar{6}$	$6/m$	622	$6mm$	$\bar{6}2m$ $\bar{6}m2$	$6/mmm$
			$P---$	$P6$ (168)	$P\bar{6}$ (174)	$P6/m$ (175)	$P622$ (177)	$P6mm$ (183)	$P\bar{6}2m$ (189) $P\bar{6}m2$ (187)	$P6/mmm$ (191)
		l	$P6_3--$	$P6_3$ (173)		$P6_3/m$ (176)	$P6_322$ (182)			
		$l=3n$	$P6_2--$	$\left\{\begin{matrix} P6_2\ (171) \\ P6_4\ (172) \end{matrix}\right\}$**			$\left\{\begin{matrix} P6_222\ (180) \\ P6_422\ (181) \end{matrix}\right\}$**			
		$l=6n$	$P6_1--$	$\left\{\begin{matrix} P6_1\ (169) \\ P6_3\ (170) \end{matrix}\right\}$**			$\left\{\begin{matrix} P6_122\ (178) \\ P6_522\ (179) \end{matrix}\right\}$**			
	l	l	$P--c$					$P6_3mc$ (186)	$P\bar{6}2c$ (190)	$P6_3/mmc$ (194)
l		l	$P-c-$					$P6_3cm$ (185)	$P\bar{6}c2$ (188)	$P6_3/mcm$ (193)
l	l	l	$P-cc$					$P6cc$ (184)		$P6/mcc$ (192)

** Pair of enantiomorphic space groups, *cf.* Section 3.1.5.

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

CUBIC, Laue classes $m\bar{3}$ and $m\bar{3}m$

Reflection conditions (Indices are permutable, apart from space group No. 205) ††				Extinction symbol	Laue class				
					$m\bar{3}$ $(2/m\ \bar{3})$		$m\bar{3}m$ $(4/m\ \bar{3}\ 2/m)$		
					Point group				
hkl	$0kl$	hhl	$00l$		23	$m\bar{3}$	432	$\bar{4}3m$	$m\bar{3}m$
				$P---$	$P23$ (195)	$Pm\bar{3}$ (200)	$P432$ (207)	$P\bar{4}3m$ (215)	$Pm\bar{3}m$ (221)
			l	$\begin{cases} P2_1-- \\ P4_2-- \end{cases}$	$P2_13$ (198)		$P4_232$ (208)		
			$l=4n$	$P4_1--$			$\left.\begin{cases} P4_132\ (213) \\ P4_332\ (212) \end{cases}\right\}$ ‡‡		
		l	l	$P--n$				$P\bar{4}3n$ (218)	$Pm\bar{3}n$ (223)
	k††		l	$Pa--$		$Pa\bar{3}$ (205)			
	$k+l$		l	$Pn--$		$Pn\bar{3}$ (201)			$Pn\bar{3}m$ (224)
	$k+l$	l	l	$Pn-n$					$Pn\bar{3}n$ (222)
$h+k+l$	$k+l$	l	l	$I---$	$\begin{bmatrix} I23\ (197) \\ I2_13\ (199) \end{bmatrix}$ §§	$Im\bar{3}$ (204)	$I432$ (211)	$I\bar{4}3m$ (217)	$Im\bar{3}m$ (229)
$h+k+l$	$k+l$	l	$l=4n$	$I4_1--$			$I4_132$ (214)		
$h+k+l$	$k+l$	$2h+l=4n, l$	$l=4n$	$I--d$				$I\bar{4}3d$ (220)	
$h+k+l$	k, l	l	l	$Ia--$		$Ia\bar{3}$ (206)			
$h+k+l$	k, l	$2h+l=4n, l$	$l=4n$	$Ia-d$					$Ia\bar{3}d$ (230)
$h+k, h+l, k+l$	k, l	$h+l$	l	$F---$	$F23$ (196)	$Fm\bar{3}$ (202)	$F432$ (209)	$F\bar{4}3m$ (216)	$Fm\bar{3}m$ (225)
$h+k, h+l, k+l$	k, l	$h+l$	$l=4n$	$F4_1--$			$F4_132$ (210)		
$h+k, h+l, k+l$	k, l	h, l	l	$F--c$				$F\bar{4}3c$ (219)	$Fm\bar{3}c$ (226)
$h+k, h+l, k+l$	$k+l=4n, k, l$	$h+l$	$l=4n$	$Fd--$		$Fd\bar{3}$ (203)			$Fd\bar{3}m$ (227)
$h+k, h+l, k+l$	$k+l=4n, k, l$	h, l	$l=4n$	$Fd-c$					$Fd\bar{3}c$ (228)

†† For No. 205, only cyclic permutations are permitted. Conditions are $0kl$: $k=2n$; $h0l$: $l=2n$; $hk0$: $h=2n$.
‡‡ Pair of enantiomorphic space groups, *cf.* Section 3.1.5.
§§ Pair of space groups with common point group and symmetry elements but differing in the relative location of these elements.

3.1.6.2. *Point-group determination by methods other than the use of X-ray diffraction*

This is discussed in Chapter 10.2. In favourable cases, suitably chosen methods can prove the absence of an inversion centre or a mirror plane.

3.1.6.3. *Study of X-ray intensity distributions*

X-ray data can give a strong clue to the presence or absence of an inversion centre if not only the symmetry of the diffraction pattern but also the distribution of the intensities of the reflection spots is taken into account. Methods have been developed by Wilson and others that involve a statistical examination of certain groups of reflections. For a textbook description, see Lipson & Cochran (1966) and Wilson (1970). In this way, the presence of an inversion centre in a three-dimensional structure or in certain projections can be tested. Usually it is difficult, however, to obtain reliable conclusions from projection data. The same applies to crystals possessing pseudo-symmetry, such as a centrosymmetric arrangement of heavy atoms in a noncentrosymmetric structure. Several computer programs performing the statistical analysis of the diffraction intensities are available.

3.1.6.4. *Consideration of maxima in Patterson syntheses*

The application of Patterson syntheses for space-group determination is described by Buerger (1950, 1959).

3.1.6.5. *Anomalous dispersion*

Friedel's rule, $|F(hkl)|^2 = |F(\bar{h}\bar{k}\bar{l})|^2$, does not hold for noncentrosymmetric crystals containing atoms showing anomalous dispersion. The difference between these intensities becomes particularly strong when use is made of a wavelength near the resonance level (absorption edge) of a particular atom in the crystal. Synchrotron radiation, from which a wide variety of wavelengths can be chosen, may be used for this purpose. In such cases, the diffraction pattern reveals the symmetry of the actual point group of the crystal (including the orientation of the point group with respect to the lattice).

3.1.6.6. *Summary*

One or more of the methods discussed above may reveal whether or not the point group of the crystal has an inversion centre. With this information, in addition to the diffraction symbol, 192 space groups can be uniquely identified. The rest consist of the eleven pairs of enantiomorphic space groups, the two 'special pairs' and six further ambiguities: 3 in the orthorhombic system (Nos. 26 & 28, 35 & 38, 36 & 40), 2 in the tetragonal system (Nos. 111 & 115, 119 & 121), and 1 in the hexagonal system (Nos. 187 & 189). If not only the point group but also its orientation with respect to the lattice can be determined, the six ambiguities can be resolved. This implies that 204 space groups can be uniquely identified, the only exceptions being the eleven pairs of enantiomorphic space groups and the two 'special pairs'.

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4.1. Introduction to the synoptic tables

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4.1.1. Introduction

The synoptic tables of this section comprise two features:

(i) Space-group symbols for various settings and choices of the unit cell. Changes of the basis vectors generally cause changes of the Hermann–Mauguin space-group symbol. These axis transformations involve not only permutations of axes, conserving the shape of the cell, but also transformations which lead to different cell shapes and even to multiple cells.

(ii) Extended Hermann–Mauguin space-group symbols, in addition to the short and full symbols. The occurrence of 'additional symmetry elements' (see below) led to the introduction of 'extended space-group symbols' in *IT* (1952); they are systematically developed in the present section. These additional symmetry elements are displayed in the space-group diagrams and are important for the tabulated '*Symmetry operations*'.

For each crystal system, the text starts with a historical note on the synoptic tables in the earlier editions of *International Tables** followed by a discussion of points (i) and (ii) above. Finally, those group–subgroup relations (*cf.* Section 8.3.3) are treated that can be recognized from the full and the extended Hermann–Mauguin space-group symbols. This applies mainly to the *translationengleiche* or *t* subgroups (type **I**, *cf.* Section 2.2.15) and to the *klassengleiche* or *k* subgroups of type **IIa**. For the *k* subgroups of types **IIb** and **IIc**, inspection of the synoptic Table 4.3.2.1 provides easy recognition of only those subgroups which originate from the decentring of certain multiple cells: *C* or *F* in the tetragonal system (Section 4.3.4), *R* and *H* in the trigonal and hexagonal systems (Section 4.3.5).

4.1.2. Additional symmetry elements

In space groups, 'due to periodicity', symmetry elements occur that are not recorded in the Hermann–Mauguin symbols. These *additional symmetry elements* are products of a symmetry translation T and a symmetry operation W. This product is TW and its geometrical representation is found in the space-group diagrams (*cf.* Sections 8.1.2 and 11.1.1).†

Two cases have to be distinguished:

(i) *Symmetry operations of the same nature*

The symmetry operations W and TW are of the *same nature* and only the locations of their symmetry elements differ. This occurs when the translation vector **t** is *perpendicular* to the symmetry element of W (symmetry plane or symmetry axis); it also holds when W is an *inversion* or a *rotoinversion* (see below).

Table 4.1.2.1 summarizes the symmetry elements, located at the origin, and the location of those 'additional symmetry elements' which are generated by periodicity in the *interior* of the unit cell. 'Additional' axes $\bar{3}$, 6, 6_1, 6_2, 6_3, 6_4, 6_5 do not occur. The first column of Table 4.1.2.1 specifies W, the second column the translation vector **t**, the third the location of the symmetry element of TW. The last column indicates space groups and plane groups with representative diagrams. Other orientations of the symmetry axes and symmetry planes can easily be derived from the table.

Example

Let W be a threefold rotation with Seitz symbol $(3/0,0,0)$ and axis along 0, 0, *z*. The product with the translation $\mathsf{T}(1,0,0)$, perpendicular to the axis, is $(3/1,0,0)$ and again is a threefold rotation, for $(3/1,0,0)^3 = (1/0,0,0)$; its location is $\frac{2}{3}, \frac{1}{3}, z$.

Table 4.1.2.1 also deals with certain powers W^p of symmetry operations W, namely with $p = 2$ for operations of order four and with $p = 2, 3, 4$ for operations of order six. These powers give rise to their own 'additional symmetry elements', as illustrated by the following list and by the example below (operations of order 2 or 3 obviously do not have to be considered).

W	4, 4_2	4_1, 4_3	$\bar{4}$	6	$\bar{6}$	$\bar{3}$	6_1	6_5	6_3	6_2	6_4
W^p	2	2_1	2	3, 2	3, *m*	3, $\bar{1}$	3_1, 2_1	3_2, 2_1	3, 2_1	3_2, 2	3_1, 2

Example

6_2 in 0, 0, *z*; the powers to be considered are

$$(6_2)^2 = 3_2; \quad (6_2)^3 = 2; \quad (6_2)^4 = (3_2)^2.$$

The axes 3_2 and 2 at 0, 0, *z* create additional symmetry elements:

$$3_2 \text{ at } \tfrac{1}{3},\tfrac{2}{3},z;\ \tfrac{2}{3},\tfrac{1}{3},z \quad \text{and} \quad 2 \text{ at } \tfrac{1}{2},0,z;\ 0,\tfrac{1}{2},z;\ \tfrac{1}{2},\tfrac{1}{2},z.$$

If W is an inversion operation with its centre of symmetry at point *M*, the operation TW creates an additional centre at the endpoint of the translation vector $\frac{1}{2}\mathbf{t}$, drawn from *M* (*cf.* Table 4.1.2.1, where *M* is in 0, 0, 0).

(ii) *Symmetry operations of different nature*

The symmetry operations W and TW are of a *different nature* and have different symbols, corresponding to rotation and screw axes, to mirror and glide planes, to screw axes of different nature, and to glide planes of different nature, respectively.‡

In this case, the translation vector **t** has a component *parallel* to the symmetry axis or symmetry plane of W. This parallel component determines the nature and the symbol of the additional symmetry element, whereas the normal component of **t** is responsible for its location, as explained in Section 11.1.1. If the normal component is zero, symmetry element and additional symmetry element coincide geometrically. Note that such additional symmetry elements with glide or screw components exist even in symmorphic space groups.

Integral and centring translations: In primitive lattices, only integral translations occur and Tables 4.1.2.1 and 4.1.2.2 are relevant. For centred lattices, Tables 4.1.2.1 and 4.1.2.2 remain valid for the integral translations, whereas Table 4.1.2.3 has to be considered for the centring translations, which cause further 'additional symmetry elements'.

4.1.2.1. *Integral translations*

Table 4.1.2.2 lists representative symmetry elements, corresponding to W, and their associated glide planes and screw axes, corresponding to TW. The upper part of the table contains the diagonal twofold axes and symmetry planes that appear as tertiary symmetry elements in tetragonal and cubic space groups and as

* *Comparison tables*, pp. 28–44, *IT* (1935); *Index of symbols of space groups,* pp. 542–553, *IT* (1952).

† W is represented by $(\boldsymbol{W}, \boldsymbol{w})$ where $\boldsymbol{W}$ is the matrix part, $\boldsymbol{w}$ the column part, referred to a conventional coordinate system. T is represented by $(\boldsymbol{I}, \boldsymbol{t})$ and TW by $(\boldsymbol{W}, \boldsymbol{w}+\boldsymbol{t})$.

‡ The location and nature (screw axis, glide plane) of these additional symmetry elements were listed in the space-group tables of *IT* (1935) under the heading *Weitere Symmetrieelemente*, but were suppressed in *IT* (1952).

Table 4.1.2.1. *Location of additional symmetry element, if the translation vector* **t** *is perpendicular to the symmetry axis along* $0, 0, z$ *or to the symmetry plane in* $x, y, 0$

The symmetry centre at $0,0,0$ is included. The table is restricted to integral translations (for centring translations, see Table 4.1.2.3). The symbol $\circlearrowleft$ indicates cyclic permutation.

Symmetry element at the origin	Translation vector **t**	Location of additional symmetry element	Representative plane and space groups (numbers)
$2, 2_1$	$1,0,0$ $0,1,0$ $1,1,0$	$\frac{1}{2},0,z$ $0,\frac{1}{2},z$ $\frac{1}{2},\frac{1}{2},z$	$P2$ (3), $P2_1$ (4), $p2$ (2)
$3, 3_1, 3_2$	$1,0,0$ $1,1,0$	$\frac{2}{3},\frac{1}{3},z$ $\frac{1}{3},\frac{2}{3},z$	$P3$ (143)–$P3_2$ (145), $p3$ (13)
$4, 4_1, 4_2, 4_3$	$1,0,0$	$\frac{1}{2},\frac{1}{2},z$	$P4$ (75)–$P4_3$ (78), $p4$(10)
$6, 6_1, 6_2, 6_3, 6_4, 6_5$	–	–	$P6$ (168)–$P6_5$ (173), $p6$ (16)
m, a, b, n, d, e	$0,0,1$	$x, y, \frac{1}{2}$	Pm (6), Pa, Pb, Pn (7), $Fddd$ (70), $Cmme$ (67)
$\bar{1}$	$1,0,0$ $\circlearrowleft$ $1,1,0$ $\circlearrowleft$ $1,1,1$	$\frac{1}{2},0,0$ $\circlearrowleft$ $\frac{1}{2},\frac{1}{2},0$ $\circlearrowleft$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$P\bar{1}$ (2)
$\bar{3}$	–	–	$P\bar{3}$ (147)
$\bar{4}$	$0,1,0$	$\frac{1}{2},\frac{1}{2},z$	$P\bar{4}$ (81)
$\bar{6}$	$0,1,0$ $1,1,0$	$\frac{1}{3},\frac{2}{3},z$ $\frac{2}{3},\frac{1}{3},z$	$P\bar{6}$ (174)

secondary symmetry elements in rhombohedral space groups (referred to rhombohedral axes). The middle part lists the twofold axes and symmetry planes that are secondary and tertiary symmetry elements in trigonal and hexagonal space groups and secondary symmetry elements in rhombohedral space groups (referred to hexagonal axes). The lower part illustrates the occurrence of threefold screw axes in rhombohedral and cubic space groups for the orientation [111].

Note that integral translations do not produce additional glide or screw components in triclinic, monoclinic and orthorhombic groups.

Example

The operation $(3/1,0,0)$ in a rhombohedral or cubic space group represents a screw rotation 3_1 with axis along [111]. Indeed, the third power of $(3/1,0,0)$ is the translation $t(1,1,1)$, *i.e.* the periodicity along the threefold axis. The translation $t(1, 0, 0)$ is decomposed uniquely into the screw component $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ parallel to and the location component $\frac{2}{3}, -\frac{1}{3}, -\frac{1}{3}$ perpendicular to the threefold axis. The location of the 3_1 axis is then found to be $x, x+\frac{2}{3}, x+\frac{1}{3}$, which can also be expressed as $x+\frac{1}{3}, x, x+\frac{2}{3}$ or $x+\frac{2}{3}, x+\frac{1}{3}, x$.

For 2, m and c, the locations of the symmetry elements at the origin and within the cell can be interchanged.

Example

According to Table 4.1.2.2, the c plane located in x, x, z implies an n plane in $x, x+\frac{1}{2}, z$. *Vice versa*, an n plane in x, x, z implies a c plane in $x, x+\frac{1}{2}, z$.

In the rhombohedral space groups $R3c$ (161) and $R\bar{3}c$ (167) and in their cubic supergroups, diagonal n planes in x, x, z and, by symmetry, in z, x, x and x, z, x coexist with c planes in $x, x+\frac{1}{2}, z$, a planes in $z, x, x+\frac{1}{2}$ and b planes in $x+\frac{1}{2}, z, x$, respectively (*cf.* Section 4.3.5).

Note that *the symbol of a glide plane depends on the reference frame.* Thus, the above-mentioned n planes in the rhombohedral description become c planes in the hexagonal description of $R3c$ and $R\bar{3}c$; similarly, the *a, b* and c planes become n planes; *cf.* Sections 1.3.1 and 1.4.4.

4.1.2.2. *Centring translations**

The general rules given under (i) and (ii) remain valid. In lattices C, A, B, I and F, a centring vector **t** with a component parallel to the symmetry element leads to an additional symmetry element of a different kind. When the centring vector **t** is perpendicular to the symmetry element or when the symmetry element is an inversion centre or a rotoinversion axis, the additional symmetry element is of the same kind.

The first part of Table 4.1.2.3 contains pairs of *symmetry planes* related by a centring translation. Each box has three or four entries, which define three or four pairs of 'associated' planes; the cell under F contains all the planes under C, A and B. Hence, their locations are not repeated under F. Again, the locations of the two planes can be interchanged.

Example

The product of the C-centring translation, *i.e.* $t(\frac{1}{2}, \frac{1}{2}, 0)$, and the reflection through a mirror plane m, located in $0, y, z$, is a glide reflection b with glide plane in $\frac{1}{4}, y, z$. Similarly, C centring associates a glide plane c in $0, y, z$ with a glide plane n in $\frac{1}{4}, y, z$.

Note that the mirror plane and 'associated' glide plane coincide geometrically when the centring translation is parallel to the mirror (*i.e.* no normal component exists); see the first cell under A, the second under B, the third cell under C. Also, two 'associated' glide planes (a, b) or (b, c) or (a, c) coincide geometrically. These 'double' glide planes are symbolized by 'e'; see Table 4.1.2.3 and Section 1.3.2, Note (x).

* For the 'R centring' see Section 4.3.5.

Table 4.1.2.2. *Additional symmetry elements and their locations, if the translation vector* **t** *is inclined to the symmetry axis or symmetry plane*

The table is restricted to integral translations and thus is valid for *P* lattices and for integral translations in centred lattices (for centring translations see Table 4.1.2.3).

Symmetry element at the origin			Additional symmetry element			Representative plane and space groups (numbers)
Symbol	Location	Translation vector **t**	Symbol	Screw or glide component	Location	
Tetragonal, rhombohedral and cubic coordinate systems						
2	$x, x, 0$	1, 0, 0 0, 1, 0	2_1	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$x, x+\frac{1}{2}, 0$	*P*422 (89) *R*32 (155) *P*432 (207)
m	x, x, z	1, 0, 0 0, 1, 0	*g*	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$x, x+\frac{1}{2}, z$	*p*4*mm* (11) *P*4*mm* (99) *R*3*m* (160) $P\bar{4}3m$ (215)
c	x, x, z	1, 0, 0 0, 1, 0	*n*	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$x, x+\frac{1}{2}, z$	$P\bar{4}2c$ (112) *R*3*c* (161) $P\bar{4}3n$ (218)
Hexagonal coordinate system						
2	$x, 0, 0$	1, 1, 0 0, 1, 0	2_1	$\frac{1}{2}, 0, 0$ $-\frac{1}{2}, 0, 0$	$x, \frac{1}{2}, 0$	*P*321 (150) *R*32 (155)
2	$x, 2x, 0$	0, 1, 0 1, 1, 0	2_1	$\frac{1}{2}, 1, 0$	$x, 2x+\frac{1}{2}, 0$	*P*312 (149) *P*622 (177)
m	$x, 2x, z$	0, 1, 0 1, 1, 0	*b*	$\frac{1}{2}, 1, 0$	$x, 2x+\frac{1}{2}, z$	*P*3*m*1 (156) *p*3*m*1 (14) *R*3*m* (160)
c	$x, 2x, z$	0, 1, 0 1, 1, 0	*n*	$\frac{1}{2}, 1, \frac{1}{2}$	$x, 2x+\frac{1}{2}, z$	*P*3*c*1 (158) $P\bar{6}c2$ (188) *R*3*c* (161)
m	$x, 0, z$	1, 1, 0 0, 1, 0	*a*	$\frac{1}{2}, 0, 0$ $-\frac{1}{2}, 0, 0$	$x, \frac{1}{2}, z$	*P*31*m* (157) *p*31*m* (15)
c	$x, 0, z$	1, 1, 0 0, 1, 0	*n*	$\frac{1}{2}, 0, \frac{1}{2}$ $-\frac{1}{2}, 0, \frac{1}{2}$	$x, \frac{1}{2}, z$	*P*31*c* (159) $P\bar{6}2c$ (190)
Rhombohedral and cubic coordinate systems						
3	x, x, x	1, 0, 0 0, 1, 0 0, 0, 1	3_1	$\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$	$x, x+\frac{2}{3}, x+\frac{1}{3}$	*R*3 (146) *P*23 (195)
3	x, x, x	2, 0, 0 0, 2, 0 0, 0, 2	3_2	$\frac{2}{3}, \frac{2}{3}, \frac{2}{3}$	$x, x+\frac{1}{3}, x+\frac{2}{3}$	

Glide reflections whose square is a pure centring translation are called *d*; other diagonal glide planes are called *g* and *n*; in each case, the glide component is given between parentheses (*cf.* Sections 2.2.9 and 11.1.2).

The second part of Table 4.1.2.3 summarizes pairs of *symmetry axes* and, in the bottom line, pairs of *symmetry centres* related by a centring translation. For instance, the *B*-centring translation $t(\frac{1}{2}, 0, \frac{1}{2})$ associates a rotation axis 2 along *x*, 0, 0 with a screw axis 2_1 along $x, 0, \frac{1}{4}$. Here, too, the locations can be interchanged.

Example

The product of the translation $t(0, \frac{1}{2}, \frac{1}{2})$ with a twofold rotation around *x*, *x*, 0 is the operation $(2/0, \frac{1}{2}, \frac{1}{2})$, which occurs, for instance, in *F*432 (209). The square of this operation is the fractional translation $t(\frac{1}{2}, \frac{1}{2}, 0)$. The translation $t(0, \frac{1}{2}, \frac{1}{2})$ is decomposed into a 'screw part' $\frac{1}{4}, \frac{1}{4}, 0$ and a 'location part' $-\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ perpendicular to it. The location of the additional symmetry element 2_1 is then found to be $x, x+\frac{1}{4}, \frac{1}{4}$ which is parallel to that of the axis 2 in *x*, *x*, 0.

Table 4.1.2.3. *Additional symmetry elements due to a centring vector* **t** *and their locations*

Symmetry element at the origin		Additional symmetry elements									Representative space groups (numbers)
		$C, t(\frac{1}{2}, \frac{1}{2}, 0)$		$A, t(0, \frac{1}{2}, \frac{1}{2})$		$B, t(\frac{1}{2}, 0, \frac{1}{2})$		$I, t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$		F	
Symbol	Location	Symbol	Location	Symbol	Location	Symbol	Location	Symbol	Location	Symbol	
m	$0, y, z$	b	$\frac{1}{4}, y, z$	n	$0, y, z$	c	$\frac{1}{4}, y, z$	n	$\frac{1}{4}, y, z$	b, n, c, e	*Cmmm*, *Ammm*, *Bmmm* (65)
c		n		b		m		b			*Immm* (71), *Fmmm* (69)
b		m		c		n		c			*Cccm*, *Amaa*, *Bbmb* (66) *Ibca* (73)
e				e							*Aem*2 (39)
$d(0, \frac{1}{4}, \frac{1}{4})$		$d(0, \frac{3}{4}, \frac{1}{4})$		$d(0, \frac{3}{4}, \frac{3}{4})$		$d(0, \frac{1}{4}, \frac{3}{4})$				d, d, d	*Fddd* (70)
m	$x, 0, z$	a	$x, \frac{1}{4}, z$	c	$x, \frac{1}{4}, z$	n	$x, 0, z$	n	$x, \frac{1}{4}, z$	a, c, n, e	As above
a		m		n		c		c			
c		n		m		a		a			
e						e					*Fmm*2 (42)
$d(\frac{1}{4}, 0, \frac{1}{4})$		$d(\frac{3}{4}, 0, \frac{1}{4})$		$d(\frac{1}{4}, 0, \frac{3}{4})$		$d(\frac{3}{4}, 0, \frac{3}{4})$				d, d, d	
m	$x, y, 0$	n	$x, y, 0$	b	$x, y, \frac{1}{4}$	a	$x, y, \frac{1}{4}$	n	$x, y, \frac{1}{4}$	n, b, a, e	As above
b		a		m		n		a			
a		b		n		m		b			
e		e									*Cmme* (67)
$d(\frac{1}{4}, \frac{1}{4}, 0)$		$d(\frac{3}{4}, \frac{3}{4}, 0)$		$d(\frac{1}{4}, \frac{3}{4}, 0)$		$d(\frac{3}{4}, \frac{1}{4}, 0)$				d, d, d	
m	x, x, z	$g(\frac{1}{2}, \frac{1}{2}, 0)$	x, x, z	$g(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$	$x, x+\frac{1}{4}, z$	$g(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$	$x, x-\frac{1}{4}, z$	$n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	x, x, z	g, g, g	*I*4*mm* (107), $F\bar{4}3m$ (216)
c		$n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$		$g(\frac{1}{4}, \frac{1}{4}, 0)$		$g(\frac{1}{4}, \frac{1}{4}, 0)$		$g(\frac{1}{2}, \frac{1}{2}, 0)$		n, g, g	$F\bar{4}3c$ (219)
e								e			*I*4*cm* (108)
$d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$								$d(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$			$I\bar{4}3d$ (220)
2	$x, 0, 0$	2_1	$x, \frac{1}{4}, 0$	2	$x, \frac{1}{4}, \frac{1}{4}$	2_1	$x, 0, \frac{1}{4}$	2_1	$x, \frac{1}{4}, \frac{1}{4}$	$2_1, 2, 2_1$	*C*222, *A*222, *B*222 (21)
2	$0, y, 0$	2_1	$\frac{1}{4}, y, 0$	2_1	$0, y, \frac{1}{4}$	2	$\frac{1}{4}, y, \frac{1}{4}$	2_1	$\frac{1}{4}, y, \frac{1}{4}$	$2_1, 2_1, 2$	*I*222 (23)
2	$0, 0, z$	2	$\frac{1}{4}, \frac{1}{4}, z$	2_1	$0, \frac{1}{4}, z$	2_1	$\frac{1}{4}, 0, z$	2_1	$\frac{1}{4}, \frac{1}{4}, z$	$2, 2_1, 2_1$	*F*222 (22)
2	$x, \bar{x}, 0$	2	$x, \bar{x}+\frac{1}{2}, 0$	$2_1(-\frac{1}{4}, \frac{1}{4}, 0)$	$x, \bar{x}+\frac{1}{4}, \frac{1}{4}$	$2_1(\frac{1}{4}, -\frac{1}{4}, 0)$	$x, \bar{x}+\frac{1}{4}, \frac{1}{4}$	2	$x, \bar{x}, \frac{1}{4}$	$2, 2_1, 2_1$	*C*422 (*P*422) (89), *I*422 (97)
4	$0, 0, z$	4	$0, \frac{1}{2}, z$	4_2	$-\frac{1}{4}, \frac{1}{4}, z$	4_2	$\frac{1}{4}, \frac{1}{4}, z$	4_2	$0, \frac{1}{2}, z$	$4, 4_2, 4_2$	*F*432 (209)
4_1	$0, 0, z$	4_1	$0, \frac{1}{2}, z$	4_3	$-\frac{1}{4}, \frac{1}{4}, z$	4_3	$\frac{1}{4}, \frac{1}{4}, z$	4_3	$0, \frac{1}{2}, z$	$4_1, 4_3, 4_3$	$F4_132$ (210)
$\bar{1}$	$0, 0, 0$	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\bar{1}$	$0, \frac{1}{4}, \frac{1}{4}$	$\bar{1}$	$\frac{1}{4}, 0, \frac{1}{4}$	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\bar{1}, \bar{1}, \bar{1}$	*Immm* (71), *Fmmm* (69)

Inversions. The 'midpoint rule' given under (i) for integral translations remains valid. When M occupies successively the eight positions of inversion centres in the primitive cell (*cf.* Table 4.1.2.1), each of the centrings C, A, B and I creates eight supplementary centres, whereas the F centring produces $3 \times 8 = 24$ supplementary centres, leading to a total of 32 inversion centres.

Example

For C centring, add $\frac{1}{4}, \frac{1}{4}, 0$ (*cf.* Table 4.1.2.3) to the eight locations of symmetry centres, given in Table 4.1.2.1, in order to obtain the eight additional symmetry centres $\frac{1}{4}, \frac{1}{4}, 0$; $\frac{3}{4}, \frac{1}{4}, 0$; $\frac{1}{4}, \frac{3}{4}, 0$; $\frac{3}{4}, \frac{3}{4}, 0$; $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$; $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$; $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$; $\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$.

Table 4.1.2.3 contains only representative cases. For 4 and 4_1 axes, only the standard orientation [001] is given. For diagonal twofold axes, only the orientation $[\bar{1}10]$ is considered. When the locations of *all* additional symmetry elements of a chosen species are desired, it is sufficient to insert the location of one of the elements into the coordinate triplets of the general position and to remove redundancies.

Example

Insert the location $x, x+\frac{2}{3}, x+\frac{1}{3}$ of a 3_1 axis (see Table 4.1.2.2) into the general position of a cubic space group to obtain four distinct locations of 3_1 axes in P groups and sixteen in F groups.

4.1.2.3. *The priority rule*

When more than one kind of symmetry element occurs for a given symmetry direction, the question of choice arises for defining the appropriate Hermann–Mauguin symbol. This choice is made in order of descending priority:

m, e, a, b, c, n, d; and rotation axes before screw axes.

This *priority rule* is explicitly stated in *IT* (1952), pages 55 and 543. It is applied to the space-group symbols in *IT* (1952) and the present edition. There are a few exceptions, however:

(i) For glide planes in *centred monoclinic* space groups, the priority rule is purposely not followed in this volume, in order to bring out the relations between the three 'cell choices' given for each setting (*cf.* Sections 2.2.16 and 4.3.2).

(ii) For *orthorhombic* space groups, the priority rule is applied only to the 'standard symbol'. The symbols for the other five settings are obtained from the standard symbol by the appropriate transformations, without invoking the priority rule again (*cf.* Table 4.3.2.1).

(iii) Space groups $I222$ (23) and $I2_12_12_1$ (24) are two distinct groups. Both contain parallel twofold rotation and screw axes and thus would receive the same symbol according to the priority rule. In $I222$, the three rotation axes and the three screw axes intersect, whereas in $I2_12_12_1$ neither the three rotation axes nor the three screw axes intersect (*cf.* Section 4.3.3).

(iv) For space group No. 73, the standard symbol *Ibca* was adopted, instead of *Ibaa* according to the rule, because *Ibca* displays the equivalence of the three symmetry directions clearly.

(v) The full symbols of space groups *Ibca* (73) and *Imma* (74) were written $I2/b\ 2/c\ 2/a$ and $I2/m\ 2/m\ 2/a$ in *IT* (1952), in application of the priority rule. In the present edition, these symbols are changed to $I2_1/b\,2_1/c\,2_1/a$ and $I2_1/m\,2_1/m\,2_1/a$, because both space groups contain $I2_12_12_1$ (and not $I222$) as subgroup.

(vi) In *tetragonal* space groups with both *a* and *b* glide planes parallel to [001], the preference was given to *b*, as in *P4bm* (100).

(vii) In *cubic* space groups where tertiary symmetry planes with glide components $\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$ and $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ coexist, the tertiary symmetry element was called *n* in *P* groups (instead of *a*, *b* or *c*) but *c* in *F* groups, because these symmetry elements intersect the origin.

(viii) Space groups $I23$ (197) and $I2_13$ (199) are two distinct space groups. For this pair, the same arguments apply as given above for $I222$ and $I2_12_12_1$.

4.2. Symbols for plane groups (two-dimensional space groups)

BY E. F. BERTAUT

4.2.1. Arrangement of the tables

Comparative tables for the 17 plane groups first appeared in *IT* (1952). The classification of plane groups is discussed in Chapter 2.1. Table 4.2.1.1 lists for each plane group its system, lattice symbol, point group and the plane-group number, followed by the short, full and extended Hermann–Mauguin symbols. Short symbols are included only where different from the full symbols. The next column contains the full symbol for another setting which corresponds to an interchange of the basis vectors **a** and **b**; it is only needed for the rectangular system. Multiple cells c and h for the square and the hexagonal system are introduced in the last column.

4.2.2. Additional symmetry elements and extended symbols

'Additional symmetry' elements are

(i) rotation points 2, 3 and 4, reproduced in the interior of the cell (*cf.* Table 4.1.2.1 and plane-group diagrams in Part 6);

(ii) glide lines g which alternate with mirror lines m.

In the extended plane-group symbols, only the additional glide lines g are listed: they are due either to c centring or to 'inclined' integral translations, as shown in Table 4.1.2.2.

4.2.3. Multiple cells

The c cell in the square system is defined as follows:

$$\mathbf{a}' = \mathbf{a} \mp \mathbf{b}; \quad \mathbf{b}' = \pm\mathbf{a} + \mathbf{b},$$

with 'centring points' at $0, 0; \frac{1}{2}, \frac{1}{2}$. It plays the same role as the three-dimensional C cell in the tetragonal system (*cf.* Section 4.3.4).

Likewise, the triple cell h in the hexagonal system is defined as follows:

$$\mathbf{a}' = \mathbf{a} - \mathbf{b}; \quad \mathbf{b}' = \mathbf{a} + 2\mathbf{b},$$

with 'centring points' at $0, 0; \frac{2}{3}, \frac{1}{3}; \frac{1}{3}, \frac{2}{3}$. It is the two-dimensional analogue of the three-dimensional H cell (*cf.* Chapter 1.2 and Section 4.3.5).

4.2.4. Group–subgroup relations

The following example illustrates the usefulness of multiple cells.

Example: $p3m1$ (14)

The symbol of this plane group, described by the triple cell h, is $h31m$, where the symmetry elements of the secondary and tertiary positions are interchanged. 'Decentring' the h cell gives rise to maximal non-isomorphic k subgroups $p31m$ of index [3], with lattice parameters $a\sqrt{3}, a\sqrt{3}$ (*cf.* Section 4.3.5).

Table 4.2.1.1. *Index of symbols for plane groups*

System and lattice symbol	Point group	No. of plane group	Hermann–Mauguin symbol: Short	Hermann–Mauguin symbol: Full	Hermann–Mauguin symbol: Extended	Full symbol for other setting	Multiple cell
Oblique	1	1		$p1$			
p	2	2		$p2$			
Rectangular p, c	m	3	pm	$p1m1$		$p11m$	
		4	pg	$p1g1$		$p11g$	
		5	cm	$c1m1$	$c1m1$ g	$c11m$	
	$2mm$	6		$p2mm$		$p2mm$	
		7		$p2mg$		$p2gm$	
		8		$p2gg$		$p2gg$	
		9		$c2mm$	$c2mm$ $g\ g$	$c2mm$	
Square	4	10		$p4$			$c4$
p	$4mm$	11		$p4mm$	$p4mm$ g		$c4mm$ g
		12		$p4gm$	$p4gm$ g		$c4mg$ g
Hexagonal	3	13		$p3$			$h3$
p	$3m$	14		$p3m1$	$p3m1$ g		$h31m$ g
		15		$p31m$	$p31m$ g		$h3m1$ g
	6	16		$p6$			$h6$
	$6mm$	17		$p6mm$	$p6mm$ $g\ g$		$h6mm$ $g\ g$

International Tables for Crystallography (2006). Vol. A, Chapter 4.3, pp. 62–76.

4.3. Symbols for space groups

BY E. F. BERTAUT

4.3.1. Triclinic system

There are only two triclinic space groups, $P1$ (1) and $P\bar{1}$ (2). $P1$ is quite outstanding because all its subgroups are also $P1$. They are listed in Table 13.2.2.1 for indices up to [7]. $P\bar{1}$ has subgroups $P\bar{1}$, isomorphic, and $P1$, non-isomorphic.

In the triclinic system, a primitive unit cell can always be selected. In some cases, however, it may be advantageous to select a larger cell, with A, B, C, I or F centring.

The two types of reduced bases (reduced cells) are discussed in Section 9.2.2.

4.3.2. Monoclinic system

4.3.2.1. *Historical note and arrangement of the tables*

In *IT* (1935) only the b axis was considered as the unique axis. In *IT* (1952) two choices were given: the c-axis setting was called the 'first setting' and the b-axis setting was designated the 'second setting'.

To avoid the presence of two standard space-group symbols side by side, in the present tables only *one standard short symbol* has been chosen, that conforming to the long-lasting tradition of the b-axis unique (*cf.* Sections 2.2.4 and 2.2.16). However, for reasons of rigour and completeness, in Table 4.3.2.1 the *full* symbols are given not only for the c-axis and the b-axis settings but also for the a-axis setting. Thus, Table 4.3.2.1 has six columns which in pairs refer to these three settings. In the headline, the unique axis of each setting is underlined.

Additional complications arise from the presence of fractional translations due to glide planes in the primitive cell [groups Pc (7), $P2/c$ (13), $P2_1/c$ (14)], due to centred cells [$C2$ (5), Cm (8), $C2/m$ (12)], or due to both [Cc (9), $C2/c$ (15)]. For these groups, three different choices of the two oblique axes are possible which are called 'cell choices' 1, 2 and 3 (see Section 2.2.16). If this is combined with the three choices of the unique axis, $3 \times 3 = 9$ symbols result. If we add the effect of the permutation of the two oblique axes (and simultaneously reversing the sense of the unique axis to keep the system right-handed, as in $\mathbf{abc}$ and $\mathbf{c\bar{b}a}$), we arrive at the $9 \times 2 = 18$ symbols listed in Table 4.3.2.1 for each of the eight space groups mentioned above.

The space-group symbols $P2$ (3), $P2_1$ (4), Pm (6), $P2/m$ (10) and $P2_1/m$ (11) do not depend on the cell choice: in these cases, one line of six space-group symbols is sufficient.

For space groups with centred lattices (A, B, C, I), extended symbols are given; the 'additional symmetry elements' (due to the centring) are printed in the half line below the space-group symbol.

The use of the present tabulation is illustrated by two examples, Pm, which does not depend on the cell choice, and $C2/c$, which does.

Examples

(1) Pm (6)

(i) *Unique axis b*

In the first column, headed by $\mathbf{a\underline{b}c}$, one finds the full symbol $P1m1$. Interchanging the labels of the oblique axes a and c does not change this symbol, which is found again in the second column headed by $\mathbf{c\underline{\bar{b}}a}$.

(ii) *Unique axis c*

In the third column, headed by $\mathbf{ab\underline{c}}$, one finds the symbol $P11m$. Again, this symbol is conserved in the interchange of the oblique axes a and b, as seen in the fourth column headed by $\mathbf{ba\underline{\bar{c}}}$.

The same applies to the setting with unique axis a, columns five and six.

(2) $C2/c$ (15)

The short symbol $C2/c$ is followed by three lines, corresponding to the cell choices 1, 2, 3. Each line contains six full space-group symbols.

(i) *Unique axis b*

The column headed by $\mathbf{a\underline{b}c}$ contains the three symbols $C\,1\,2/c\,1$, $A1\,2/n\,1$ and $I1\,2/a\,1$, equivalent to the short symbol $C2/c$ and corresponding to the cell choices 1, 2, 3. In the half line below each symbol, the additional symmetry elements are indicated (extended symbol). If the oblique axes a and c are interchanged, the column under $\mathbf{c\underline{\bar{b}}a}$ lists the symbols $A1\,2/a\,1$, $C1\,2/n\,1$ and $I1\,2/c\,1$ for the three cell choices.

(ii) *Unique axis c*

The column under $\mathbf{ab\underline{c}}$ contains the symbols $A112/a$, $B112/n$ and $I112/b$, corresponding to the cell choices 1, 2 and 3. If the oblique axes a and b are interchanged, the column under $\mathbf{ba\underline{\bar{c}}}$ applies.

Similar considerations apply to the a-axis setting.

4.3.2.2. *Transformation of space-group symbols*

How does a monoclinic space-group symbol transform for the various settings of the same unit cell? This can be easily recognized with the help of the headline of Table 4.3.2.1, completed to the following scheme:

$\mathbf{a\underline{b}c}$	$\mathbf{c\underline{\bar{b}}a}$	$\mathbf{cab}$	$\mathbf{ac\bar{b}}$	$\mathbf{bca}$	$\mathbf{\bar{b}ac}$	Unique axis b
$\mathbf{bca}$	$\mathbf{a\bar{c}b}$	$\mathbf{ab\underline{c}}$	$\mathbf{ba\underline{\bar{c}}}$	$\mathbf{cab}$	$\mathbf{\bar{c}ba}$	Unique axis c
$\mathbf{cab}$	$\mathbf{b\bar{a}c}$	$\mathbf{bca}$	$\mathbf{cb\bar{a}}$	$\mathbf{\underline{a}bc}$	$\mathbf{\underline{\bar{a}}cb}$	Unique axis a.

The use of this three-line scheme is illustrated by the following examples.

Examples

(1) $C2/c$ (15, unique axis b, cell choice 1)

Extended symbol: $C1\,2/c\,1$.
$2_1/n$

Consider the setting $\mathbf{cab}$, first line, third column. Compared to the initial setting $\mathbf{a\underline{b}c}$, it contains the 'unique axis b' in the third place and, consequently, must be identified with the setting $\mathbf{ab\underline{c}}$, unique axis c, in the third column, for which in Table 4.3.2.1 the new symbol for cell choice 1 is listed as $A11\,2/a$
$2_1/n$.

(2) $C2/c$ (15, unique axis b, cell choice 3)

Extended symbol: $I1\,2/a\;\;1$.
$2_1/c$

Consider the setting $\mathbf{\bar{b}ac}$ in the first line, sixth column. It contains the 'unique axis b' in the first place and thus must be identified with the setting $\mathbf{\underline{\bar{a}}cb}$, unique axis a, in the sixth column. From Table 4.3.2.1, the appropriate space-group symbol for cell choice 3 is found as $I\,2/b\,11$.
$2_1/c$

4.3.2.3. *Group–subgroup relations*

It is easy to read all monoclinic maximal t and k subgroups of types **I** and **IIa** directly from the extended full symbols of a space group. Maximal subgroups of types **IIb** and **IIc** cannot be recognized by simple inspection of the synoptic Table 4.3.2.1

Table 4.3.2.1. *Index of symbols for space groups for various settings and cells*

TRICLINIC SYSTEM

No. of space group	Schoenflies symbol	Hermann–Mauguin symbol for all settings of the same unit cell
1	C_1^1	$P1$
2	C_i^1	$P\bar{1}$

MONOCLINIC SYSTEM

No. of space group	Schoenflies symbol	Standard short Hermann–Mauguin symbol	Extended Hermann–Mauguin symbols for various settings and cell choices						
			$\mathbf{a\underline{b}c}$	$\mathbf{c\underline{\bar{b}}a}$	$\mathbf{ab\underline{c}}$	$\mathbf{ba\underline{\bar{c}}}$	$\mathbf{\underline{a}bc}$	$\mathbf{\underline{\bar{a}}cb}$	Unique axis *b* Unique axis *c* Unique axis *a*
3	C_2^1	$P2$	$P121$	$P121$	$P112$	$P112$	$P211$	$P211$	
4	C_2^2	$P2_1$	$P12_11$	$P12_11$	$P112_1$	$P112_1$	$P2_111$	$P2_111$	
5	C_2^3	$C2$	$C121$ 2_1	$A121$ 2_1	$A112$ 2_1	$B112$ 2_1	$B211$ 2_1	$C211$ 2_1	Cell choice 1
			$A121$ 2_1	$C121$ 2_1	$B112$ 2_1	$A112$ 2_1	$C211$ 2_1	$B211$ 2_1	Cell choice 2
			$I121$ 2_1	$I121$ 2_1	$I112$ 2_1	$I112$ 2_1	$I211$ 2_1	$I211$ 2_1	Cell choice 3
6	C_s^1	Pm	$P1m1$	$P1m1$	$P11m$	$P11m$	$Pm11$	$Pm11$	
7	C_s^2	Pc	$P1c1$	$P1a1$	$P11a$	$P11b$	$Pb11$	$Pc11$	Cell choice 1
			$P1n1$	$P1n1$	$P11n$	$P11n$	$Pn11$	$Pn11$	Cell choice 2
			$P1a1$	$P1c1$	$P11b$	$P11a$	$Pc11$	$Pb11$	Cell choice 3
8	C_s^3	Cm	$C1m1$ a	$A1m1$ c	$A11m$ b	$B11m$ a	$Bm11$ c	$Cm11$ b	Cell choice 1
			$A1m1$ c	$C1m1$ a	$B11m$ a	$A11m$ b	$Cm11$ b	$Bm11$ c	Cell choice 2
			$I1m1$ n	$I1m1$ n	$I11m$ n	$I11m$ n	$Im11$ n	$Im11$ n	Cell choice 3
9	C_s^4	Cc	$C1c1$ n	$A1a1$ n	$A11a$ n	$B11b$ n	$Bb11$ n	$Cc11$ n	Cell choice 1
			$A1n1$ a	$C1n1$ c	$B11n$ b	$A11n$ a	$Cn11$ c	$Bn11$ b	Cell choice 2
			$I1a1$ c	$I1c1$ a	$I11b$ a	$I11a$ b	$Ic11$ b	$Ib11$ c	Cell choice 3
10	C_{2h}^1	$P2/m$	$P1\frac{2}{m}1$	$P1\frac{2}{m}1$	$P11\frac{2}{m}$	$P11\frac{2}{m}$	$P\frac{2}{m}11$	$P\frac{2}{m}11$	
11	C_{2h}^2	$P2_1/m$	$P1\frac{2_1}{m}1$	$P1\frac{2_1}{m}1$	$P11\frac{2_1}{m}$	$P11\frac{2_1}{m}$	$P\frac{2_1}{m}11$	$P\frac{2_1}{m}11$	
12	C_{2h}^3	$C2/m$	$C1\frac{2}{m}1$ $\frac{2_1}{a}$	$A1\frac{2}{m}1$ $\frac{2_1}{c}$	$A11\frac{2}{m}$ $\frac{2_1}{b}$	$B11\frac{2}{m}$ $\frac{2_1}{a}$	$B\frac{2}{m}11$ $\frac{2_1}{c}$	$C\frac{2}{m}11$ $\frac{2_1}{b}$	Cell choice 1
			$A1\frac{2}{m}1$ $\frac{2_1}{c}$	$C1\frac{2}{m}1$ $\frac{2_1}{a}$	$B11\frac{2}{m}$ $\frac{2_1}{a}$	$A11\frac{2}{m}$ $\frac{2_1}{b}$	$C\frac{2}{m}11$ $\frac{2_1}{b}$	$B\frac{2}{m}11$ $\frac{2_1}{c}$	Cell choice 2
			$I1\frac{2}{m}1$ $\frac{2_1}{n}$	$I1\frac{2}{m}1$ $\frac{2_1}{n}$	$I11\frac{2}{m}$ $\frac{2_1}{n}$	$I11\frac{2}{m}$ $\frac{2_1}{n}$	$I\frac{2}{m}11$ $\frac{2_1}{n}$	$I\frac{2}{m}11$ $\frac{2_1}{n}$	Cell choice 3
13	C_{2h}^4	$P2/c$	$P1\frac{2}{c}1$	$P1\frac{2}{a}1$	$P11\frac{2}{a}$	$P11\frac{2}{b}$	$P\frac{2}{b}11$	$P\frac{2}{c}11$	Cell choice 1
			$P1\frac{2}{n}1$	$P1\frac{2}{n}1$	$P11\frac{2}{n}$	$P11\frac{2}{n}$	$P\frac{2}{n}11$	$P\frac{2}{n}11$	Cell choice 2
			$P1\frac{2}{a}1$	$P1\frac{2}{c}1$	$P11\frac{2}{b}$	$P11\frac{2}{a}$	$P\frac{2}{c}11$	$P\frac{2}{b}11$	Cell choice 3

Table 4.3.2.1. *Index of symbols for space groups for various settings and cells* (*cont.*)

MONOCLINIC SYSTEM (*cont.*)

No. of space group	Schoenflies symbol	Standard short Hermann–Mauguin symbol	Extended Hermann–Mauguin symbols for various settings and cell choices						Unique axis *b* Unique axis *c* Unique axis *a*
			$\mathbf{a\underline{b}c}$	$\mathbf{c\underline{\bar{b}}a}$	$\mathbf{ab\underline{c}}$	$\mathbf{ba\underline{\bar{c}}}$	$\mathbf{\underline{a}bc}$	$\mathbf{\underline{\bar{a}}cb}$	
14	C_{2h}^5	$P2_1/c$	$P1\frac{2_1}{c}1$	$P1\frac{2_1}{a}1$	$P11\frac{2_1}{a}$	$P11\frac{2_1}{b}$	$P\frac{2_1}{b}11$	$P\frac{2_1}{c}11$	Cell choice 1
			$P1\frac{2_1}{n}1$	$P1\frac{2_1}{n}1$	$P11\frac{2_1}{n}$	$P11\frac{2_1}{n}$	$P\frac{2_1}{n}11$	$P\frac{2_1}{n}11$	Cell choice 2
			$P1\frac{2_1}{a}1$	$P1\frac{2_1}{c}1$	$P11\frac{2_1}{b}$	$P11\frac{2_1}{a}$	$P\frac{2_1}{c}11$	$P\frac{2_1}{b}11$	Cell choice 3
15	C_{2h}^6	$C2/c$	$C1\frac{2}{c}1$ $\frac{2_1}{n}$	$A1\frac{2}{a}1$ $\frac{2_1}{n}$	$A11\frac{2}{a}$ $\frac{2_1}{n}$	$B11\frac{2}{b}$ $\frac{2_1}{n}$	$B\frac{2}{b}11$ $\frac{2_1}{n}$	$C\frac{2}{c}11$ $\frac{2_1}{n}$	Cell choice 1
			$A1\frac{2}{n}1$ $\frac{2_1}{a}$	$C1\frac{2}{n}1$ $\frac{2_1}{c}$	$B11\frac{2}{n}$ $\frac{2_1}{b}$	$A11\frac{2}{n}$ $\frac{2_1}{a}$	$C\frac{2}{n}11$ $\frac{2_1}{c}$	$B\frac{2}{n}11$ $\frac{2_1}{b}$	Cell choice 2
			$I1\frac{2}{a}1$ $\frac{2_1}{c}$	$I1\frac{2}{c}1$ $\frac{2_1}{a}$	$I11\frac{2}{b}$ $\frac{2_1}{a}$	$I11\frac{2}{a}$ $\frac{2_1}{b}$	$I\frac{2}{c}11$ $\frac{2_1}{b}$	$I\frac{2}{b}11$ $\frac{2_1}{c}$	Cell choice 3

ORTHORHOMBIC SYSTEM

No. of space group	Schoenflies symbol	Standard full Hermann–Mauguin symbol	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
		abc	**abc** (standard)	$\mathbf{ba\bar{c}}$	**cab**	$\mathbf{\bar{c}ba}$	**bca**	$\mathbf{a\bar{c}b}$
16	D_2^1	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$
17	D_2^2	$P222_1$	$P222_1$	$P222_1$	$P2_122$	$P2_122$	$P22_12$	$P22_12$
18	D_2^3	$P2_12_12$	$P2_12_12$	$P2_12_12$	$P22_12_1$	$P22_12_1$	$P2_122_1$	$P2_122_1$
19	D_2^4	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
20	D_2^5	$C222_1$	$C222_1$ $2_12_12_1$	$C222_1$ $2_12_12_1$	$A2_122$ $2_12_12_1$	$A2_122$ $2_12_12_1$	$B22_12$ $2_12_12_1$	$B22_12$ $2_12_12_1$
21	D_2^6	$C222$	$C222$ 2_12_12	$C222$ 2_12_12	$A222$ 22_12_1	$A222$ 22_12_1	$B222$ 2_122_1	$B222$ 2_122_1
22	D_2^7	$F222$	$F222$ 2_12_12 22_12_1 2_122_1	$F222$ 2_12_12 2_122_1 22_12_1	$F222$ 22_12_1 2_122_1 2_12_12	$F222$ 22_12_1 2_12_12 2_122_1	$F222$ 2_122_1 2_12_12 22_12_1	$F222$ 2_122_1 22_12_1 2_12_12
23	D_2^8	$I222$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$
24	D_2^9	$I2_12_12_1$	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222
25	C_{2v}^1	$Pmm2$	$Pmm2$	$Pmm2$	$P2mm$	$P2mm$	$Pm2m$	$Pm2m$
26	C_{2v}^2	$Pmc2_1$	$Pmc2_1$	$Pcm2_1$	$P2_1ma$	$P2_1am$	$Pb2_1m$	$Pm2_1b$
27	C_{2v}^3	$Pcc2$	$Pcc2$	$Pcc2$	$P2aa$	$P2aa$	$Pb2b$	$Pb2b$
28	C_{2v}^4	$Pma2$	$Pma2$	$Pbm2$	$P2mb$	$P2cm$	$Pc2m$	$Pm2a$
29	C_{2v}^5	$Pca2_1$	$Pca2_1$	$Pbc2_1$	$P2_1ab$	$P2_1ca$	$Pc2_1b$	$Pb2_1a$
30	C_{2v}^6	$Pnc2$	$Pnc2$	$Pcn2$	$P2na$	$P2an$	$Pb2n$	$Pn2b$
31	C_{2v}^7	$Pmn2_1$	$Pmn2_1$	$Pnm2_1$	$P2_1mn$	$P2_1nm$	$Pn2_1m$	$Pm2_1n$
32	C_{2v}^8	$Pba2$	$Pba2$	$Pba2$	$P2cb$	$P2cb$	$Pc2a$	$Pc2a$
33	C_{2v}^9	$Pna2_1$	$Pna2_1$	$Pbn2_1$	$P2_1nb$	$P2_1cn$	$Pc2_1n$	$Pn2_1a$
34	C_{2v}^{10}	$Pnn2$	$Pnn2$	$Pnn2$	$P2nn$	$P2nn$	$Pn2n$	$Pn2n$

Table 4.3.2.1. *Index of symbols for space groups for various settings and cells* (*cont.*)

ORTHORHOMBIC SYSTEM (*cont.*)

No. of space group	Schoenflies symbol	Standard full Hermann–Mauguin symbol **abc**	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
			abc (standard)	**ba$\bar{\mathbf{c}}$**	**cab**	**$\bar{\mathbf{c}}$ba**	**bca**	**a$\bar{\mathbf{c}}$b**
35	C_{2v}^{11}	*Cmm*2	*Cmm*2 *ba*2	*Cmm*2 *ba*2	*A*2*mm* 2*cb*	*A*2*mm* 2*cb*	*Bm*2*m* *c*2*a*	*Bm*2*m* *c*2*a*
36	C_{2v}^{12}	$Cmc2_1$	$Cmc2_1$ $bn2_1$	$Ccm2_1$ $na2_1$	$A2_1ma$ 2_1cn	$A2_1am$ 2_1nb	$Bb2_1m$ $n2_1a$	$Bm2_1b$ $c2_1n$
37	C_{2v}^{13}	*Ccc*2	*Ccc*2 *nn*2	*Ccc*2 *nn*2	*A*2*aa* 2*nn*	*A*2*aa* 2*nn*	*Bb*2*b* *n*2*n*	*Bb*2*b* *n*2*n*
38	C_{2v}^{14}	*Amm*2	*Amm*2 $nc2_1$	*Bmm*2 $cn2_1$	*B*2*mm* 2_1na	*C*2*mm* 2_1an	*Cm*2*m* $b2_1n$	*Am*2*m* $n2_1b$
39*	C_{2v}^{15}	*Aem*2	*Aem*2 $ec2_1$	*Bme*2 $ce2_1$	*B*2*em* 2_1ea	*C*2*me* 2_1ae	*Cm*2*e* $b2_1e$	*Ae*2*m* $e2_1b$
40	C_{2v}^{16}	*Ama*2	*Ama*2 $nn2_1$	*Bbm*2 $nn2_1$	*B*2*mb* 2_1nn	*C*2*cm* 2_1nn	*Cc*2*m* $n2_1n$	*Am*2*a* $n2_1n$
41*	C_{2v}^{17}	*Aea*2	*Aea*2 $en2_1$	*Bbe*2 $ne2_1$	*B*2*eb* 2_1en	*C*2*ce* 2_1ne	*Cc*2*e* $n2_1e$	*Ae*2*a* $e2_1n$
42	C_{2v}^{18}	*Fmm*2	*Fmm*2 *ba*2 $nc2_1$ $cn2_1$	*Fmm*2 *ba*2 $cn2_1$ $nc2_1$	*F*2*mm* 2*cb* 2_1na 2_1an	*F*2*mm* 2*cb* 2_1an 2_1na	*Fm*2*m* *c*2*a* $b2_1n$ $n2_1b$	*Fm*2*m* *c*2*a* $n2_1b$ $b2_1n$
43	C_{2v}^{19}	*Fdd*2	*Fdd*2 $dd2_1$	*Fdd*2 $dd2_1$	*F*2*dd* 2_1dd	*F*2*dd* 2_1dd	*Fd*2*d* $d2_1d$	*Fd*2*d* $d2_1d$
44	C_{2v}^{20}	*Imm*2	*Imm*2 $nn2_1$	*Imm*2 $nn2_1$	*I*2*mm* 2_1nn	*I*2*mm* 2_1nn	*Im*2*m* $n2_1n$	*Im*2*m* $n2_1n$
45	C_{2v}^{21}	*Iba*2	*Iba*2 $cc2_1$	*Iba*2 $cc2_1$	*I*2*cb* 2_1aa	*I*2*cb* 2_1aa	*Ic*2*a* $b2_1b$	*Ic*2*a* $b2_1b$
46	C_{2v}^{22}	*Ima*2	*Ima*2 $nc2_1$	*Ibm*2 $cn2_1$	*I*2*mb* 2_1na	*I*2*cm* 2_1an	*Ic*2*m* $b2_1n$	*Im*2*a* $n2_1b$
47	D_{2h}^{1}	$P\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*Pmmm*	*Pmmm*	*Pmmm*	*Pmmm*	*Pmmm*	*Pmmm*
48	D_{2h}^{2}	$P\frac{2}{n}\frac{2}{n}\frac{2}{n}$	*Pnnn*	*Pnnn*	*Pnnn*	*Pnnn*	*Pnnn*	*Pnnn*
49	D_{2h}^{3}	$P\frac{2}{c}\frac{2}{c}\frac{2}{m}$	*Pccm*	*Pccm*	*Pmaa*	*Pmaa*	*Pbmb*	*Pbmb*
50	D_{2h}^{4}	$P\frac{2}{b}\frac{2}{a}\frac{2}{n}$	*Pban*	*Pban*	*Pncb*	*Pncb*	*Pcna*	*Pcna*
51	D_{2h}^{5}	$P\frac{2_1}{m}\frac{2}{m}\frac{2}{a}$	*Pmma*	*Pmmb*	*Pbmm*	*Pcmm*	*Pmcm*	*Pmam*
52	D_{2h}^{6}	$P\frac{2}{n}\frac{2_1}{n}\frac{2}{a}$	*Pnna*	*Pnnb*	*Pbnn*	*Pcnn*	*Pncn*	*Pnan*
53	D_{2h}^{7}	$P\frac{2}{m}\frac{2}{n}\frac{2_1}{a}$	*Pmna*	*Pnmb*	*Pbmn*	*Pcnm*	*Pncm*	*Pman*
54	D_{2h}^{8}	$P\frac{2_1}{c}\frac{2}{c}\frac{2}{a}$	*Pcca*	*Pccb*	*Pbaa*	*Pcaa*	*Pbcb*	*Pbab*
55	D_{2h}^{9}	$P\frac{2_1}{b}\frac{2_1}{a}\frac{2}{m}$	*Pbam*	*Pbam*	*Pmcb*	*Pmcb*	*Pcma*	*Pcma*
56	D_{2h}^{10}	$P\frac{2_1}{c}\frac{2_1}{c}\frac{2}{n}$	*Pccn*	*Pccn*	*Pnaa*	*Pnaa*	*Pbnb*	*Pbnb*
57	D_{2h}^{11}	$P\frac{2}{b}\frac{2_1}{c}\frac{2_1}{m}$	*Pbcm*	*Pcam*	*Pmca*	*Pmab*	*Pbma*	*Pcmb*
58	D_{2h}^{12}	$P\frac{2_1}{n}\frac{2_1}{n}\frac{2}{m}$	*Pnnm*	*Pnnm*	*Pmnn*	*Pmnn*	*Pnmn*	*Pnmn*
59	D_{2h}^{13}	$P\frac{2_1}{m}\frac{2_1}{m}\frac{2}{n}$	*Pmmn*	*Pmmn*	*Pnmm*	*Pnmm*	*Pmnm*	*Pmnm*
60	D_{2h}^{14}	$P\frac{2_1}{b}\frac{2}{c}\frac{2_1}{n}$	*Pbcn*	*Pcan*	*Pnca*	*Pnab*	*Pbna*	*Pcnb*
61	D_{2h}^{15}	$P\frac{2_1}{b}\frac{2_1}{c}\frac{2_1}{a}$	*Pbca*	*Pcab*	*Pbca*	*Pcab*	*Pbca*	*Pcab*

Table 4.3.2.1. *Index of symbols for space groups for various settings and cells* (*cont.*)

ORTHORHOMBIC SYSTEM (*cont.*)

No. of space group	Schoenflies symbol	Standard full Hermann–Mauguin symbol **abc**	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
			abc (standard)	**ba$\bar{\mathbf{c}}$**	**cab**	**$\bar{\mathbf{c}}$ba**	**bca**	**a$\bar{\mathbf{c}}$b**
62	D_{2h}^{16}	$P\frac{2_1}{n}\frac{2_1}{m}\frac{2_1}{a}$	*Pnma*	*Pmnb*	*Pbnm*	*Pcmn*	*Pmcn*	*Pnam*
63	D_{2h}^{17}	$C\frac{2}{m}\frac{2}{c}\frac{2_1}{m}$	*Cmcm* *bnn*	*Ccmm* *nan*	*Amma* *ncn*	*Amam* *nnb*	*Bbmm* *nna*	*Bmmb* *cnn*
64*†	D_{2h}^{18}	$C\frac{2}{m}\frac{2}{c}\frac{2_1}{e}$	*Cmce* *bne*	*Ccme* *nae*	*Aema* *ecn*	*Aeam* *enb*	*Bbem* *nea*	*Bmeb* *cen*
65	D_{2h}^{19}	$C\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*Cmmm* *ban*	*Cmmm* *ban*	*Ammm* *ncb*	*Ammm* *ncb*	*Bmmm* *cna*	*Bmmm* *cna*
66	D_{2h}^{20}	$C\frac{2}{c}\frac{2}{c}\frac{2}{m}$	*Cccm* *nnn*	*Cccm* *nnn*	*Amaa* *nnn*	*Amaa* *nnn*	*Bbmb* *nnn*	*Bbmb* *nnn*
67*†	D_{2h}^{21}	$C\frac{2}{m}\frac{2}{m}\frac{2}{e}$	*Cmme* *bae*	*Cmme* *bae*	*Aemm* *ecb*	*Aemm* *ecb*	*Bmem* *cea*	*Bmem* *cea*
68*	D_{2h}^{22}	$C\frac{2}{c}\frac{2}{c}\frac{2}{e}$	*Ccce* *nne*	*Ccce* *nne*	*Aeaa* *enn*	*Aeaa* *enn*	*Bbeb* *nen*	*Bbeb* *nen*
69	D_{2h}^{23}	$F\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*Fmmm* *ban* *ncb* *cna*	*Fmmm* *ban* *cna* *ncb*	*Fmmm* *ncb* *cna* *ban*	*Fmmm* *ncb* *ban* *cna*	*Fmmm* *cna* *ban* *ncb*	*Fmmm* *cna* *ncb* *ban*
70	D_{2h}^{24}	$F\frac{2}{d}\frac{2}{d}\frac{2}{d}$	*Fddd*	*Fddd*	*Fddd*	*Fddd*	*Fddd*	*Fddd*
71	D_{2h}^{25}	$I\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*
72	D_{2h}^{26}	$I\frac{2}{b}\frac{2}{a}\frac{2}{m}$	*I bam* *ccn*	*I bam* *ccn*	*I mcb* *naa*	*I mcb* *naa*	*I cma* *bnb*	*I cma* *bnb*
73	D_{2h}^{27}	$I\frac{2_1}{b}\frac{2_1}{c}\frac{2_1}{a}$	*I bca* *cab*	*I cab* *bca*	*I bca* *cab*	*I cab* *bca*	*I bca* *cab*	*I cab* *bca*
74†	D_{2h}^{28}	$I\frac{2_1}{m}\frac{2_1}{m}\frac{2_1}{a}$	*I mma* *nnb*	*I mmb* *nna*	*I bmm* *cnn*	*I cmm* *bnn*	*I mcm* *nan*	*I mam* *ncn*

* For the five space groups *Aem*2 (39), *Aea*2 (41), *Cmce* (64), *Cmme* (67) and *Ccce* (68), the 'new' space-group symbols, containing the symbol '*e*' for the 'double' glide plane, are given for all settings. These symbols were first introduced in the Fourth Edition of this volume (*IT* 1995); *cf. Foreword to the Fourth Edition.* For further explanations, see Section 1.3.2, Note (x) and the space-group diagrams.

† For space groups *Cmca* (64), *Cmma* (67) and *Imma* (74), the first lines of the extended symbols, as tabulated here, correspond with the symbols for the six settings in the diagrams of these space groups (Part 7). An alternative formulation which corresponds with the coordinate triplets is given in Section 4.3.3.

TETRAGONAL SYSTEM

No. of space group	Schoen-flies symbol	Hermann–Mauguin symbols for standard cell P or I		Multiple cell C or F	
		Short	Extended	Short	Extended
75	C_4^1	$P4$		$C4$	
76	C_4^2	$P4_1$		$C4_1$	
77	C_4^3	$P4_2$		$C4_2$	
78	C_4^4	$P4_3$		$C4_3$	
79	C_4^5	$I\,4$	$I4$ 4_2	$F4$	$F4$ 4_2
80	C_4^6	$I\,4_1$	$I4_1$ 4_3	$F4_1$	$F4_1$ 4_3
81	S_4^1	$P\bar{4}$		$C\bar{4}$	
82	S_4^2	$I\bar{4}$		$F\bar{4}$	

No. of space group	Schoen-flies symbol	Hermann–Mauguin symbols for standard cell P or I		Multiple cell C or F	
		Short	Extended	Short	Extended
83	C_{4h}^1	$P4/m$		$C4/m$	$C4_2/m$ n
84	C_{4h}^2	$P4_2/m$		$C4_2/m$	$C4_2/m$ n
85	C_{4h}^3	$P4/n$		$C4/a$	$C4/a$ b
86	C_{4h}^4	$P4_2/n$		$C4_2/a$	$C4_2/a$ b
87	C_{4h}^5	$I\,4/m$	$I4/m$ $4_2/n$	$F4/m$	$F4/m$ $4_2/a$
88	C_{4h}^6	$I\,4_1/a$	$I4_1/a$ $4_3/b$	$F4_1/d$	$F4_1/d$ $4_3/d$

Table 4.3.2.1. *Index of symbols for space groups for various settings and cells* (*cont.*)

TETRAGONAL SYSTEM (*cont.*)

No. of space group	Schoen-flies symbol	Hermann–Mauguin symbols for standard cell P or I		Multiple cell C or F	
		Short	Extended	Short	Extended
89	D_4^1	$P422$	$P422$ 2_1	$C422$	$C422$ 2_1
90	D_4^2	$P42_12$	$P42_12$ 2_1	$C422_1$	$C422_1$ 2_1
91	D_4^3	$P4_122$	$P4_122$ 2_1	$C4_122$	$C4_122$ 2_1
92	D_4^4	$P4_12_12$	$P4_12_12$ 2_1	$C4_122_1$	$C4_122_1$ 2_1
93	D_4^5	$P4_222$	$P4_222$ 2_1	$C4_222$	$C4_222$ 2_1
94	D_4^6	$P4_22_12$	$P4_22_12$ 2_1	$C4_222_1$	$C4_222_1$ 2_1
95	D_4^7	$P4_322$	$P4_322$ 2_1	$C4_322$	$C4_322$ 2_1
96	D_4^8	$P4_32_12$	$P4_32_12$ 2_1	$C4_322_1$	$C4_322_1$ 2_1
97	D_4^9	$I\,422$	$I\,422$ $4_22_12_1$	$F422$	$F422$ $4_22_12_1$
98	D_4^{10}	$I4_122$	$I\,4_122$ $4_32_12_1$	$F4_122$	$F4_122$ $4_32_12_1$
99	C_{4v}^1	$P4mm$	$P4mm$ g	$C4mm$	$C4mm$ b
100	C_{4v}^2	$P4bm$	$P4bm$ g	$C4mg_1$	$C4mg_1$ b
101	C_{4v}^3	$P4_2cm$	$P4_2cm$ g	$C4_2mc$	$C4_2mc$ b
102	C_{4v}^4	$P4_2nm$	$P4_2nm$ g	$C4_2mg_2$	$C4_2mg_2$ b
103	C_{4v}^5	$P4cc$	$P4cc$ n	$C4cc$	$C4cc$ n
104	C_{4v}^6	$P4nc$	$P4nc$ n	$C4cg_2$	$C4cg_2$ n
105	C_{4v}^7	$P4_2mc$	$P4_2mc$ n	$C4_2cm$	$C4_2cm$ n
106	C_{4v}^8	$P4_2bc$	$P4_2bc$ n	$C4_2cg_1$	$C4_2cg_1$ n
107	C_{4v}^9	$I\,4mm$	$I\,4mm$ 4_2ne	$F4mm$	$F4mm$ 4_2eg_2
108	C_{4v}^{10}	$I\,4cm$	$I\,4ce$ 4_2bm	$F4mc$	$F4ec$ 4_2mg_1
109	C_{4v}^{11}	$I\,4_1md$	$I\,4_1md$ 4_1nd	$F4_1dm$	$F4_1dm$ 4_3dg_2
110	C_{4v}^{12}	$I\,4_1cd$	$I\,4_1cd$ 4_3bd	$F4_1dc$	$F4_1dc$ 4_3dg_1
111	D_{2d}^1	$P\bar{4}2m$	$P\bar{4}2m$ g	$C\bar{4}m2$	$C\bar{4}m2$ b
112	D_{2d}^2	$P\bar{4}2c$	$P\bar{4}2c$ n	$C\bar{4}c2$	$C\bar{4}c2$ n
113	D_{2d}^3	$P\bar{4}2_1m$	$P\bar{4}2_1m$ g	$C\bar{4}m2_1$	$C\bar{4}m2_1$ b
114	D_{2d}^4	$P\bar{4}2_1c$	$P\bar{4}2_1c$ n	$C\bar{4}c2_1$	$C\bar{4}c2_1$ n
115	D_{2d}^5	$P\bar{4}m2$	$P\bar{4}m2$ 2_1	$C\bar{4}2m$	$C\bar{4}2m$ 2_1
116	D_{2d}^6	$P\bar{4}c2$	$P\bar{4}c2$ 2_1	$C\bar{4}2c$	$C\bar{4}2c$ 2_1
117	D_{2d}^7	$P\bar{4}b2$	$P\bar{4}b2$ 2_1	$C\bar{4}2g_1$	$C\bar{4}2g_1$ 2_1
118	D_{2d}^8	$P\bar{4}n2$	$P\bar{4}n2$ 2_1	$C\bar{4}2g_2$	$C\bar{4}2g_2$ 2_1

TETRAGONAL SYSTEM (*cont.*)

No. of space group	Schoen-flies symbol	Hermann–Mauguin symbols for standard cell P or I		Multiple cell C or F	
		Short	Extended	Short	Extended
119	D_{2d}^9	$I\bar{4}m2$	$I\bar{4}m2$ $n2_1$	$F\bar{4}2m$	$F\bar{4}2m$ 2_1g_2
120	D_{2d}^{10}	$I\bar{4}c2$	$I\bar{4}c2$ $b2_1$	$F\bar{4}2c$	$F\bar{4}2c$ 2_1n
121	D_{2d}^{11}	$I\bar{4}2m$	$I\bar{4}2m$ 2_1e	$F\bar{4}m2$	$F\bar{4}m2$ $e2_1$
122	D_{2d}^{12}	$I\bar{4}2d$	$I\bar{4}2d$ 2_1d	$F\bar{4}d2$	$F\bar{4}d2$ $d2_1$
123	D_{4h}^1	$P4/mmm$	$P4/m\ 2/m\ 2/m$ $2_1/g$	$C4/mmm$	$C4/mmm$ nb
124	D_{4h}^2	$P4/mcc$	$P4/m\ 2/c\ 2/c$ $2_1/n$	$C4/mcc$	$C4/mcc$ nn
125	D_{4h}^3	$P4/nbm$	$P4/n\ 2/b\ 2/m$ $2_1/g$	$C4/amg_1$	$C4/amg_1$ bb
126	D_{4h}^4	$P4/nnc$	$P4/n\ 2/n\ 2/c$ $2_1/n$	$C4/acg_2$	$C4/acg_2$ bn
127	D_{4h}^5	$P4/mbm$	$P4/m\ 2_1/b\ 2/m$ $2_1/g$	$C4/mmg_1$	$C4/mmg_1$ nb
128	D_{4h}^6	$P4/mnc$	$P4/m\ 2_1/n\ 2/c$ $2_1/n$	$C4/mcg_2$	$C4/mcg_2$ nn
129	D_{4h}^7	$P4/nmm$	$P4/n\ 2_1/m\ 2/m$ $2_1/g$	$C4/amm$	$C4amm$ bb
130	D_{4h}^8	$P4/ncc$	$P4/n\ 2_1/c\ 2/c$ $2_1/n$	$C4/acc$	$C4/acc$ bn
131	D_{4h}^9	$P4_2/mmc$	$P4_2/m2/m\ 2/c$ $2_1/n$	$C4_2/mcm$	$C4_2/mcm$ nn
132	D_{4h}^{10}	$P4_2/mcm$	$P4_2/m2/c\ 2/m$ $2_1/g$	$C4_2/mmc$	$C4_2/mmc$ nb
133	D_{4h}^{11}	$P4_2/nbc$	$P4_2/n2/b\ 2/c$ $2_1/n$	$C4_2/acg_1$	$C4_2/acg_1$ bn
134	D_{4h}^{12}	$P4_2/nnm$	$P4_2/n2/n\ 2/m$ $2_1/g$	$C4_2/amg_2$	$C4_2/amg_2$ bb
135	D_{4h}^{13}	$P4_2/mbc$	$P4_2/m2_1/b\ 2/c$ $2_1/n$	$C4_2/mcg_1$	$C4_2/mcg_1$ nn
136	D_{4h}^{14}	$P4_2/mnm$	$P4_2/m2_1/n\ 2/m$ $2_1/g$	$C4_2/mmg_2$	$C4_2/mmg_2$ nb
137	D_{4h}^{15}	$P4_2/nmc$	$P4_2/n\ 2_1/m\ 2/c$ $2_1/n$	$C4_2/acm$	$C4_2/acm$ bn
138	D_{4h}^{16}	$P4_2/ncm$	$P4_2/n\ 2_1/c\ 2/m$ $2_1/g$	$C4_2/amc$	$C4_2/amc$ bb
139	D_{4h}^{17}	$I4/mmm$	$I4/m\ 2/m\ 2/m$ $4_2/n\ 2_1/n\ 2_1/e$	$F4/mmm$	$F4/mmm$ $4_2/aeg_2$
140	D_{4h}^{18}	$I4/mcm$	$I4/m\ 2/c\ 2/e$ $4_2/n\ 2_1/b\ 2_1/m$	$F4/mmc$	$F4/mec$ $4_2/amg_1$
141	D_{4h}^{19}	$I4_1/amd$	$I4_1/a\ 2/m\ 2/d$ $4_3/b\ 2_1/n\ 2_1/d$	$F4_1/ddm$	$F4_1/ddm$ $4_3/ddg_2$
142	D_{4h}^{20}	$I4_1/acd$	$I4_1/a\ 2/c\ 2/d$ $4_3/b\ 2_1/b\ 2_1/d$	$F4_1/ddc$	$F4_1/ddc$ $4_3/ddg_1$

Note: The glide planes g, g_1 and g_2 have the glide components $g(\frac{1}{2}, \frac{1}{2}, 0)$, $g_1(\frac{1}{4}, \frac{1}{4}, 0)$ and $g_2(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$. For the glide plane symbol 'e', see the *Foreword to the Fourth Edition* (*IT* 1995) and Section 1.3.2, Note (x).

Table 4.3.2.1. *Index of symbols for space groups for various settings and cells* (*cont.*)

TRIGONAL SYSTEM

No. of space group	Schoen-flies symbol	Hermann-Mauguin symbols for standard cell P or R			Triple cell H
		Short	Full	Extended	
143	C_3^1	$P3$			$H3$
144	C_3^2	$P3_1$			$H3_1$
145	C_3^3	$P3_2$			$H3_2$
146	C_3^4	$R3$		$R3$ $3_{1,2}$	
147	C_{3i}^1	$P\bar{3}$			$H\bar{3}$
148	C_{3i}^2	$R\bar{3}$		$R\bar{3}$ $3_{1,2}$	
149	D_3^1	$P312$		$P312$ 2_1	$H321$
150	D_3^2	$P321$		$P321$ 2_1	$H312$
151	D_3^3	$P3_112$		$P3_112$ 2_1	$H3_121$
152	D_3^4	$P3_121$		$P3_121$ 2_1	$H3_112$
153	D_3^5	$P3_212$		$P3_212$ 2_1	$H3_221$
154	D_3^6	$P3_221$		$P3_221$ 2_1	$H3_212$
155	D_3^7	$R32$		$R3\ \ 2$ $3_{1,2}2_1$	
156	C_{3v}^1	$P3m1$		$P3m1$ b	$H31m$
157	C_{3v}^2	$P31m$		$P31m$ a	$H3m1$
158	C_{3v}^3	$P3c1$		$P3c1$ n	$H31c$
159	C_{3v}^4	$P31c$		$P31c$ n	$H3c1$
160	C_{3v}^5	$R3m$		$R3\ \ m$ $3_{1,2}b$	
161	C_{3v}^6	$R3c$		$R3\ \ c$ $3_{1,2}n$	
162	D_{3d}^1	$P\bar{3}1m$	$P\bar{3}12/m$	$P\bar{3}12/m$ $2_1/a$	$H\bar{3}m1$
163	D_{3d}^2	$P\bar{3}1c$	$P\bar{3}12/c$	$P\bar{3}12/c$ $2_1/n$	$H\bar{3}c1$
164	D_{3d}^3	$P\bar{3}m1$	$P\bar{3}2/m1$	$P\bar{3}2/m1$ $2_1/b$	$H\bar{3}1m$
165	D_{3d}^4	$P\bar{3}c1$	$P\bar{3}2/c1$	$P\bar{3}2/c1$ $2_1/n$	$H\bar{3}1c$
166	D_{3d}^5	$R\bar{3}m$	$R\bar{3}2/m$	$R\bar{3}\ \ 2/m$ $3_{1,2}2_1/b$	
167	D_{3d}^6	$R\bar{3}c$	$R\bar{3}2/c$	$R\bar{3}\ \ 2/c$ $3_{1,2}2_1/n$	

HEXAGONAL SYSTEM

No. of space group	Schoen-flies symbol	Hermann–Mauguin symbols for standard cell P			Triple cell H
		Short	Full	Extended	
168	C_6^1	$P6$			$H6$
169	C_6^2	$P6_1$			$H6_1$
170	C_6^3	$P6_5$			$H6_5$
171	C_6^4	$P6_2$			$H6_2$
172	C_6^5	$P6_4$			$H6_4$
173	C_6^6	$P6_3$			$H6_3$
174	C_{3h}^1	$P\bar{6}$			$H\bar{6}$
175	C_{6h}^1	$P6/m$			$H6/m$
176	C_{6h}^2	$P6_3/m$			$H6_3/m$
177	D_6^1	$P622$		$P62\ 2$ 2_12_1	$H622$
178	D_6^2	$P6_122$		$P6_12\ 2$ 2_12_1	$H6_122$
179	D_6^3	$P6_522$		$P6_52\ 2$ 2_12_1	$H6_522$
180	D_6^4	$P6_222$		$P6_22\ 2$ 2_12_1	$H6_222$
181	D_6^5	$P6_422$		$P6_42\ 2$ 2_12_1	$H6_422$
182	D_6^6	$P6_322$		$P6_32\ 2$ 2_12_1	$H6_322$
183	C_{6v}^1	$P6mm$		$P6mm$ ba	$H6mm$
184	C_{6v}^2	$P6cc$		$P6cc$ nn	$H6cc$
185	C_{6v}^3	$P6_3cm$		$P6_3cm$ na	$H6_3mc$
186	C_{6v}^4	$P6_3mc$		$P6_3mc$ bn	$H6_3cm$
187	D_{3h}^1	$P\bar{6}m2$		$P\bar{6}m2$ $b2_1$	$H\bar{6}2m$
188	D_{3h}^2	$P\bar{6}c2$		$P\bar{6}c2$ $n2_1$	$H\bar{6}2c$
189	D_{3h}^3	$P\bar{6}2m$		$P\bar{6}2m$ 2_1a	$H\bar{6}m2$
190	D_{3h}^4	$P\bar{6}2c$		$P\bar{6}2\ c$ 2_1n	$H\bar{6}c2$
191	D_{6h}^1	$P6/mmm$	$P6/m2/m2/m$	$P6/m\ 2/m\ 2/m$ $2_1/b\ 2_1/a$	$H6/mmm$
192	D_{6h}^2	$P6/mcc$	$P6/m2/c2/c$	$P6/m\ 2/c\ 2/c$ $2_1/n\ 2_1/n$	$H6/mcc$
193	D_{6h}^3	$P6_3/mcm$	$P6_3/m2/c2/m$	$P6_3/m\ 2/c\ 2/m$ $2_1/b\ 2_1/a$	$H6_3/mmc$
194	D_{6h}^4	$P6_3/mmc$	$P6_3/m2/m2/c$	$P6_3/m\ 2/m\ 2/c$ $2_1/b\ 2_1/n$	$H6_3/mcm$

Example: $B\ 2/b\ 11$ (15, unique axis a)
$\quad 2_1/n$

The t subgroups of index [2] (type **I**) are $B211(C2)$; $Bb11(Cc)$; $B\bar{1}(P\bar{1})$.

The k subgroups of index [2] (type **IIa**) are $P2/b11(P2/c)$: $P2_1/b11(P2_1/c)$; $P2/n11(P2/c)$; $P2_1/n11(P2_1/c)$.

Some subgroups of index [4] (not maximal) are $P211(P2)$; $P2_111(P2_1)$; $Pb11(Pc)$; $Pn11(Pc)$; $P\bar{1}$; $B1(P1)$.

4.3.3. Orthorhombic system

4.3.3.1. *Historical note and arrangement of the tables*

The synoptic table of *IT* (1935) contained space-group symbols for the six orthorhombic 'settings', corresponding to the six permutations of the basis vectors **a**, **b**, **c**. In *IT* (1952), left-handed systems like $\bar{\mathbf{c}}\mathbf{ba}$ were changed to right-handed systems by reversing the orientation of the c axis, as in **cba**. Note that reversal

Table 4.3.2.1. *Index of symbols for space groups for various settings and cells* (*cont.*)

CUBIC SYSTEM

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols		
		Short	Full	Extended†
195	T^1	$P23$		
196	T^2	$F23$		$F23$ 2 2_1 2_1
197	T^3	$I23$		$I23$ 2_1
198	T^4	$P2_13$		
199	T^5	$I2_13$		$I2_13$ 2
200	T_h^1	$Pm\bar{3}$	$P2/m\bar{3}$	
201	T_h^2	$Pn\bar{3}$	$P2/n\bar{3}$	
202	T_h^3	$Fm\bar{3}$	$F/2m\bar{3}$	$F2/m\bar{3}$ $2/n$ $2_1/e$ $2_1/e$
203	T_h^4	$Fd\bar{3}$	$F2/d\bar{3}$	$F2/d\bar{3}$ $2/d$ $2_1/d$ $2_1/d$
204	T_h^5	$Im\bar{3}$	$I2/m\bar{3}$	$I2/m\bar{3}$ $2_1/n$
205	T_h^6	$Pa\bar{3}$	$P2_1/a\bar{3}$	
206	T_h^7	$Ia\bar{3}$	$I2_1/a\bar{3}$	$I2_1/a\bar{3}$ $2/b$
207	O^1	$P432$		$P4\ 32$ 2_1
208	O^2	$P4_232$		$P4_232$ 2_1
209	O^3	$F432$		$F4\ 32$ $4\ 2$ 4_22_1 4_22_1
210	O^4	$F4_132$		$F4_132$ $4_1\ 2$ $4_3\ 2_1$ $4_3\ 2_1$
211	O^5	$I432$		$I4\ 32$ $4_2\ 2_1$
212	O^6	$P4_332$		$P4_3\ 32$ 2_1
213	O^7	$P4_132$		$P4_132$ 2_1
214	O^8	$I4_132$		$I4_132$ $4_3\ 2_1$

CUBIC SYSTEM (*cont.*)

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols		
		Short	Full	Extended†
215	T_d^1	$P\bar{4}3m$		$P\bar{4}3m$ g
216	T_d^2	$F\bar{4}3m$		$F\bar{4}3m$ g g_2 g_2
217	T_d^3	$I\bar{4}3m$		$I\bar{4}3m$ e
218	T_d^4	$P\bar{4}3n$		$P\bar{4}3n$ c
219	T_d^5	$F\bar{4}3c$		$F\bar{4}3n$ c g_1 g_1
220	T_d^6	$I\bar{4}3d$		$I\bar{4}3d$ d
221	O_h^1	$Pm\bar{3}m$	$P4/m\bar{3}2/m$	$P4/m\bar{3}2/m$ $2_1/g$
222	O_h^2	$Pn\bar{3}n$	$P4/n\bar{3}2/n$	$P4/n\bar{3}2/n$ $2_1/c$
223	O_h^3	$Pm\bar{3}n$	$P4_2/m\bar{3}2/n$	$P4_2/m\bar{3}2/n$ $2_1/c$
224	O_h^4	$Pn\bar{3}m$	$P4_2/n\bar{3}2/m$	$P4_2/n\bar{3}2/m$ $2_1/g$
225	O_h^5	$Fm\bar{3}m$	$F4/m\bar{3}2/m$	$F4/m\ \bar{3}2/m$ $4/n\ \ 2/g$ $4_2/e\ \ 2_1/g_2$ $4_2/e\ \ 2_1/g_2$
226	O_h^6	$Fm\bar{3}c$	$F4/m\bar{3}2/c$	$F4/m\bar{3}2/n$ $4/n\ \ 2/c$ $4_2/e\ 2_1/g_1$ $4_2/e\ 2_1/g_1$
227	O_h^7	$Fd\bar{3}m$	$F4_1/d\bar{3}2/m$	$F4_1/d\bar{3}2/m$ $4_1/d\ 2/g$ $4_3/d\ 2_1/g_2$ $4_3/d\ 2_1/g_2$
228	O_h^8	$Fd\bar{3}c$	$F4_1/d\bar{3}2/c$	$F4_1/d\bar{3}2/n$ $4_1/d\ 2/c$ $4_3/d\ 2_1/g_1$ $4_3/d\ 2_1/g_1$
229	O_h^9	$Im\bar{3}m$	$I4/m\bar{3}2/m$	$I4/m\bar{3}2/m$ $4_2/n\ 2_1/e$
230	O_h^{10}	$Ia\bar{3}d$	$I4_1/a\bar{3}2/d$	$I4_1/a\bar{3}2/d$ $4_3/b\ \ 2_1/d$

† Axes 3_1 and 3_2 parallel to axes 3 are not indicated in the extended symbols: *cf.* Chapter 4.1. For the glide-plane symbol '*e*', see the *Foreword to the Fourth Edition* (*IT* 1995) and Section 1.3.2, Note (x).

Note: The glide planes g, g_1 and g_2 have the glide components $g(\frac{1}{2}, \frac{1}{2}, 0)$, $g_1(\frac{1}{4}, \frac{1}{4}, 0)$ and $g_2(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$.

of two axes does not change the handedness of a coordinate system, so that the settings $\bar{\mathbf{c}}\mathbf{ba}$, $\mathbf{c}\bar{\mathbf{b}}\mathbf{a}$, $\mathbf{cb}\bar{\mathbf{a}}$ and $\bar{\mathbf{c}}\bar{\mathbf{b}}\bar{\mathbf{a}}$ are equivalent in this respect. The tabulation thus deals with the $6 \times 4 = 24$ possible right-handed settings. For further details see Section 2.2.6.4.

An important innovation of *IT* (1952) was the introduction of extended symbols for the centred groups *A*, *B*, *C*, *I*, *F*. These symbols are systematically developed in Table 4.3.2.1. Settings which permute the two axes **a** and **b** are listed side by side so that the two *C* settings appear together, followed by the two *A* and the two *B* settings.

In crystal classes *mm*2 and 222, the last symmetry element is the product of the first two and thus is not independent. It was omitted in the short Hermann–Mauguin symbols of *IT* (1935) for all space groups of class $mm2$, but was restored in *IT* (1952). In space groups of class 222, the last symmetry element cannot be omitted (see examples below).

For the new 'double' glide plane symbol '*e*', see the *Foreword to the Fourth Edition* (*IT* 1995) and Section 1.3.2, Note (x).

4.3.3.2. *Group–subgroup relations*

The present section emphasizes the use of the extended and full symbols for the derivation of maximal subgroups of types **I** and **IIa**; maximal orthorhombic subgroups of types **IIb** and **IIc** cannot be recognized by inspection of the synoptic Table 4.3.2.1.

4.3.3.2.1. *Maximal non-isomorphic k subgroups of type* **IIa** *(decentred)*

(i) *Extended symbols of centred groups A, B, C, I*

By convention, the second line of the extended space-group symbol is the result of the multiplication of the first line by the centring translation (*cf.* Table 4.1.2.3). As a consequence, the product of any two terms in one line is equal to the product of the corresponding two terms in the other line.

(*a*) *Class* 222

The extended symbol of $I222$ (23) is $\begin{matrix} I2\,2\,2; \\ 2_12_12_1 \end{matrix}$ the twofold axes intersect and one obtains $2_x \times 2_y = 2_z = 2_{1x} \times 2_{1y}$.

Maximal *k* subgroups are $P222$ and $P2_12_12$ (plus permutations) but *not* $P2_12_12_1$.

The extended symbol of $I2_12_12_1$ (24) is $\begin{matrix} I2_12_12_1 \\ 2\,2\,2 \end{matrix}$, where one obtains $2_{1x} \times 2_{1y} = 2_{1z} = 2_x \times 2_y$; the twofold axes do *not* intersect. Thus, maximal non-isomorphic *k* subgroups are $P2_12_12_1$ and $P222_1$ (plus permutations), but *not* $P222$.

(*b*) *Class mm*2

The extended symbol of $Aea2$ (41) is $\begin{matrix} Aba2; \\ cn2_1 \end{matrix}$ the following relations hold: $b \times a = 2 = c \times n$ and $b \times n = 2_1 = c \times a$.

Maximal *k* subgroups are $Pba2$; $Pcn2$ ($Pnc2$); $Pbn2_1$ ($Pna2_1$); $Pca2_1$.

(*c*) *Class mmm*

By convention, the first line of the extended symbol contains those symmetry elements for which the coordinate triplets are explicitly printed under *Positions.* From the two-line symbols, as defined in the example below, one reads not only the eight maximal *k* subgroups *P* of class *mmm* but also the location of their centres of symmetry, by applying the following rules:

If in the symbol of the *P* subgroup the number of symmetry planes, chosen from the first line of the extended symbol, is odd (three or one), the symmetry centre is at 0, 0, 0; if it is even (two or zero), the symmetry centre is at $\frac{1}{4}, \frac{1}{4}, 0$ for the subgroups of *C* groups and at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ for the subgroups of *I* groups (Bertaut, 1976).

Examples

(1) According to these rules, the extended symbol of *Cmce* (64) is $\begin{matrix} Cmcb \\ bna \end{matrix}$ (see above). The four *k* subgroups with symmetry centres at 0, 0, 0 are *Pmcb* (*Pbam*); *Pmna*; *Pbca*; *Pbnb* (*Pccn*); those with symmetry centres at $\frac{1}{4}, \frac{1}{4}, 0$ are *Pbna* (*Pbcn*); *Pmca* (*Pbcm*); *Pmnb* (*Pnma*); *Pbcb* (*Pcca*). These rules can easily be transposed to other settings.

(2) The extended symbol of *Ibam* (72) is $\begin{matrix} Ibam \\ ccn \end{matrix}$. The four subgroups with symmetry centre at 0, 0, 0 are *Pbam*; *Pbcn*; *Pcan* (*Pbcn*); *Pccm*;
those with symmetry centre at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ are *Pccn*; *Pcam* (*Pbcm*); *Pbcm*; *Pban.*

(ii) *Extended symbols of F-centred space groups*

Maximal *k* subgroups of the groups $F222$, $Fmm2$ and $Fmmm$ are *C*, *A* and *B* groups. The corresponding centring translations are $w = t(\frac{1}{2}, \frac{1}{2}, 0)$, $u = t(0, \frac{1}{2}, \frac{1}{2})$ and $v = w \times u = t(\frac{1}{2}, 0, \frac{1}{2})$.

The (four-line) extended symbols of these groups can be obtained from the following scheme:

	$F222$ (22)	$Fmm2$ (42)	$Fmmm$ (69)
1	222	$mm2$	mmm
w	$2_12_12^w$	$ba2^w$	ban
u	$2^u2_1^v2_1$	$nc2_1$	ncb
v	$2_1^u2^v2_1^w$	$cn2_1^w$	cna

The second, third, and fourth lines are the result of the multiplication of the first line by the centring translations *w*, *u* and *v*, respectively.

The following abbreviations are used:

$$2_z^w = w \times 2_z; \quad 2_{1z}^w = w \times 2_{1z}; \ etc.$$

For the location of the symmetry elements in the above scheme, see Table 4.1.2.3. In Table 4.3.2.1, the centring translations and the superscripts *u*, *v*, *w* have been omitted. The first two lines of the scheme represent the extended symbols of $C222$, $Cmm2$ and *Cmmm.* An interchange of the symmetry elements in the first two lines does not change the group. To obtain further maximal *C* subgroups, one has to replace symmetry elements of the first line by corresponding elements of the third or fourth line. Note that the symbol '*e*' is not used in the four-line symbols for $Fmm2$ and *Fmmm* in order to keep the above scheme transparent.

Examples

(1) $F222$ (22). In the first line replace 2_x by 2_x^u (third line, same column) and keep 2_y. Complete the first line by the product $2_x^u \times 2_y = 2_{1z}$ and obtain the maximal *C* subgroup $C2^u22_1$.

Similarly, in the first line keep 2_x and replace 2_y with 2_y^v (fourth line, same column). Complete the first line by the product $2_x \times 2_y^v = 2_{1z}$ and obtain the maximal *C* subgroup $C22^v2_1$.

Finally, replace 2_x and 2_y by 2_x^u and 2_y^v and form the product $2_x^u \times 2_y^v = 2_z^w$, to obtain the maximal *C* subgroup $C2^u2^v2^w$ (where 2^w can be replaced by 2). Note that $C222$ and $C2^u2^v2$ are two different subgroups, as are $C2^u22_1$ and $C22^v2_1$.

(2) $Fmm2$ (42). A similar procedure leads to the four maximal *k* subgroups $Cmm2$; $Cmc2_1$; $Ccm2_1^w$ ($Cmc2_1$); and $Ccc2$.

(3) *Fmmm* (69). One finds successively the eight maximal *k* subgroups *Cmmm*; *Cmma*; *Cmcm*; *Ccmm* (*Cmcm*); *Cmca*; *Ccma* (*Cmca*); *Cccm*; and *Ccca.*

Maximal *A*- and *B*-centred subgroups can be obtained from the *C* subgroups by simple symmetry arguments.

In space groups $Fdd2$ (43) and *Fddd* (70), the nature of the *d* planes is not altered by the translations of the *F* lattice; for this reason, a two-line symbol for $Fdd2$ and a one-line symbol for *Fddd* are sufficient. There exist no maximal non-isomorphic *k* subgroups for these two groups.

4.3.3.2.2. *Maximal t subgroups of type* **I**

(i) *Orthorhombic subgroups*

The standard full symbol of a P group of class mmm indicates all the symmetry elements, so that maximal t subgroups can be read at once.

Example

$P\,2_1/m2/m2/a$ (51) has the following four t subgroups: $P2_122$ ($P222_1$); $Pmm2$; $P2_1ma$ ($Pmc2_1$); $Pm2a$ ($Pma2$).

From the standard full symbol of an I group of class mmm, the t subgroup of class 222 is read directly. It is either $I222$ [for $Immm$ (71) and $Ibam$ (72)] or $I2_12_12_1$ [for $Ibca$ (73) and $Imma$ (74)]. Use of the two-line symbols results in three maximal t subgroups of class $mm2$.

Example

$Ibam$ (72) has the following three maximal t subgroups of ccn

class $mm2$: $Iba2$; $Ib2_1m$ ($Ima2$); $I2_1am$ ($Ima2$).

From the standard full symbol of a C group of class mmm, one immediately reads the maximal t subgroup of class 222, which is either $C222_1$ [for $Cmcm$ (63) and $Cmce$ (64)] or $C222$ (for all other cases). For the three maximal t subgroups of class $mm2$, the two-line symbols are used.

Example

$Cmce$ (64) has the following three maximal t subgroups of bna

class $mm2$: $Cmc2_1$; $Cm2e$ ($Aem2$); $C2ce$ ($Aea2$).

Finally, $Fmmm$ (69) has maximal t subgroups $F222$ and $Fmm2$ (plus permutations), whereas $Fddd$ (70) has $F222$ and $Fdd2$ (plus permutations).

(ii) *Monoclinic subgroups*

These subgroups are obtained by substituting the symbol '1' in two of the three positions. Non-standard centred cells are reduced to primitive cells.

Examples

(1) $C222_1$ (20) has the maximal t subgroups $C211$ ($C2$), $C121$ ($C2$) and $C112_1$. The last one reduces to $P112_1$ ($P2_1$).
(2) $Ama2$ (40) has the maximal t subgroups $Am11$, reducible to Pm, $A1a1$ (Cc) and $A112$ ($C2$).
(3) $Pnma$ (62) has the standard full symbol $P2_1/n2_1/m2_1/a$, from which the maximal t subgroups $P2_1/n11$ ($P2_1/c$), $P12_1/m1$ ($P2_1/m$) and $P112_1/a$ ($P2_1/c$) are obtained.
(4) $Fddd$ (70) has the maximal t subgroups $F2/d11$, $F12/d1$ and $F112/d$, each one reducible to $C2/c$.

4.3.4. Tetragonal system

4.3.4.1. *Historical note and arrangement of the tables*

In the 1935 edition of *International Tables*, for each tetragonal P and I space group an additional C-cell and F-cell description was given. In the corresponding space-group symbols, secondary and tertiary symmetry elements were simply interchanged. Coordinate triplets for these larger cells were not printed, except for the space groups of class $\bar{4}m2$. In *IT* (1952), the C and F cells were dropped from the space-group tables but kept in the comparative tables.

In the present edition, the C and F cells reappear in the sub- and supergroup tabulations of Part 7, as well as in the synoptic Table 4.3.2.1, where short and extended (two-line) symbols are given for P and C cells, as well as for I and F cells.

4.3.4.2. *Relations between symmetry elements*

In the crystal classes 42(2), $4m(m)$, $\bar{4}2(m)$ or $\bar{4}m(2)$, $4/m\,2/m\,(2/m)$, where the tertiary symmetry elements are between parentheses, one finds

$$4\times m=(m)=\bar{4}\times 2;\ 4\times 2=(2)=\bar{4}\times m.$$

Analogous relations hold for the space groups. In order to have the symmetry direction of the tertiary symmetry elements along [1$\bar{1}$0] (*cf.* Table 2.2.4.1), one has to choose the primary and secondary symmetry elements in the product rule along [001] and [010].

Example

In $P4_12(2)$ (91), one has $4_1\times 2=(2)$ so that $P4_12$ would be the short symbol. In fact, in *IT* (1935), the tertiary symmetry element was suppressed for all groups of class 422, but re-established in *IT* (1952), the main reason being the generation of the fourfold rotation as the product of the secondary and tertiary symmetry operations: $4=(m)\times m$ *etc.*

4.3.4.3. *Additional symmetry elements*

As a result of periodicity, in all space groups of classes 422, $\bar{4}m2$ and $4/m\,2/m\,2/m$, the two tertiary diagonal axes 2, along [1$\bar{1}$0] and [110], alternate with axes 2_1, the screw component being $\frac{1}{2},\mp\frac{1}{2},0$ (*cf.* Table 4.1.2.2).

Likewise, tertiary diagonal mirrors m in x,x,z and $x,\bar{x},z$ in space groups of classes $4mm$, $\bar{4}2m$ and $4/m\,2/m\,2/m$ alternate with glide planes called g,* the glide components being $\frac{1}{2}$, $\pm\frac{1}{2}$, 0. The same glide components produce also an alternation of diagonal glide planes c and n (*cf.* Table 4.1.2.2).

4.3.4.4. *Multiple cells*

The transformations from the P to the two C cells, or from the I to the two F cells, are

$$C_1 \text{ or } F_1\text{: (i)}\quad \mathbf{a}'=\mathbf{a}-\mathbf{b},\quad \mathbf{b}'=\mathbf{a}+\mathbf{b},\quad \mathbf{c}'=\mathbf{c}$$
$$C_2 \text{ or } F_2\text{: (ii)}\quad \mathbf{a}'=\mathbf{a}+\mathbf{b},\quad \mathbf{b}'=-\mathbf{a}+\mathbf{b},\quad \mathbf{c}'=\mathbf{c}$$

(*cf.* Fig. 5.1.3.5). The secondary and tertiary symmetry directions are interchanged in the double cells. It is important to know how primary, secondary and tertiary symmetry elements change in the new cells $\mathbf{a}',\mathbf{b}',\mathbf{c}'$.

(i) *Primary symmetry elements*

In P groups, only two kinds of planes, m and n, occur perpendicular to the fourfold axis: a and b planes are forbidden. A plane m in the P cell corresponds to a plane in the C cell which has the character of both a mirror plane m and a glide plane n. This is due to the centring translation $\frac{1}{2},\frac{1}{2},0$ (*cf.* Chapter 4.1). Thus, the C-cell description shows† that $P4/m..$ (cell $\mathbf{a},\mathbf{b},\mathbf{c}$) has two maximal k subgroups of index [2], $P4/m..$ and $P4/n..$ (cells $\mathbf{a}',\mathbf{b}',\mathbf{c}'$), originating from the decentring of the C cell. The same reasoning is valid for $P4_2/m...$

A glide plane n in the P cell is associated with glide planes a and b in the C cell. Since such planes do not exist in tetragonal P groups, the C cell cannot be decentred, *i.e.* $P4/n..$ and $P4_2/n..$ have no k subgroups of index [2] and cells $\mathbf{a}',\mathbf{b}',\mathbf{c}'$.

Glide planes a perpendicular to $\mathbf{c}$ only occur in $I4_1/a$ (88) and groups containing $I4_1/a$ [$I4_1/amd$ (141) and $I4_1/acd$ (142)]; they are associated with d planes in the F cell. These groups cannot be decentred, *i.e.* they have no P subgroups at all.

* For other g planes see (ii), *Secondary symmetry elements.*

† In this section, a dot stands for a symmetry element to be inserted in the corresponding position of the space-group symbol.

(ii) *Secondary symmetry elements*

In the tetragonal space-group symbols, one finds two kinds of secondary symmetry elements:

(1) $2, m, c$ without glide components in the *ab* plane occur in *P* and *I* groups. They transform to tertiary symmetry elements $2, m, c$ in the *C* or *F* cells, from which *k* subgroups can be obtained by decentring.

(2) $2_1, b, n$ with glide components $\frac{1}{2}, 0, 0$; $0, \frac{1}{2}, 0$; $\frac{1}{2}, \frac{1}{2}, 0$ in the *ab* plane occur only in *P* groups. In the *C* cell, they become tertiary symmetry elements with glide components $\frac{1}{4}, -\frac{1}{4}, 0$; $\frac{1}{4}, \frac{1}{4}, 0$; $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$. One has the following correspondence between *P*- and *C*-cell symbols:

$$P.2_1. = C..2_1$$
$$P.b. = C..g_1 \text{ with } g(\tfrac{1}{4},\tfrac{1}{4},0) \text{ in } \quad x, x-\tfrac{1}{4}, z$$
$$P.n. = C..g_2 \text{ with } g(\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{2}) \text{ in } \quad x, x-\tfrac{1}{4}, z,$$

where $(g_1)^2$ and $(g_2)^2$ are the centring translations $\frac{1}{2}, \frac{1}{2}, 0$ and $\frac{1}{2}, \frac{1}{2}, 1$. Thus, the *C* cell cannot be decentred, *i.e.* tetragonal *P* groups having secondary symmetry elements 2_1, *b* or *n* cannot have *klassengleiche P* subgroups of index [2] and cells $\mathbf{a}', \mathbf{b}', \mathbf{c}'$.

(iii) *Tertiary symmetry elements*

Tertiary symmetry elements 2, *m*, *c* in *P* groups transform to secondary symmetry elements in the *C* cell, from which *k* subgroups can easily be deduced ($\rightarrow$):

$$\begin{array}{ccc} P..m = & C.m. \longrightarrow & P.m. \\ g & b & P.b. \\ P..c = & C.c. \longrightarrow & P.c. \\ n & n & P.n. \\ P..2 = & C.2. \longrightarrow & P.2. \\ 2_1 & 2_1 & P.2_1. \end{array}$$

Decentring leads in each case to two *P* subgroups (cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$), when allowed by (i) and (ii).

In *I* groups, 2, *m* and *d* occur as tertiary symmetry elements. They are transformed to secondary symmetry elements in the *F* cells. *I* groups with tertiary *d* glides cannot be decentred to *P* groups, whereas *I* groups with diagonal symmetry elements 2 and *m* have maximal *P* subgroups, due to decentring.

4.3.4.5. *Group–subgroup relations*

Examples are given for maximal *k* subgroups of *P* groups (i), of *I* groups (ii), and for maximal tetragonal, orthorhombic and monoclinic *t* subgroups.

4.3.4.5.1. *Maximal k subgroups*

(i) *Subgroups of P groups*

The discussion is limited to maximal *P* subgroups, obtained by decentring the larger *C* cell (*cf.* Section 4.3.4.4 *Multiple cells*).

Classes $\bar{4}$, 4 *and* 422

Examples

(1) Space groups $P\bar{4}$ (81) and $P4_p$ $(p = 0, 1, 2, 3)$ (75–78) have isomorphic *k* subgroups of index [2], cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$.

(2) Space groups $P4_p22$ $(p = 0, 1, 2, 3)$ (89, 91, 93, 95) have the extended *C*-cell symbol $C4_p2\genfrac{}{}{0pt}{}{2}{2_1}$, from which one deduces two *k* subgroups, $P4_p22$ (isomorphic, type **IIc**) and $P4_p2_12$ (non-isomorphic, type **IIb**), cell $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$.

(3) Space groups $P4_p2_12$ (90, 92, 94, 96) have no *k* subgroups of index [2], cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$.

Classes $\bar{4}m2$, 4*mm*, 4/*m*, *and* 4/*mmm*

Examples

(1) $P\bar{4}c2$ (116) has the *C*-cell symbol $C\bar{4}\genfrac{}{}{0pt}{}{2}{2_1}c$, wherefrom one deduces two *k* subgroups, $P\bar{4}2c$ and $P\bar{4}2_1c$, cell $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$.

(2) $P4_2mc$ (105) has the *C*-cell symbol $C4_2\genfrac{}{}{0pt}{}{c}{n}m$, from which the *k* subgroups $P4_2cm$ (101) and $P4_2nm$ (102), cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$, are obtained.

(3) $P4_2/mcm$ (132) has the extended *C* symbol $C4_2/\genfrac{}{}{0pt}{}{m}{n}\genfrac{}{}{0pt}{}{m}{b}c$, wherefrom one reads the following *k* subgroups of index [2], cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$: $P4_2/mmc$, $P4_2/mbc$, $P4_2/nmc$, $P4_2/nbc$.

(4) $P4/nbm$ (125) has the extended *C* symbol $C4/a\genfrac{}{}{0pt}{}{m}{b}\genfrac{}{}{0pt}{}{g_1}{b}$ and has *no k* subgroups of index [2], as explained above in Section 4.3.4.4.

(ii) *Subgroups of I groups*

Note that *I* groups with *a* glides perpendicular to [001] or with diagonal *d* planes cannot be decentred (*cf.* above). The discussion is limited to *P* subgroups of index [2], obtained by decentring the *I* cell. These subgroups are easily read from the two-line symbols of the *I* groups in Table 4.3.2.1.

Examples

(1) *I*4*cm* (108) has the extended symbol $I\genfrac{}{}{0pt}{}{4}{4_2}\genfrac{}{}{0pt}{}{c}{b}\genfrac{}{}{0pt}{}{e}{m}$. The multiplication rules $4 \times b = m = 4_2 \times c$ give rise to the maximal *k* subgroups: $P4cc$, $P4_2bc$, $P4bm$, $P4_2cm$.

Similarly, *I*4*mm* (107) has the *P* subgroups $P4mm$, $P4_2nm$, $P4nc$, $P4_2mc$, *i.e.* *I*4*mm* and *I*4*cm* have all *P* groups of class 4*mm* as maximal *k* subgroups.

(2) $I4/mcm$ (140) has the extended symbol $I\genfrac{}{}{0pt}{}{4/m}{4_2/n}\genfrac{}{}{0pt}{}{c}{b}\genfrac{}{}{0pt}{}{e}{m}$. One obtains the subgroups of example (1) with an additional *m* or *n* plane perpendicular to $\mathbf{c}$.

As in example (1), $I4/mcm$ (140) and $I4/mmm$ (139) have all *P* groups of class $4/mmm$ as maximal *k* subgroups.

4.3.4.5.2. *Maximal t subgroups*

(i) *Tetragonal subgroups*

The class $4/mmm$ contains the classes $4/m, 422, 4mm$ and $\bar{4}2m$. Maximal *t* subgroups belonging to these classes are read directly from the standard full symbol.

Examples

(1) $P4_2/m\,bc$ (135) has the full symbol $P4_2/m\,2_1/b\,2/c$ and the tetragonal maximal *t* subgroups: $P4_2/m$, $P4_22_12$, $P4_2bc$, $P\bar{4}2_1c$, $P\bar{4}b2$.

(2) $I4/m\,cm$ (140) has the extended full symbol $I\genfrac{}{}{0pt}{}{4/m}{4_2/n}\genfrac{}{}{0pt}{}{2/c}{2_1/b}\genfrac{}{}{0pt}{}{2/e}{2_1/m}$ and the tetragonal maximal *t* subgroups $I4/m$, $I422$, $I4cm$, $I\bar{4}2m$, $I\bar{4}c2$. Note that the *t* subgroups of class $\bar{4}m2$ always exist in pairs.

(ii) *Orthorhombic subgroups*

In the orthorhombic subgroups, the symmetry elements belonging to directions [100] and [010] are the same, except that a glide plane *b* perpendicular to [100] is accompanied by a glide plane *a* perpendicular to [010].

Examples

(1) $P4_2/mbc$ (135). From the full symbol, the *first* maximal t subgroup is found to be $P2_1/b\,2_1/a\,2/m$ ($Pbam$). The C-cell symbol is $C4_2/m\,cg_1$ and gives rise to the *second* maximal orthorhombic t subgroup $Cccm$, cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$.

(2) $I4/m\,cm$ (140). Similarly, the *first* orthorhombic maximal t subgroup is $Iccm$ ($Ibam$); the *second* maximal orthorhombic t subgroup is obtained from the F-cell symbol as $F\begin{array}{c} b\,a\,n \\ c\,c\,m \\ m\,m\,n \end{array}$ ($Fmmm$), cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$.

These examples show that P- and C-cell, as well as I- and F-cell descriptions of tetragonal groups have to be considered together.

(iii) *Monoclinic subgroups*

Only space groups of classes 4, $\bar{4}$ and $4/m$ have maximal monoclinic t subgroups.

Examples

(1) $P4_1$ (76) has the subgroup $P112_1$ ($P2_1$). The C-cell description does not add new features: $C112_1$ is reducible to $P2_1$.

(2) $I4_1/a$ (88) has the subgroup $I112_1/a$, equivalent to $I112/a$ ($C2/c$). The F-cell description yields the same subgroup $F11\,2/d$, again reducible to $C2/c$.

4.3.5. Trigonal and hexagonal systems

The trigonal and hexagonal crystal systems are considered together, because they form the hexagonal 'crystal family', as explained in Chapter 2.1. Hexagonal lattices occur in both systems, whereas rhombohedral lattices occur only in the trigonal system.

4.3.5.1. *Historical note*

The 1935 edition of *International Tables* contains the symbols C and H for the *hexagonal lattice* and R for the *rhombohedral lattice*. C recalls that the hexagonal lattice can be described by a double rectangular C-centred cell (orthohexagonal axes); H was used for a hexagonal triple cell (see below); R designates the rhombohedral lattice and is used for both the rhombohedral description (primitive cell) and the hexagonal description (triple cell).

In the 1952 edition the following changes took place (*cf.* pages x, 51 and 544 of *IT* 1952): The lattice symbol C was replaced by P for reasons of consistency; the H description was dropped. The symbol R was kept for both descriptions, rhombohedral and hexagonal. The tertiary symmetry element in the short Hermann–Mauguin symbols of class 622, which was omitted in *IT* (1935), was re-established.

In the present volume, the use of P and R is the same as in *IT* (1952). The H cell, however, reappears in the sub- and supergroup data of Part 7 and in Table 4.3.2.1 of this section, where short symbols for the H description of trigonal and hexagonal space groups are given. The C cell reappears in the subgroup data for all trigonal and hexagonal space groups having symmetry elements orthogonal to the main axis.

4.3.5.2. *Primitive cells*

The primitive cells of the hexagonal and the rhombohedral lattice, hP and hR, are defined in Table 2.1.2.1 In Part 7, the 'rhombohedral' description of the hR lattice is designated by 'rhombohedral axes'; *cf.* Chapter 1.2.

4.3.5.3. *Multiple cells*

Multiple cells are frequently used to describe both the hexagonal and the rhombohedral lattice.

(i) *The triple hexagonal R cell; cf. Chapters 1.2 and 2.1*

When the lattice is *rhombohedral hR* (primitive cell $\mathbf{a}, \mathbf{b}, \mathbf{c}$), the triple R cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ corresponds to the 'hexagonal description' of the rhombohedral lattice. There are three right-handed *obverse R* cells:

$$\begin{array}{llll} R_1: & \mathbf{a}' = \mathbf{a} - \mathbf{b}; & \mathbf{b}' = \mathbf{b} - \mathbf{c}; & \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}; \\ R_2: & \mathbf{a}' = \mathbf{b} - \mathbf{c}; & \mathbf{b}' = \mathbf{c} - \mathbf{a}; & \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}; \\ R_3: & \mathbf{a}' = \mathbf{c} - \mathbf{a}; & \mathbf{b}' = \mathbf{a} - \mathbf{b}; & \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}. \end{array}$$

Three further right-handed R cells are obtained by changing $\mathbf{a}'$ and $\mathbf{b}'$ to $-\mathbf{a}'$ and $-\mathbf{b}'$, *i.e.* by a 180° rotation around $\mathbf{c}'$. These cells are *reverse*. The transformations between the triple R cells and the primitive rhombohedral cell are given in Table 5.1.3.1 and Fig. 5.1.3.6.

The obverse triple R cell has 'centring points' at

$$0,0,0; \quad \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3}; \quad \tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3},$$

whereas the reverse R cell has 'centring points' at

$$0,0,0; \quad \tfrac{1}{3},\tfrac{2}{3},\tfrac{1}{3}; \quad \tfrac{2}{3},\tfrac{1}{3},\tfrac{2}{3}.$$

In the space-group tables of Part 7, the obverse R_1 cell is used, as illustrated in Fig. 2.2.6.9. This 'hexagonal description' is designated by 'hexagonal axes'.

(ii) *The triple rhombohedral D cell*

Parallel to the 'hexagonal description of the rhombohedral lattice' there exists a 'rhombohedral description of the hexagonal lattice'. Six right-handed rhombohedral cells (here denoted by D) with cell vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ of equal lengths are obtained from the hexagonal P cell $\mathbf{a}, \mathbf{b}, \mathbf{c}$ by the following transformations and by cyclic permutations of $\mathbf{a}', \mathbf{b}', \mathbf{c}'$:

$$\begin{array}{llll} D_1: & \mathbf{a}' = \mathbf{a} + \mathbf{c}; & \mathbf{b}' = \mathbf{b} + \mathbf{c}; & \mathbf{c}' = -(\mathbf{a} + \mathbf{b}) + \mathbf{c} \\ D_2: & \mathbf{a}' = -\mathbf{a} + \mathbf{c}; & \mathbf{b}' = -\mathbf{b} + \mathbf{c}; & \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}. \end{array}$$

The transformation matrices are listed in Table 5.1.3.1. D_2 follows from D_1 by a 180° rotation around [111]. The D cells are triple rhombohedral cells with 'centring' points at

$$0,0,0; \quad \tfrac{1}{3},\tfrac{1}{3},\tfrac{1}{3}; \quad \tfrac{2}{3},\tfrac{2}{3},\tfrac{2}{3}.$$

The D cell, not used in practice and not considered explicitly in the present volume, is useful for a deeper understanding of the relations between hexagonal and rhombohedral lattices.

(iii) *The triple hexagonal H cell; cf. Chapter 1.2*

Generally, a hexagonal lattice hP is described by means of the smallest hexagonal P cell. An alternative description employs a larger hexagonal H-centred cell of three times the volume of the P cell; this cell was extensively used in *IT* (1935), see *Historical note* above.

There are three right-handed orientations of the H cell (basis vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$) with respect to the basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of the P cell:

$$\begin{array}{llll} H_1: & \mathbf{a}' = \mathbf{a} - \mathbf{b}; & \mathbf{b}' = \mathbf{a} + 2\mathbf{b}; & \mathbf{c}' = \mathbf{c} \\ H_2: & \mathbf{a}' = 2\mathbf{a} + \mathbf{b}; & \mathbf{b}' = -\mathbf{a} + \mathbf{b}; & \mathbf{c}' = \mathbf{c} \\ H_3: & \mathbf{a}' = \mathbf{a} + 2\mathbf{b}; & \mathbf{b}' = -2\mathbf{a} - \mathbf{b}; & \mathbf{c}' = \mathbf{c}. \end{array}$$

The transformations are given in Table 5.1.3.1 and Fig. 5.1.3.8. The new vectors $\mathbf{a}'$ and $\mathbf{b}'$ are rotated in the ab plane by $-30°(H_1)$, $+30°(H_2)$, $+90°(H_3)$ with respect to the old vectors $\mathbf{a}$ and $\mathbf{b}$. Three further right-handed H cells are obtained by changing $\mathbf{a}'$ and $\mathbf{b}'$ to $-\mathbf{a}'$ and $-\mathbf{b}'$, *i.e.* by a rotation of 180° around $\mathbf{c}'$.

The H cell has 'centring' points at

$$0,0,0; \quad \tfrac{2}{3},\tfrac{1}{3},0; \quad \tfrac{1}{3},\tfrac{2}{3},0.$$

Secondary and tertiary symmetry elements of the P cell are interchanged in the H cell, and the general position in the H cell is easily obtained, as illustrated by the following example.

Example

The space-group symbol $P3m1$ in the P cell $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ becomes $H31m$ in the H cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$. To obtain the general position of $H31m$, consider the coordinate triplets of $P31m$ and add the centring translations $0,0,0;\ \frac{2}{3},\frac{1}{3},0;\ \frac{1}{3},\frac{2}{3},0$.

(iv) *The double orthohexagonal C cell*

The C-centred cell which is defined by the so-called 'orthohexagonal' vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ has twice the volume of the P cell. There are six right-handed orientations of the C cell, which are C_1, C_2 and C_3 plus three further ones obtained by changing $\mathbf{a}'$ and $\mathbf{b}'$ to $-\mathbf{a}'$ and $-\mathbf{b}'$:

$$\begin{aligned} C_1 &: \mathbf{a}' = \mathbf{a}\quad; & \mathbf{b}' &= \mathbf{a} + 2\mathbf{b}; & \mathbf{c}' &= \mathbf{c} \\ C_2 &: \mathbf{a}' = \mathbf{a} + \mathbf{b}; & \mathbf{b}' &= -\mathbf{a} + \mathbf{b}; & \mathbf{c}' &= \mathbf{c} \\ C_3 &: \mathbf{a}' = \mathbf{b}; & \mathbf{b}' &= -2\mathbf{a} - \mathbf{b}; & \mathbf{c}' &= \mathbf{c}. \end{aligned}$$

Transformation matrices are given in Table 5.1.3.1 and illustrations in Fig. 5.1.3.7. Here $\mathbf{b}'$ is the long axis.

4.3.5.4. *Relations between symmetry elements*

In the hexagonal crystal classes $62(2)$, $6m(m)$ and $\bar{6}2(m)$ or $\bar{6}m(2)$, where the tertiary symmetry element is between parentheses, the following products hold:

$$6 \times 2 = (2) = \bar{6} \times m; \quad 6 \times m = (m) = \bar{6} \times 2$$

or

$$6 \times 2 \times (2) = 6 \times m \times (m) = \bar{6} \times 2 \times (m) = \bar{6} \times m \times (2) = 1.$$

The same relations hold for the corresponding Hermann–Mauguin space-group symbols.

4.3.5.5. *Additional symmetry elements*

Parallel axes 2 and 2_1 occur perpendicular to the principal symmetry axis. Examples are space groups $R32$ (155), $P321$ (150) and $P312$ (149), where the screw components are $\frac{1}{2},\frac{1}{2},0$ (rhombohedral axes) or $\frac{1}{2},0,0$ (hexagonal axes) for $R32$; $\frac{1}{2},0,0$ for $P321$; and $\frac{1}{2},1,0$ for $P312$. Hexagonal examples are $P622$ (177) and $P\bar{6}2c$ (190).

Likewise, mirror planes m parallel to the main symmetry axis alternate with glide planes, the glide components being perpendicular to the principal axis. Examples are $P3m1$ (156), $P31m$ (157), $R3m$ (160) and $P6mm$ (183).

Glide planes c parallel to the main axis are interleaved by glide planes n. Examples are $P3c1$ (158), $P31c$ (159), $R3c$ (161, hexagonal axes), $P\bar{6}c2$ (188). In $R3c$ and $R\bar{3}c$, the glide component $0,0,\frac{1}{2}$ for hexagonal axes becomes $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ for rhombohedral axes, *i.e.* the c glide changes to an n glide. Thus, if the space group is referred to rhombohedral axes, diagonal n planes alternate with diagonal a, b or c planes (*cf.* Section 1.4.4).

In R space groups, all additional symmetry elements with glide and screw components have their origin in the action of an integral lattice translation. This is also true for the axes 3_1 and 3_2 which appear in all R space groups (*cf.* Table 4.1.2.2). For this reason, the 'rhombohedral centring' R is not included in Table 4.1.2.3, which contains only the centrings A, B, C, I, F.

4.3.5.6. *Group–subgroup relations*

4.3.5.6.1. *Maximal k subgroups*

Maximal k subgroups of index [3] are obtained by 'decentring' the triple cells R (hexagonal description), D and H in the trigonal system, H in the hexagonal system. Any one of the three centring points may be taken as origin of the subgroup.

(i) *Trigonal system*

Examples

(1) $P3m1$ (156) (cell $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$) is equivalent to $H31m$ ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}$). Decentring of the H cell yields maximal non-isomorphic k subgroups of type $P31m$. Similarly, $P31m$ (157) has maximal subgroups of type $P3m1$; thus, one can construct infinite chains of subgroup relations of index [3], tripling the cell at each step:

$$P3m1 \to P31m \to P3m1 \ldots$$

(2) $R3$ (146), by decentring the triple hexagonal R cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$, yields the subgroups $P3$, $P3_1$ and $P3_2$ of index [3].

(3) Likewise, decentring of the triple rhombohedral cells D_1 and D_2 gives rise, for each cell, to the rhombohedral subgroups of a trigonal P group, again of index [3].

Combining (2) and (3), one may construct infinite chains of subgroup relations, tripling the cell at each step:

$$P3 \to R3 \to P3 \to R3 \ldots$$

These chains illustrate best the connections between rhombohedral and hexagonal lattices.

(4) Special care must be applied when secondary or tertiary symmetry elements are present. Combining (1), (2) and (3), one has for instance:

$$P31c \to R3c \to P3c1 \to P31c \to R3c \ldots$$

(5) Rhombohedral subgroups, found by decentring the triple cells D_1 and D_2, are given under block **IIb** and are referred there to hexagonal axes, $\mathbf{a}', \mathbf{b}', \mathbf{c}$ as listed below. Examples are space groups $P3$ (143) and $P\bar{3}1c$ (163)

$$\begin{aligned} \mathbf{a}' &= \mathbf{a} - \mathbf{b}, & \mathbf{b}' &= \mathbf{a} + 2\mathbf{b}, & \mathbf{c}' &= 3\mathbf{c}; \\ \mathbf{a}' &= 2\mathbf{a} + \mathbf{b}, & \mathbf{b}' &= -\mathbf{a} + \mathbf{b}, & \mathbf{c}' &= 3\mathbf{c}. \end{aligned}$$

(ii) *Hexagonal system*

Examples

(1) $P\bar{6}2c$ (190) is described as $H\bar{6}c2$ in the triple cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$; decentring yields the non-isomorphic subgroup $P\bar{6}c2$.

(2) $P6/mcc$ (192) (cell $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$) keeps the same symbol in the H cell and, consequently, gives rise to the maximal isomorphic subgroup $P6/mcc$ with cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$. An analogous result applies whenever secondary and tertiary symmetry elements in the Hermann–Mauguin symbol are the same and also to space groups of classes 6, $\bar{6}$ and $6/m$.

4.3.5.6.2. *Maximal t subgroups*

Maximal t subgroups of index [2] are read directly from the full symbol of the space groups of classes 32, $3m$, $\bar{3}m$, 622, $6mm$, $\bar{6}2m$, $6/mmm$.

Maximal t subgroups of index [3] follow from the third power of the main-axis operation. Here the C-cell description is valuable.

(i) *Trigonal system*

(*a*) *Trigonal subgroups*

Examples

(1) $R\bar{3}2/c$ (167) has $R3c$, $R32$ and $R\bar{3}$ as maximal t subgroups of index [2].

(2) $P\bar{3}c1$ (165) has $P3c1$, $P321$ and $P\bar{3}$ as maximal t subgroups of index [2].

(*b*) *Orthorhombic subgroups*

No orthorhombic subgroups of trigonal space groups exist, in spite of the existence of an orthohexagonal C cell.

(*c*) *Monoclinic subgroups*

All trigonal space groups with secondary or tertiary symmetry elements have monoclinic C-centred maximal t subgroups of index [3].

Example

$P\bar{3}1c$ (163), $P\bar{3}c1$ (165) and $R\bar{3}c$ (167) have subgroups of type $C2/c$.

(*d*) *Triclinic subgroups*

All trigonal space groups without secondary or tertiary symmetry elements have triclinic maximal t subgroups of index [3].

Example

$P\bar{3}$ (147) and $R\bar{3}$ (148) have subgroups $P\bar{1}$.

(ii) *Hexagonal system*

(*a*) *Hexagonal subgroups*

Example

$P6_3/m\,2/c\,2/m$ (193) has maximal t subgroups $P6_3/m$, $P6_322$, $P6_3cm$, $P\bar{6}2m$ and $P\bar{6}c2$ of index [2].

(*b*) *Trigonal subgroups*

The second and fourth powers of sixfold operations are threefold operations; thus, all hexagonal space groups have maximal trigonal t subgroups of index [2]. In space groups of classes 622, $6mm$, $\bar{6}2m$, $6/mmm$ with secondary and tertiary symmetry elements, trigonal t subgroups always occur in pairs.

Examples

(1) $P6_1$ (169) contains $P3_1$ of index [2].

(2) $P\bar{6}2c$ (190) has maximal t subgroups $P321$ and $P31c$; $P6_122$ (178) has subgroups $P3_121$ and $P3_112$, all of index [2].

(3) $P6_3/mcm$ (193) contains the operation $\bar{3}$ $[= (6_3)^2 \times \bar{1}]$ and thus has maximal t subgroups $P\bar{3}c1$ and $P\bar{3}1m$ of index [2].

(*c*) *Orthorhombic and monoclinic subgroups*

The third power of the sixfold operation is a twofold operation: accordingly, maximal orthorhombic t subgroups of index [3] are derived from the C-cell description of space groups of classes 622, $6mm$, $\bar{6}2m$ and $6/mmm$. Monoclinic P subgroups of index [3] occur in crystal classes 6, $\bar{6}$ and $6/m$.

Examples

(1) $P\bar{6}2c$ (190) becomes $C\bar{6}2c$ in the C cell; with $(\bar{6})^3 = m$, one obtains $C2cm$ (sequence **a**, **b**, **c**) as a maximal t subgroup of index [3]. The standard symbol is $Ama2$.

(2) $P6_3/mcm$ (193) has maximal orthorhombic t subgroups of type $Cmcm$ of index [3]. With the examples under (*a*) and (*b*), this exhausts all maximal t subgroups of $P6_3/mcm$.

(3) $P6_1$ (169) has a maximal t subgroup $P2_1$; $P6_3/m$ (176) has $P2_1/m$ as a maximal t subgroup.

4.3.6. Cubic system

4.3.6.1. *Historical note and arrangement of tables*

In the synoptic tables of *IT* (1935) and *IT* (1952), for cubic space groups short and full Hermann–Mauguin symbols were listed. They agree, except that in *IT* (1935) the tertiary symmetry element of the space groups of class 432 was omitted; it was re-established in *IT* (1952).

In the present edition, the symbols of *IT* (1952) are retained, with one exception. In the space groups of crystal classes $m\bar{3}$ and $m\bar{3}m$, the short symbols contain $\bar{3}$ instead of 3 (*cf.* Section 2.2.4). In Table 4.3.2.1, short and full symbols for all cubic space groups are given. In addition, for centred groups F and I and for P groups with tertiary symmetry elements, extended space-group symbols are listed. In space groups of classes 432 and $\bar{4}3m$, the product rule (as defined below) is applied in the first line of the extended symbol.

4.3.6.2. *Relations between symmetry elements*

Conventionally, the representative directions of the primary, secondary and tertiary symmetry elements are chosen as [001], [111], and $[1\bar{1}0]$ (*cf.* Table 2.2.4.1 for the equivalent directions). As in tetragonal and hexagonal space groups, tertiary symmetry elements are not independent. In classes 432, $\bar{4}3m$ and $m\bar{3}m$, there are product rules

$$4 \times 3 = (2); \quad \bar{4} \times 3 = (m) = 4 \times \bar{3},$$

where the tertiary symmetry element is in parentheses; analogous rules hold for the space groups belonging to these classes. When the symmetry directions of the primary and secondary symmetry elements are chosen along [001] and [111], respectively, the tertiary symmetry direction is $[0\bar{1}1]$, according to the product rule. In order to have the tertiary symmetry direction along $[1\bar{1}0]$, one has to choose the somewhat awkward primary and secondary symmetry directions [010] and $[\bar{1}1\bar{1}]$.

Examples

(1) In $P\bar{4}3n$ (218), with the choice of the 3 axis along $[\bar{1}1\bar{1}]$ and of the $\bar{4}$ axis parallel to [010], one finds $\bar{4} \times 3 = n$, the n glide plane being in x, x, z, as shown in the space-group diagram.

(2) In $F\bar{4}3c$ (219), one has the same product rule as above; the centring translation $t(\frac{1}{2}, \frac{1}{2}, 0)$, however, associates with the n glide plane a c glide plane, also located in x, x, z (*cf.* Table 4.1.2.3). In the space-group diagram and symbol, c was preferred to n.

4.3.6.3. *Additional symmetry elements*

Owing to periodicity, the tertiary symmetry elements alternate; diagonal axes 2 alternate with parallel screw axes 2_1; diagonal planes m alternate with parallel glide planes g; diagonal n planes, *i.e.* planes with glide components $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, alternate with glide planes a, b or c (*cf.* Chapter 4.1 and Tables 4.1.2.2 and 4.1.2.3). For the meaning of the various glide planes g, see Section 11.1.2 and the entries *Symmetry operations* in Part 7.

4.3.6.4. *Group–subgroup relations*

4.3.6.4.1. *Maximal k subgroups*

The extended symbol of $Fm\bar{3}$ (202) shows clearly that $Pm\bar{3}$, $Pn\bar{3}$, $Pb\bar{3}$ ($Pa\bar{3}$) and $Pa\bar{3}$ are maximal subgroups. $Pm\bar{3}m$, $Pn\bar{3}n$, $Pm\bar{3}n$ and $Pn\bar{3}m$ are maximal subgroups of $Im\bar{3}m$ (229). Space groups with d glide planes have no k subgroup of lattice P.

4.3.6.4.2. *Maximal t subgroups*

(*a*) *Cubic subgroups*

The cubic space groups of classes $m\bar{3}$, 432 and $\bar{4}3m$ have maximal cubic subgroups of class 23 which are found by simple inspection of the full symbol.

Examples

$Ia\bar{3}$ (206), full symbol $I2_1/a\bar{3}$, contains $I2_13$. $P2_13$ is a maximal subgroup of $P4_132$ (213) and its enantiomorph $P4_332$ (212). A more difficult example is $I\bar{4}3d$ (220) which contains $I2_13$.*

The cubic space groups of class $m\bar{3}m$ have maximal subgroups which belong to classes 432 and $\bar{4}3m$.

Examples

$F4/m\bar{3}2/c$ (226) contains $F432$ *and* $F\bar{4}3c$; $I4_1/a\bar{3}2/d$ (230) contains $I4_132$ *and* $I\bar{4}3d$.

(*b*) *Tetragonal subgroups*

In the cubic space groups of classes 432 and $\bar{4}3m$, the primary and tertiary symmetry elements are relevant for deriving maximal tetragonal subgroups.

Examples

The groups $P432$ (207), $P4_232$ (208), $P4_332$ (212) and $P4_132$ (213) have maximal tetragonal *t* subgroups of index [3]: $P422$, $P4_222, P4_32_12$ and $P4_12_12$. $I432$ (211) gives rise to $I422$ with the same cell. $F432$ (209) also gives rise to $I422$, but *via* $F422$, so that the final unit cell is $a\sqrt{2}/2, a\sqrt{2}/2, a$.

In complete analogy, the groups $P\bar{4}3m$ (215) and $P\bar{4}3n$ (218) have maximal subgroups $P\bar{4}2m$ and $P\bar{4}2c$.†

For the space groups of class $m\bar{3}m$, the full symbols are needed to recognize their tetragonal maximal subgroups of class $4/mmm$. The primary symmetry planes of the cubic space group are conserved in the primary *and* secondary symmetry elements of the tetragonal subgroup: *m*, *n* and *d* remain in the tetragonal symbol; *a* remains *a* in the primary and becomes *c* in the secondary symmetry element of the tetragonal symbol.

Example

$P4_2/n\,\bar{3}\,2/m$ (224) and $I4_1/a\,\bar{3}\,2/d$ (230) have maximal subgroups $P4_2/n\,2/n\,2/m$ and $I4_1/a\,2/c\,2/d$, respectively, $F4_1/d\,\bar{3}\,2/c$ (228) gives rise to $F4_1/d\,2/d\,2/c$, which is equivalent to $I4_1/a\,2/c\,2/d$, all of index [3].

(*c*) *Rhombohedral subgroups*‡

Here the secondary and tertiary symmetry elements of the cubic space-group symbols are relevant. For space groups of classes 23, $m\bar{3}$, 432, the maximal *R* subgroups are $R3$, $R\bar{3}$ and $R32$, respectively. For space groups of class $\bar{4}3m$, the maximal *R* subgroup is $R3m$ when the tertiary symmetry element is *m* and $R3c$ otherwise. Finally, for space groups of class $m\bar{3}m$, the maximal *R* subgroup is $R\bar{3}m$ when the tertiary symmetry element is *m* and $R\bar{3}c$ otherwise. All subgroups are of index [4].

(*d*) *Orthorhombic subgroups*

Maximal orthorhombic space groups of index [3] are easily derived from the cubic space-group symbols of classes 23 and $m\bar{3}$.‡ Thus, $P23$, $F23$, $I23$, $P2_13$, $I2_13$ (195–199) have maximal subgroups $P222$, $F222$, $I222$, $P2_12_12_1$, $I2_12_12_1$, respectively. Likewise, maximal subgroups of $Pm\bar{3}$, $Pn\bar{3}$, $Fm\bar{3}$, $Fd\bar{3}$, $Im\bar{3}$, $Pa\bar{3}$, $Ia\bar{3}$ (200–206) are *Pmmm*, *Pnnn*, *Fmmm*, *Fddd*, *Immm*, *Pbca*, *Ibca*, respectively. The lattice type (*P*, *F*, *I*) is conserved and only the primary symmetry element has to be considered.

* From the product rule it follows that $\bar{4}$ and *d* have the same translation component so that $(\bar{4})^2 = 2_1$.

† The tertiary cubic symmetry element *n* becomes *c* in tetragonal notation.

‡ They have already been given in *IT* (1935).

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4.1

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5.1. Transformations of the coordinate system (unit-cell transformations)

BY H. ARNOLD

5.1.1. Introduction

There are two main uses of transformations in crystallography.

(i) *Transformation of the coordinate system* and the unit cell while keeping the crystal at rest. This aspect forms the main topic of the present part. Transformations of coordinate systems are useful when nonconventional descriptions of a crystal structure are considered, for instance in the study of relations between different structures, of phase transitions and of group–subgroup relations. Unit-cell transformations occur particularly frequently when different settings or cell choices of monoclinic, orthorhombic or rhombohedral space groups are to be compared or when 'reduced cells' are derived.

(ii) Description of the *symmetry operations* (motions) of an object (crystal structure). This involves the transformation of the coordinates of a point or the components of a position vector while keeping the coordinate system unchanged. Symmetry operations are treated in Chapter 8.1 and Part 11. They are briefly reviewed in Chapter 5.2.

5.1.2. Matrix notation

Throughout this volume, matrices are written in the following notation:

As (1 × 3) row matrices:

$(\mathbf{a}, \mathbf{b}, \mathbf{c})$	the basis vectors of direct space
(h, k, l)	the Miller indices of a plane (or a set of planes) in direct space or the coordinates of a point in reciprocal space

As (3 × 1) or (4 × 1) column matrices:

$x = (x/y/z)$	the coordinates of a point in direct space
$(\mathbf{a}^*/\mathbf{b}^*/\mathbf{c}^*)$	the basis vectors of reciprocal space
$(u/v/w)$	the indices of a direction in direct space
$\boldsymbol{p} = (p_1/p_2/p_3)$	the components of a shift vector from origin O to the new origin O'
$\boldsymbol{q} = (q_1/q_2/q_3)$	the components of an inverse origin shift from origin O' to origin O, with $\boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p}$
$\boldsymbol{w} = (w_1/w_2/w_3)$	the translation part of a symmetry operation W in direct space
$\mathbb{X} = (x/y/z/1)$	the augmented (4×1) column matrix of the coordinates of a point in direct space

As (3 × 3) or (4 × 4) square matrices:

$\boldsymbol{P}, \boldsymbol{Q} = \boldsymbol{P}^{-1}$	linear parts of an affine transformation; if $\boldsymbol{P}$ is applied to a (1×3) row matrix, $\boldsymbol{Q}$ must be applied to a (3×1) column matrix, and *vice versa*
$\boldsymbol{W}$	the rotation part of a symmetry operation W in direct space
$\mathbb{P} = \begin{pmatrix} \boldsymbol{P} & \boldsymbol{p} \\ \boldsymbol{o} & 1 \end{pmatrix}$	the augmented affine (4×4) transformation matrix, with $\boldsymbol{o} = (0, 0, 0)$
$\mathbb{Q} = \begin{pmatrix} \boldsymbol{Q} & \boldsymbol{q} \\ \boldsymbol{o} & 1 \end{pmatrix}$	the augmented affine (4×4) transformation matrix, with $\mathbb{Q} = \mathbb{P}^{-1}$
$\mathbb{W} = \begin{pmatrix} \boldsymbol{W} & \boldsymbol{w} \\ \boldsymbol{o} & 1 \end{pmatrix}$	the augmented (4×4) matrix of a symmetry operation in direct space (*cf.* Chapter 8.1 and Part 11).

5.1.3. General transformation

Here the crystal structure is considered to be at rest, whereas the coordinate system and the unit cell are changed. Specifically, a point X in a crystal is defined with respect to the basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ and the origin O by the coordinates x, y, z, *i.e.* the position vector $\mathbf{r}$ of point X is given by

$$\mathbf{r} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c} = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

The same point X is given with respect to a new coordinate system, *i.e.* the new basis vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ and the new origin O' (Fig. 5.1.3.1), by the position vector

$$\mathbf{r}' = x'\mathbf{a}' + y'\mathbf{b}' + z'\mathbf{c}'.$$

In this section, the relations between the primed and unprimed quantities are treated.

The general transformation (affine transformation) of the coordinate system consists of two parts, a linear part and a shift of origin. The (3×3) matrix $\boldsymbol{P}$ of the linear part and the (3×1) column matrix $\boldsymbol{p}$, containing the components of the shift vector $\boldsymbol{p}$, define the transformation uniquely. It is represented by the symbol $(\boldsymbol{P}, \boldsymbol{p})$.

(i) The *linear part* implies a change of orientation or length or both of the basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$, *i.e.*

$$\begin{aligned}(\mathbf{a}', \mathbf{b}', \mathbf{c}') &= (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P} \\ &= (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \\ &= (P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c}, \\ &\quad P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c}, \\ &\quad P_{13}\mathbf{a} + P_{23}\mathbf{b} + P_{33}\mathbf{c}).\end{aligned}$$

For a pure linear transformation, the shift vector $\mathbf{p}$ is zero and the symbol is $(\boldsymbol{P}, \boldsymbol{o})$.

The determinant of $\boldsymbol{P}$, $\det(\boldsymbol{P})$, should be positive. If $\det(\boldsymbol{P})$ is negative, a right-handed coordinate system is transformed into a left-handed one (or *vice versa*). If $\det(\boldsymbol{P}) = 0$, the new basis vectors are linearly dependent and do not form a complete coordinate system.

In this chapter, transformations in three-dimensional space are treated. A change of the basis vectors in two dimensions, *i.e.* of the basis vectors $\mathbf{a}$ and $\mathbf{b}$, can be considered as a three-dimensional transformation with invariant $\mathbf{c}$ axis. This is achieved by setting $P_{33} = 1$ and $P_{13} = P_{23} = P_{31} = P_{32} = 0$.

(ii) A *shift of origin* is defined by the shift vector

$$\mathbf{p} = p_1\mathbf{a} + p_2\mathbf{b} + p_3\mathbf{c}.$$

The basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are fixed at the origin O; the new basis vectors are fixed at the new origin O' which has the coordinates p_1, p_2, p_3 in the old coordinate system (Fig. 5.1.3.1).

For a pure origin shift, the basis vectors do not change their lengths or orientations. In this case, the transformation matrix $\boldsymbol{P}$ is the unit matrix $\boldsymbol{I}$ and the symbol of the pure shift becomes $(\boldsymbol{I}, \boldsymbol{p})$.

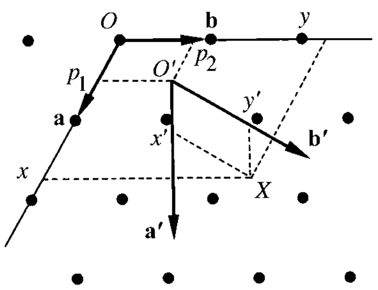

Fig. 5.1.3.1. General affine transformation, consisting of a shift of origin from O to O' by a shift vector $\mathbf{p}$ with components p_1 and p_2 and a change of basis from $\mathbf{a}$, $\mathbf{b}$ to $\mathbf{a}'$, $\mathbf{b}'$. This implies a change in the coordinates of the point X from x, y to x', y'.

Also, the inverse matrices of $\boldsymbol{P}$ and $\boldsymbol{p}$ are needed. They are

$$\boldsymbol{Q} = \boldsymbol{P}^{-1}$$

and

$$\boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p}.$$

The matrix $\boldsymbol{q}$ consists of the components of the negative shift vector $\mathbf{q}$ which refer to the coordinate system $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$, *i.e.*

$$\mathbf{q} = q_1\mathbf{a}' + q_2\mathbf{b}' + q_3\mathbf{c}'.$$

Thus, the transformation ($\boldsymbol{Q}$, $\boldsymbol{q}$) is the inverse transformation of ($\boldsymbol{P}$, $\boldsymbol{p}$). Applying ($\boldsymbol{Q}$, $\boldsymbol{q}$) to the basis vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ and the origin O', the old basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ with origin O are obtained.

For a two-dimensional transformation of $\mathbf{a}'$ and $\mathbf{b}'$, some elements of $\boldsymbol{Q}$ are set as follows: $Q_{33} = 1$ and $Q_{13} = Q_{23} = Q_{31} = Q_{32} = 0$.

The quantities which transform in the same way as the basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ are called *covariant* quantities and are written as row matrices. They are:

the *Miller indices of a plane* (or a set of planes), (hkl), in direct space and

the *coordinates of a point in reciprocal space*, h, k, l.

Both are transformed by

$$(h', k', l') = (h, k, l)\boldsymbol{P}.$$

Usually, the Miller indices are made relative prime before and after the transformation.

The quantities which are covariant with respect to the basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ are *contravariant* with respect to the basis vectors $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ of reciprocal space.

The *basis vectors of reciprocal space* are written as a column matrix and their transformation is achieved by the matrix $\boldsymbol{Q}$:

$$\begin{pmatrix} \mathbf{a}^{*\prime} \\ \mathbf{b}^{*\prime} \\ \mathbf{c}^{*\prime} \end{pmatrix} = \boldsymbol{Q}\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix} = \begin{pmatrix} Q_{11}\mathbf{a}^* + Q_{12}\mathbf{b}^* + Q_{13}\mathbf{c}^* \\ Q_{21}\mathbf{a}^* + Q_{22}\mathbf{b}^* + Q_{23}\mathbf{c}^* \\ Q_{31}\mathbf{a}^* + Q_{32}\mathbf{b}^* + Q_{33}\mathbf{c}^* \end{pmatrix}.$$

The inverse transformation is obtained by the inverse matrix $\boldsymbol{P} = \boldsymbol{Q}^{-1}$:

$$\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix} = \boldsymbol{P}\begin{pmatrix} \mathbf{a}^{*\prime} \\ \mathbf{b}^{*\prime} \\ \mathbf{c}^{*\prime} \end{pmatrix}.$$

These transformation rules apply also to the quantities covariant with respect to the basis vectors $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ and contravariant with respect to $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, which are written as column matrices. They are the *indices of a direction* in direct space, [uvw], which are transformed by

$$\begin{pmatrix} u' \\ v' \\ w' \end{pmatrix} = \boldsymbol{Q}\begin{pmatrix} u \\ v \\ w \end{pmatrix}.$$

In contrast to all quantities mentioned above, the *components of a position vector* $\mathbf{r}$ or the *coordinates of a point X in direct space* x, y, z depend also on the shift of the origin in direct space. The general (affine) transformation is given by

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \boldsymbol{Q}\begin{pmatrix} x \\ y \\ z \end{pmatrix} + \boldsymbol{q} = \begin{pmatrix} Q_{11}x + Q_{12}y + Q_{13}z + q_1 \\ Q_{21}x + Q_{22}y + Q_{23}z + q_2 \\ Q_{31}x + Q_{32}y + Q_{33}z + q_3 \end{pmatrix}.$$

Example

If no shift of origin is applied, *i.e.* $\boldsymbol{p} = \boldsymbol{q} = \boldsymbol{o}$, the position vector $\mathbf{r}$ of point X is transformed by

$$\mathbf{r}' = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{PQ}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = (\mathbf{a}', \mathbf{b}', \mathbf{c}')\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}.$$

In this case, $\mathbf{r} = \mathbf{r}'$, *i.e.* the position vector is invariant, although the basis vectors and the components are transformed. For a pure shift of origin, *i.e.* $\boldsymbol{P} = \boldsymbol{Q} = \boldsymbol{I}$, the transformed position vector $\mathbf{r}'$ becomes

$$\begin{aligned} \mathbf{r}' &= (x + q_1)\mathbf{a} + (y + q_2)\mathbf{b} + (z + q_3)\mathbf{c} \\ &= \mathbf{r} + q_1\mathbf{a} + q_2\mathbf{b} + q_3\mathbf{c} \\ &= (x - p_1)\mathbf{a} + (y - p_2)\mathbf{b} + (z - p_3)\mathbf{c} \\ &= \mathbf{r} - p_1\mathbf{a} - p_2\mathbf{b} - p_3\mathbf{c}. \end{aligned}$$

Here the transformed vector $\mathbf{r}'$ is no longer identical with $\mathbf{r}$.

It is convenient to introduce the augmented (4×4) matrix $\mathbb{Q}$ which is composed of the matrices $\boldsymbol{Q}$ and $\boldsymbol{q}$ in the following manner (*cf.* Chapter 8.1):

$$\mathbb{Q} = \begin{pmatrix} \boldsymbol{Q} & \boldsymbol{q} \\ \boldsymbol{o} & 1 \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

with $\boldsymbol{o}$ the (1×3) row matrix containing zeros. In this notation, the transformed coordinates x', y', z' are obtained by

Table 5.1.3.1. *Selected 3×3 transformation matrices $\boldsymbol{P}$ and $\boldsymbol{Q} = \boldsymbol{P}^{-1}$*

For inverse transformations (against the arrow) replace $\boldsymbol{P}$ by $\boldsymbol{Q}$ and *vice versa.*

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
$\mathbf{c} \to \frac{1}{2}\mathbf{c}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	All systems
$\mathbf{b} \to \frac{1}{2}\mathbf{b}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	All systems
$\mathbf{a} \to \frac{1}{2}\mathbf{a}$	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	All systems
Cell choice 1 → cell choice 2: $\left\{\begin{matrix} P \to P \\ C \to A \end{matrix}\right.$ Cell choice 2 → cell choice 3: $\left\{\begin{matrix} P \to P \\ A \to I \end{matrix}\right.$ Unique axis **b** invariant Cell choice 3 → cell choice 1: $\left\{\begin{matrix} P \to P \\ I \to C \end{matrix}\right.$ (Fig. 5.1.3.2*a*)	$\begin{pmatrix} \bar{1} & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & \bar{1} \end{pmatrix}$	Monoclinic (*cf.* Section 2.2.16)
Cell choice 1 → cell choice 2: $\left\{\begin{matrix} P \to P \\ A \to B \end{matrix}\right.$ Cell choice 2 → cell choice 3: $\left\{\begin{matrix} P \to P \\ B \to I \end{matrix}\right.$ Unique axis **c** invariant Cell choice 3 → cell choice 1: $\left\{\begin{matrix} P \to P \\ I \to A \end{matrix}\right.$ (Fig. 5.1.3.2*b*)	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Monoclinic (*cf.* Section 2.2.16)
Cell choice 1 → cell choice 2: $\left\{\begin{matrix} P \to P \\ B \to C \end{matrix}\right.$ Cell choice 2 → cell choice 3: $\left\{\begin{matrix} P \to P \\ C \to I \end{matrix}\right.$ Unique axis **a** invariant Cell choice 3 → cell choice 1: $\left\{\begin{matrix} P \to P \\ I \to B \end{matrix}\right.$ (Fig. 5.1.3.2*c*)	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 1 \\ 0 & \bar{1} & 0 \end{pmatrix}$	Monoclinic (*cf.* Section 2.2.16)
Unique axis **b** → unique axis **c** Cell choice 1: $\left\{\begin{matrix} P \to P \\ C \to A \end{matrix}\right.$ Cell choice 2: $\left\{\begin{matrix} P \to P \\ A \to B \end{matrix}\right.$ Cell choice invariant Cell choice 3: $\left\{\begin{matrix} P \to P \\ I \to I \end{matrix}\right.$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	Monoclinic (*cf.* Section 2.2.16)
Unique axis **b** → unique axis **a** Cell choice 1: $\left\{\begin{matrix} P \to P \\ C \to B \end{matrix}\right.$ Cell choice 2: $\left\{\begin{matrix} P \to P \\ A \to C \end{matrix}\right.$ Cell choice invariant Cell choice 3: $\left\{\begin{matrix} P \to P \\ I \to I \end{matrix}\right.$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	Monoclinic (*cf.* Section 2.2.16)
Unique axis **c** → unique axis **a** Cell choice 1: $\left\{\begin{matrix} P \to P \\ A \to B \end{matrix}\right.$ Cell choice 2: $\left\{\begin{matrix} P \to P \\ B \to C \end{matrix}\right.$ Cell choice invariant Cell choice 3: $\left\{\begin{matrix} P \to P \\ I \to I \end{matrix}\right.$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	Monoclinic (*cf.* Section 2.2.16)
$I \to P$ (Fig. 5.1.3.3) $\quad \frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c}) \to (\mathbf{a}' + \mathbf{b}' + \mathbf{c}')$	$\begin{pmatrix} \frac{\bar{1}}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{\bar{1}}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{\bar{1}}{2} \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$	Orthorhombic Tetragonal Cubic

Table 5.1.3.1. *Selected 3 × 3 transformation matrices $\boldsymbol{P}$ and $\boldsymbol{Q} = \boldsymbol{P}^{-1}$* (*cont.*)

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
$F \rightarrow P$ (Fig. 5.1.3.4) $(\mathbf{a}+\mathbf{b}+\mathbf{c})$ invariant vector	$\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$	Orthorhombic Tetragonal Cubic
$(\mathbf{b}, \mathbf{a}, \bar{\mathbf{c}}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	Unconventional orthorhombic setting
$(\mathbf{c}, \mathbf{a}, \mathbf{b}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	Unconventional orthorhombic setting
$(\bar{\mathbf{c}}, \mathbf{b}, \mathbf{a}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	Unconventional orthorhombic setting
$(\mathbf{b}, \mathbf{c}, \mathbf{a}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	Unconventional orthorhombic setting
$(\mathbf{a}, \bar{\mathbf{c}}, \mathbf{b}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & \bar{1} & 0 \end{pmatrix}$	Unconventional orthorhombic setting
$\left.\begin{matrix} P \rightarrow C_1 \\ I \rightarrow F_1 \end{matrix}\right\}$ (Fig. 5.1.3.5) **c** axis invariant	$\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{\bar{1}}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Tetragonal (*cf.* Section 4.3.4)
$\left.\begin{matrix} P \rightarrow C_2 \\ I \rightarrow F_2 \end{matrix}\right\}$ (Fig. 5.1.3.5) **c** axis invariant	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{\bar{1}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Tetragonal (*cf.* Section 4.3.4)
Primitive rhombohedral cell → triple hexagonal cell R_1, obverse setting (Fig. 5.1.3.6*c*)	$\begin{pmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{2}{3} & \frac{\bar{1}}{3} & \frac{\bar{1}}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{\bar{2}}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → triple hexagonal cell R_2, obverse setting (Fig. 5.1.3.6*c*)	$\begin{pmatrix} 0 & \bar{1} & 1 \\ 1 & 0 & 1 \\ \bar{1} & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{\bar{1}}{3} & \frac{2}{3} & \frac{\bar{1}}{3} \\ \frac{\bar{2}}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → triple hexagonal cell R_3, obverse setting (Fig. 5.1.3.6*c*)	$\begin{pmatrix} \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \\ 1 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{\bar{1}}{3} & \frac{\bar{1}}{3} & \frac{2}{3} \\ \frac{1}{3} & \frac{\bar{2}}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → triple hexagonal cell R_1, reverse setting (Fig. 5.1.3.6*d*)	$\begin{pmatrix} \bar{1} & 0 & 1 \\ 1 & \bar{1} & 1 \\ 0 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{\bar{2}}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{\bar{1}}{3} & \frac{\bar{1}}{3} & \frac{2}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → triple hexagonal cell R_2, reverse setting (Fig. 5.1.3.6*d*)	$\begin{pmatrix} 0 & 1 & 1 \\ \bar{1} & 0 & 1 \\ 1 & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{3} & \frac{\bar{2}}{3} & \frac{1}{3} \\ \frac{2}{3} & \frac{\bar{1}}{3} & \frac{\bar{1}}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → triple hexagonal cell R_3, reverse setting (Fig. 5.1.3.6*d*)	$\begin{pmatrix} 1 & \bar{1} & 1 \\ 0 & 1 & 1 \\ \bar{1} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & \frac{\bar{2}}{3} \\ \frac{\bar{1}}{3} & \frac{2}{3} & \frac{\bar{1}}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Hexagonal cell P → orthohexagonal centred cell C_1 (Fig. 5.1.3.7)	$\begin{pmatrix} 1 & 1 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \frac{\bar{1}}{2} & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)
Hexagonal cell P → orthohexagonal centred cell C_2 (Fig. 5.1.3.7)	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{\bar{1}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)
Hexagonal cell P → orthohexagonal centred cell C_3 (Fig. 5.1.3.7)	$\begin{pmatrix} 0 & \bar{2} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{\bar{1}}{2} & 1 & 0 \\ \frac{\bar{1}}{2} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)

Table 5.1.3.1. *Selected 3 × 3 transformation matrices* $\boldsymbol{P}$ *and* $\boldsymbol{Q} = \boldsymbol{P}^{-1}$ (*cont.*)

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
Hexagonal cell P → triple hexagonal cell H_1 (Fig. 5.1.3.8)	$\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{2}{3} & \frac{\bar{1}}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)
Hexagonal cell P → triple hexagonal cell H_2 (Fig. 5.1.3.8)	$\begin{pmatrix} 2 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & 0 \\ \frac{\bar{1}}{3} & \frac{2}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)
Hexagonal cell P → triple hexagonal cell H_3 (Fig. 5.1.3.8)	$\begin{pmatrix} 1 & \bar{2} & 0 \\ 2 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{\bar{1}}{3} & \frac{2}{3} & 0 \\ \frac{\bar{2}}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)
Hexagonal cell P → triple rhombohedral cell D_1	$\begin{pmatrix} 1 & 0 & \bar{1} \\ 0 & 1 & \bar{1} \\ 1 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{2}{3} & \frac{\bar{1}}{3} & \frac{1}{3} \\ \frac{\bar{1}}{3} & \frac{2}{3} & \frac{1}{3} \\ \frac{\bar{1}}{3} & \frac{\bar{1}}{3} & \frac{1}{3} \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)
Hexagonal cell P → triple rhombohedral cell D_2	$\begin{pmatrix} \bar{1} & 0 & 1 \\ 0 & \bar{1} & 1 \\ 1 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{\bar{2}}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{\bar{2}}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)
Triple hexagonal cell R, obverse setting → C-centred monoclinic cell, unique axis **b**, cell choice 1 (Fig. 5.1.3.9*a*) **c** and **b** axes invariant	$\begin{pmatrix} \frac{2}{3} & 0 & 0 \\ \frac{1}{3} & 1 & 0 \\ \frac{\bar{2}}{3} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{3}{2} & 0 & 0 \\ \frac{\bar{1}}{2} & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Triple hexagonal cell R, obverse setting → C-centred monoclinic cell, unique axis **b**, cell choice 2 (Fig. 5.1.3.9*a*) **c** axis invariant	$\begin{pmatrix} \frac{\bar{1}}{3} & \bar{1} & 0 \\ \frac{1}{3} & \bar{1} & 0 \\ \frac{\bar{2}}{3} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{\bar{3}}{2} & \frac{3}{2} & 0 \\ \frac{\bar{1}}{2} & \frac{\bar{1}}{2} & 0 \\ \bar{1} & 1 & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Triple hexagonal cell R, obverse setting → C-centred monoclinic cell, unique axis **b**, cell choice 3 (Fig. 5.1.3.9*a*) $\mathbf{a}_{\rm h} \rightarrow \mathbf{b}_{\rm m}, \mathbf{c}$ axis invariant	$\begin{pmatrix} \frac{\bar{1}}{3} & 1 & 0 \\ \frac{\bar{2}}{3} & 0 & 0 \\ \frac{\bar{2}}{3} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & \frac{\bar{3}}{2} & 0 \\ 1 & \frac{\bar{1}}{2} & 0 \\ 0 & \bar{1} & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Triple hexagonal cell R, obverse setting → A-centred monoclinic cell, unique axis **c**, cell choice 1 (Fig. 5.1.3.9*b*) $\mathbf{b}_{\rm h} \rightarrow \mathbf{c}_{\rm m}, \mathbf{c}_{\rm h} \rightarrow \mathbf{a}_{\rm m}$	$\begin{pmatrix} 0 & \frac{2}{3} & 0 \\ 0 & \frac{1}{3} & 1 \\ 1 & \frac{\bar{2}}{3} & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 1 \\ \frac{3}{2} & 0 & 0 \\ \frac{\bar{1}}{2} & 1 & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Triple hexagonal cell R, obverse setting → A-centred monoclinic cell, unique axis **c**, cell choice 2 (Fig. 5.1.3.9*b*) $\mathbf{c}_{\rm h} \rightarrow \mathbf{a}_{\rm m}$	$\begin{pmatrix} 0 & \frac{\bar{1}}{3} & \bar{1} \\ 0 & \frac{1}{3} & \bar{1} \\ 1 & \frac{\bar{2}}{3} & 0 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 1 \\ \frac{\bar{3}}{2} & \frac{3}{2} & 0 \\ \frac{\bar{1}}{2} & \frac{\bar{1}}{2} & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Triple hexagonal cell R, obverse setting → A-centred monoclinic cell, unique axis **c**, cell choice 3 (Fig. 5.1.3.9*b*) $\mathbf{a}_{\rm h} \rightarrow \mathbf{c}_{\rm m}, \mathbf{c}_{\rm h} \rightarrow \mathbf{a}_{\rm m}$	$\begin{pmatrix} 0 & \frac{\bar{1}}{3} & 1 \\ 0 & \frac{\bar{2}}{3} & 0 \\ 1 & \frac{\bar{2}}{3} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \bar{1} & 1 \\ 0 & \frac{\bar{3}}{2} & 0 \\ 1 & \frac{\bar{1}}{2} & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → C-centred monoclinic cell, unique axis **b**, cell choice 1 (Fig. 5.1.3.10*a*) $[111]_{\rm r} \rightarrow \mathbf{c}_{\rm m}$	$\begin{pmatrix} 0 & 0 & 1 \\ \bar{1} & 1 & 1 \\ \bar{1} & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \frac{\bar{1}}{2} & \frac{\bar{1}}{2} \\ 0 & \frac{1}{2} & \frac{\bar{1}}{2} \\ 1 & 0 & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → C-centred monoclinic cell, unique axis **b**, cell choice 2 (Fig. 5.1.3.10*a*) $[111]_{\rm r} \rightarrow \mathbf{c}_{\rm m}$	$\begin{pmatrix} \bar{1} & \bar{1} & 1 \\ 0 & 0 & 1 \\ \bar{1} & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{\bar{1}}{2} & 1 & \frac{\bar{1}}{2} \\ \frac{\bar{1}}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → C-centred monoclinic cell, unique axis **b**, cell choice 3 (Fig. 5.1.3.10*a*) $[111]_{\rm r} \rightarrow \mathbf{c}_{\rm m}$	$\begin{pmatrix} \bar{1} & 1 & 1 \\ \bar{1} & \bar{1} & 1 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{\bar{1}}{2} & \frac{\bar{1}}{2} & 1 \\ \frac{1}{2} & \frac{\bar{1}}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → A-centred monoclinic cell, unique axis **c**, cell choice 1 (Fig. 5.1.3.10*b*) $[111]_{\rm r} \rightarrow \mathbf{a}_{\rm m}$	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 1 \\ 1 & \bar{1} & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & \frac{\bar{1}}{2} & \frac{\bar{1}}{2} \\ 0 & \frac{1}{2} & \frac{\bar{1}}{2} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → A-centred monoclinic cell, unique axis **c**, cell choice 2 (Fig. 5.1.3.10*b*) $[111]_{\rm r} \rightarrow \mathbf{a}_{\rm m}$	$\begin{pmatrix} 1 & \bar{1} & \bar{1} \\ 1 & 0 & 0 \\ 1 & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ \frac{\bar{1}}{2} & 1 & \frac{\bar{1}}{2} \\ \frac{\bar{1}}{2} & 0 & \frac{1}{2} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)

Table 5.1.3.1. *Selected 3 × 3 transformation matrices* $\boldsymbol{P}$ *and* $\boldsymbol{Q} = \boldsymbol{P}^{-1}$ (*cont.*)

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
Primitive rhombohedral cell → *A*-centred monoclinic cell, unique axis **c**, cell choice 3 (Fig. 5.1.3.10*b*) $[111]_{\rm r} \rightarrow \mathbf{a}_{\rm m}$	$\begin{pmatrix} 1 & \bar{1} & 1 \\ 1 & \bar{1} & \bar{1} \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ \frac{\bar{1}}{2} & \frac{\bar{1}}{2} & 1 \\ \frac{1}{2} & \frac{\bar{1}}{2} & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)

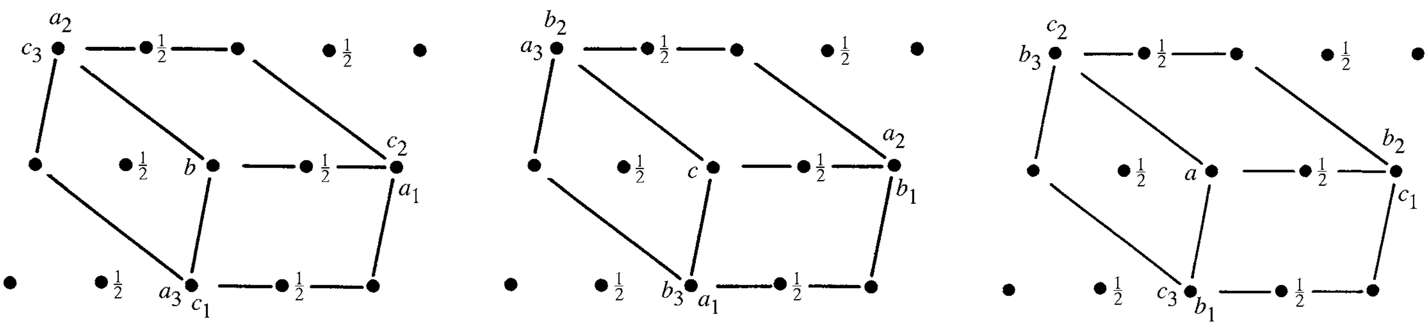

Fig. 5.1.3.2. Monoclinic centred lattice, projected along the unique axis. Origin for all cells is the same.

(*a*) Unique axis *b:*
Cell choice 1: *C*-centred cell a_1, b, c_1.
Cell choice 2: *A*-centred cell a_2, b, c_2.
Cell choice 3: *I*-centred cell a_3, b, c_3.

(*b*) Unique axis *c:*
Cell choice 1: *A*-centred cell a_1, b_1, c.
Cell choice 2: *B*-centred cell a_2, b_2, c.
Cell choice 3: *I*-centred cell a_3, b_3, c.

(*c*) Unique axis *a:*
Cell choice 1: *B*-centred cell a, b_1, c_1.
Cell choice 2: *C*-centred cell a, b_2, c_2.
Cell choice 3: *I*-centred cell a, b_3, c_3.

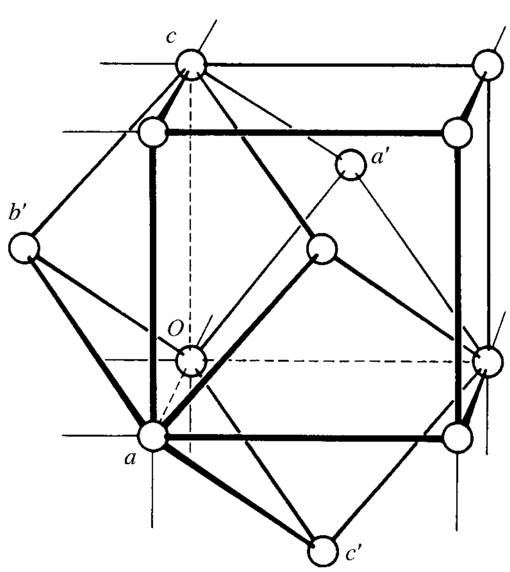

Fig. 5.1.3.3. Body-centred cell *I* with *a*, *b*, *c* and a corresponding primitive cell *P* with *a*′, *b*′, *c*′. Origin for both cells *O*. A cubic *I* cell with lattice constant a_c can be considered as a primitive rhombohedral cell with $a_r = a_c \frac{1}{2}\sqrt{3}$ and $\alpha = 109.47°$ (rhombohedral axes) or a triple hexagonal cell with $a_h = a_c\sqrt{2}$ and $c_h = a_c \frac{1}{2}\sqrt{3}$ (hexagonal axes).

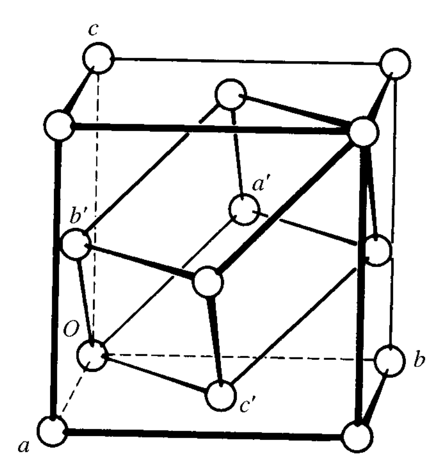

Fig. 5.1.3.4. Face-centred cell *F* with *a*, *b*, *c* and a corresponding primitive cell *P* with *a*′, *b*′, *c*′. Origin for both cells *O*. A cubic *F* cell with lattice constant a_c can be considered as a primitive rhombohedral cell with $a_r = a_c \frac{1}{2}\sqrt{2}$ and $\alpha = 60°$ (rhombohedral axes) or a triple hexagonal cell with $a_h = a_c \frac{1}{2}\sqrt{2}$ and $c_h = a_c\sqrt{3}$ (hexagonal axes).

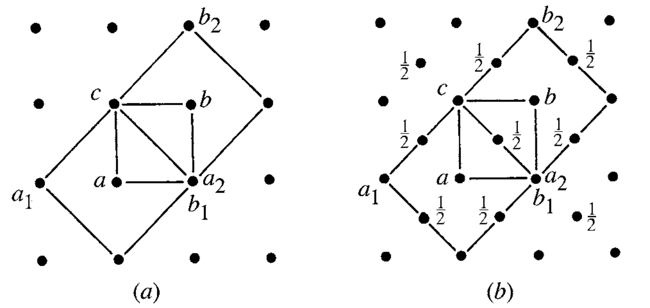

Fig. 5.1.3.5. Tetragonal lattices, projected along $[00\bar{1}]$. (*a*) Primitive cell *P* with a, b, c and the *C*-centred cells C_1 with a_1, b_1, c and C_2 with a_2, b_2, c. Origin for all three cells is the same. (*b*) Body-centred cell *I* with a, b, c and the *F*-centred cells F_1 with a_1, b_1, c and F_2 with a_2, b_2, c. Origin for all three cells is the same.

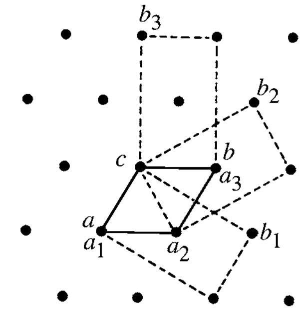

Fig. 5.1.3.7. Hexagonal lattice projected along $[00\bar{1}]$. Primitive hexagonal cell *P* with a, b, c and the three *C*-centred (orthohexagonal) cells a_1, b_1, c; a_2, b_2, c; a_3, b_3, c. Origin for all cells is the same.

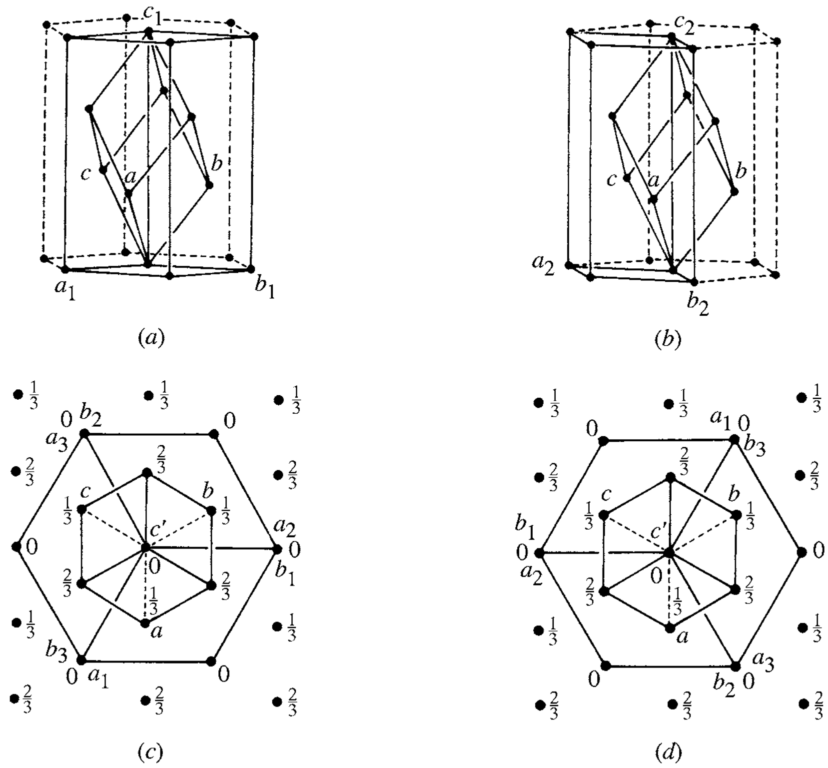

Fig. 5.1.3.6. Unit cells in the rhombohedral lattice: same origin for all cells. The basis of the rhombohedral cell is labelled a, b, c. Two settings of the triple hexagonal cell are possible with respect to a primitive rhombohedral cell: The *obverse setting* with the lattice points $0, 0, 0; \frac{2}{3}, \frac{1}{3}, \frac{1}{3}; \frac{1}{3}, \frac{2}{3}, \frac{2}{3}$ has been used in *International Tables* since 1952. Its general reflection condition is $-h + k + l = 3n$. The *reverse setting* with lattice points $0, 0, 0; \frac{1}{3}, \frac{2}{3}, \frac{1}{3}; \frac{2}{3}, \frac{1}{3}, \frac{2}{3}$ was used in the 1935 edition. Its general reflection condition is $h - k + l = 3n$. (*a*) Obverse setting of triple hexagonal cell a_1, b_1, c_1 in relation to the primitive rhombohedral cell a, b, c. (*b*) Reverse setting of triple hexagonal cell a_2, b_2, c_2 in relation to the primitive rhombohedral cell a, b, c. (*c*) Primitive rhombohedral cell (--- lower edges), a, b, c in relation to the three triple hexagonal cells in obverse setting a_1, b_1, c'; a_2, b_2, c'; a_3, b_3, c'. Projection along c'. (*d*) Primitive rhombohedral cell (- - - lower edges), a, b, c in relation to the three triple hexagonal cells in reverse setting a_1, b_1, c'; a_2, b_2, c'; a_3, b_3, c'. Projection along c'.

$$\begin{pmatrix} x' \\ y' \\ z' \\ 1 \end{pmatrix} = \mathbb{Q} \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix} = \begin{pmatrix} Q_{11}x + Q_{12}y + Q_{13}z + q_1 \\ Q_{21}x + Q_{22}y + Q_{23}z + q_2 \\ Q_{31}x + Q_{32}y + Q_{33}z + q_3 \\ 1 \end{pmatrix}.$$

The inverse of the augmented matrix $\mathbb{Q}$ is the augmented matrix $\mathbb{P}$ which contains the matrices $\boldsymbol{P}$ and $\boldsymbol{p}$, specifically,

$$\mathbb{P} = \mathbb{Q}^{-1} = \begin{pmatrix} \boldsymbol{P} & \boldsymbol{p} \\ \boldsymbol{o} & 1 \end{pmatrix} = \begin{pmatrix} \boldsymbol{Q}^{-1} & -\boldsymbol{Q}^{-1}\boldsymbol{q} \\ \boldsymbol{o} & 1 \end{pmatrix}.$$

The advantage of the use of (4×4) matrices is that a sequence of affine transformations corresponds to the product of the correspond-

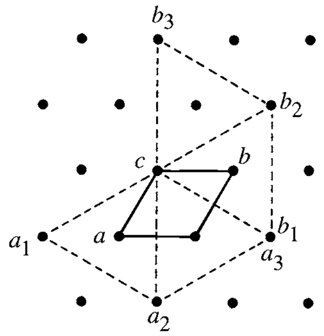

Fig. 5.1.3.8. Hexagonal lattice projected along $[00\bar{1}]$. Primitive hexagonal cell P with a, b, c and the three triple hexagonal cells H with a_1, b_1, c; a_2, b_2, c; a_3, b_3, c. Origin for all cells is the same.

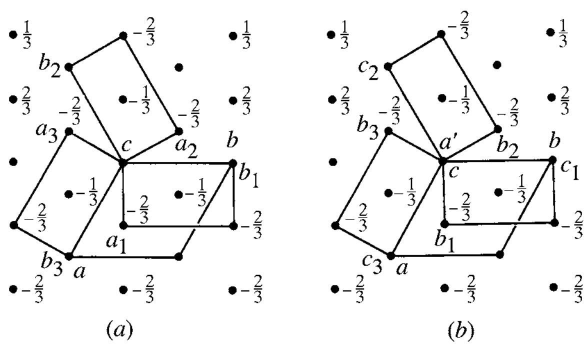

Fig. 5.1.3.9. Rhombohedral lattice with a triple hexagonal unit cell a, b, c in obverse setting (*i.e.* unit cell a_1, b_1, c in Fig. 5.1.3.6*c*) and the three centred monoclinic cells. (*a*) *C*-centred cells C_1 with a_1, b_1, c; C_2 with a_2, b_2, c; and C_3 with a_3, b_3, c. The unique monoclinic axes are b_1, b_2 and b_3, respectively. Origin for all four cells is the same. (*b*) *A*-centred cells A_1 with a', b_1, c_1; A_2 with a', b_2, c_2; and A_3 with a', b_3, c_3. The unique monoclinic axes are c_1, c_2 and c_3, respectively. Origin for all four cells is the same.

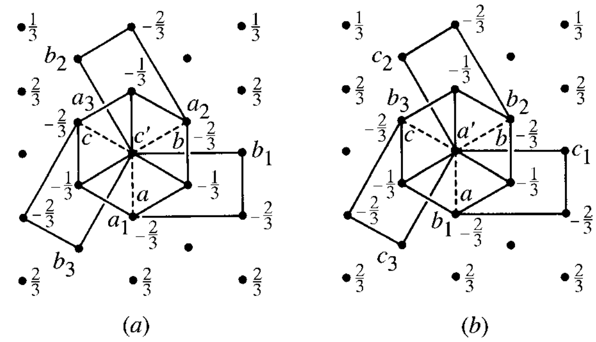

Fig. 5.1.3.10. Rhombohedral lattice with primitive rhombohedral cell a, b, c and the three centred monoclinic cells. (*a*) *C*-centred cells C_1 with a_1, b_1, c'; C_2 with a_2, b_2, c'; and C_3 with a_3, b_3, c'. The unique monoclinic axes are b_1, b_2 and b_3, respectively. Origin for all four cells is the same. (*b*) *A*-centred cells A_1 with a', b_1, c_1; A_2 with a', b_2, c_2; and A_3 with a', b_3, c_3. The unique monoclinic axes are c_1, c_2 and c_3, respectively. Origin for all four cells is the same.

ing matrices. However, the order of the factors in the product must be observed. If $\mathbb{Q}$ is the product of n transformation matrices $\mathbb{Q}_i$,

$$\mathbb{Q} = \mathbb{Q}_n \ldots \mathbb{Q}_2\mathbb{Q}_1,$$

the sequence of the corresponding inverse matrices $\mathbb{P}_i$ is reversed in the product

$$\mathbb{P} = \mathbb{P}_1\mathbb{P}_2 \ldots \mathbb{P}_n.$$

The following items are also affected by a transformation:

(i) The *metric matrix of direct lattice* $\boldsymbol{G}$ [more exactly: the matrix of geometrical coefficients (metric tensor)] is transformed by the matrix $\boldsymbol{P}$ as follows:

$$\boldsymbol{G}' = \boldsymbol{P}^t\boldsymbol{G}\boldsymbol{P}$$

with $\boldsymbol{P}^t$ the transposed matrix of $\boldsymbol{P}$, *i.e.* rows and columns of $\boldsymbol{P}$ are interchanged. Specifically,

$$\begin{aligned}\boldsymbol{G}' &= \begin{pmatrix} \mathbf{a}'\cdot\mathbf{a}' & \mathbf{a}'\cdot\mathbf{b}' & \mathbf{a}'\cdot\mathbf{c}' \\ \mathbf{b}'\cdot\mathbf{a}' & \mathbf{b}'\cdot\mathbf{b}' & \mathbf{b}'\cdot\mathbf{c}' \\ \mathbf{c}'\cdot\mathbf{a}' & \mathbf{c}'\cdot\mathbf{b}' & \mathbf{c}'\cdot\mathbf{c}' \end{pmatrix} \\ &= \begin{pmatrix} P_{11} & P_{21} & P_{31} \\ P_{12} & P_{22} & P_{32} \\ P_{13} & P_{23} & P_{33} \end{pmatrix} \begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c} \\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \end{pmatrix} \\ &\quad\times \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}.\end{aligned}$$

(ii) The *metric matrix of reciprocal lattice* $\boldsymbol{G}^*$ [more exactly: the matrix of geometrical coefficients (metric tensor)] is transformed by

$$\boldsymbol{G}^{*\prime} = \boldsymbol{Q}\boldsymbol{G}^*\boldsymbol{Q}^t.$$

Here, the transposed matrix $\boldsymbol{Q}^t$ is on the right-hand side of $\boldsymbol{G}^*$.

(iii) The *volume of the unit cell* V changes with the transformation. The volume of the new unit cell V' is obtained by

$$V' = \det(\boldsymbol{P})V = \begin{vmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{vmatrix} V$$

with $\det(\boldsymbol{P})$ the determinant of the matrix $\boldsymbol{P}$. The corresponding equation for the volume of the unit cell in reciprocal space V^* is

$$V^{*\prime} = \det(\boldsymbol{Q})V^*.$$

Matrices $\boldsymbol{P}$ and $\boldsymbol{Q}$ that frequently occur in crystallography are listed in Table 5.1.3.1.

International Tables for Crystallography (2006). Vol. A, Chapter 5.2, pp. 86–89.

5.2. Transformations of symmetry operations (motions)

BY H. ARNOLD

5.2.1. Transformations

Symmetry operations are transformations in which the coordinate system, *i.e.* the basis vectors **a**, **b**, **c** and the origin O, are considered to be at rest, whereas the object is mapped onto itself. This can be visualized as a 'motion' of an object in such a way that the object before and after the 'motion' cannot be distinguished.

A symmetry operation W transforms every point X with the coordinates x, y, z to a symmetrically equivalent point $\tilde{X}$ with the coordinates $\tilde{x}, \tilde{y}, \tilde{z}$. In matrix notation, this transformation is performed by

$$\begin{pmatrix}\tilde{x}\\ \tilde{y}\\ \tilde{z}\end{pmatrix} = \begin{pmatrix}W_{11} & W_{12} & W_{13}\\ W_{21} & W_{22} & W_{23}\\ W_{31} & W_{32} & W_{33}\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} + \begin{pmatrix}w_1\\ w_2\\ w_3\end{pmatrix} = \begin{pmatrix}W_{11}x + W_{12}y + W_{13}z + w_1\\ W_{21}x + W_{22}y + W_{23}z + w_2\\ W_{31}x + W_{32}y + W_{33}z + w_3\end{pmatrix}.$$

The (3×3) matrix $\boldsymbol{W}$ is the rotation part and the (3×1) column matrix $\boldsymbol{w}$ the translation part of the symmetry operation W. The pair $(\boldsymbol{W}, \boldsymbol{w})$ characterizes the operation uniquely. Matrices $\boldsymbol{W}$ for point-group operations are given in Tables 11.2.2.1 and 11.2.2.2.

Again, we can introduce the augmented (4×4) matrix (*cf.* Chapter 8.1)

$$\mathbb{W} = \begin{pmatrix}\boldsymbol{W} & \boldsymbol{w}\\ \boldsymbol{o} & 1\end{pmatrix} = \begin{pmatrix}W_{11} & W_{12} & W_{13} & w_1\\ W_{21} & W_{22} & W_{23} & w_2\\ W_{31} & W_{32} & W_{33} & w_3\\ 0 & 0 & 0 & 1\end{pmatrix}.$$

The coordinates $\tilde{x}, \tilde{y}, \tilde{z}$ of the point $\tilde{X}$, symmetrically equivalent to X with the coordinates x, y, z, are obtained by

$$\begin{pmatrix}\tilde{x}\\ \tilde{y}\\ \tilde{z}\\ 1\end{pmatrix} = \begin{pmatrix}W_{11} & W_{12} & W_{13} & w_1\\ W_{21} & W_{22} & W_{23} & w_2\\ W_{31} & W_{32} & W_{33} & w_3\\ 0 & 0 & 0 & 1\end{pmatrix}\begin{pmatrix}x\\ y\\ z\\ 1\end{pmatrix} = \begin{pmatrix}W_{11}x + W_{12}y + W_{13}z + w_1\\ W_{21}x + W_{22}y + W_{23}z + w_2\\ W_{31}x + W_{32}y + W_{33}z + w_3\\ 1\end{pmatrix},$$

or, in short notation,

$$\tilde{\mathbb{x}} = \mathbb{W}\mathbb{x}.$$

A sequence of symmetry operations can be obtained as a product of (4×4) matrices $\mathbb{W}$.

An affine transformation of the coordinate system transforms the coordinates $\mathbb{x}$ of the starting point

$$\mathbb{x}' = \mathbb{Q}\mathbb{x}$$

as well as the coordinates $\tilde{\mathbb{x}}$ of a symmetrically equivalent point

$$\begin{aligned}\tilde{\mathbb{x}}' &= \mathbb{Q}\tilde{\mathbb{x}}\\ &= \mathbb{Q}\mathbb{W}\mathbb{x}\\ &= \mathbb{Q}\mathbb{W}\mathbb{P}\mathbb{Q}\mathbb{x} \qquad (\text{with } \mathbb{P} = \mathbb{Q}^{-1})\\ &= \mathbb{Q}\mathbb{W}\mathbb{P}\mathbb{x}'.\end{aligned}$$

Thus, the affine transformation transforms also the symmetry-operation matrix $\mathbb{W}$ and the new matrix $\mathbb{W}'$ is obtained by

$$\mathbb{W}' = \mathbb{Q}\mathbb{W}\mathbb{P}.$$

Example

Space group $P4/n$ (85) is listed in the space-group tables with two origins; origin choice 1 with $\bar{4}$, origin choice 2 with $\bar{1}$ as point symmetry of the origin. How does the matrix $\mathbb{W}$ of the symmetry operation $\bar{4}^+$ $0, 0, z$; $0, 0, 0$ of origin choice 1 transform to the matrix $\mathbb{W}'$ of symmetry operation $\bar{4}^+ \frac{1}{4}, -\frac{1}{4}, z$; $\frac{1}{4}, -\frac{1}{4}, 0$ of origin choice 2?

In the space-group tables, origin choice 1, the transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z} = y, \bar{x}, \bar{z}$ are listed. The translation part is zero, *i.e.* $\boldsymbol{w} = (0/0/0)$. In Table 11.2.2.1, the matrix $\boldsymbol{W}$ can be found. Thus, the (4×4) matrix $\mathbb{W}$ is obtained:

$$\mathbb{W} = \begin{pmatrix}\boldsymbol{W} & \boldsymbol{w}\\ \boldsymbol{o} & \mathbf{1}\end{pmatrix} = \begin{pmatrix}0 & 1 & 0 & 0\\ \bar{1} & 0 & 0 & 0\\ 0 & 0 & \bar{1} & 0\\ 0 & 0 & 0 & 1\end{pmatrix}.$$

The transformation to origin choice 2 is accomplished by a shift vector **p** with components $\frac{1}{4}, -\frac{1}{4}, 0$. Since this is a pure shift, the matrices $\boldsymbol{P}$ and $\boldsymbol{Q}$ are the unit matrix $\boldsymbol{I}$. Now the shift vector $\boldsymbol{q}$ is derived: $\boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p} = -\boldsymbol{I}\boldsymbol{p} = -\boldsymbol{p}$. Thus, the matrices $\mathbb{P}$ and $\mathbb{Q}$ are

$$\mathbb{P} = \begin{pmatrix}1 & 0 & 0 & \frac{1}{4}\\ 0 & 1 & 0 & \frac{\bar{1}}{4}\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}, \quad \mathbb{Q} = \begin{pmatrix}1 & 0 & 0 & \frac{\bar{1}}{4}\\ 0 & 1 & 0 & \frac{1}{4}\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}.$$

By matrix multiplication, the new matrix $\mathbb{W}'$ is obtained:

$$\mathbb{W}' = \mathbb{Q}\mathbb{W}\mathbb{P} = \begin{pmatrix}0 & 1 & 0 & \frac{\bar{1}}{2}\\ \bar{1} & 0 & 0 & 0\\ 0 & 0 & \bar{1} & 0\\ 0 & 0 & 0 & 1\end{pmatrix}.$$

If the matrix $\mathbb{W}'$ is applied to x', y', z', the coordinates of the starting point in the new coordinate system, we obtain the transformed coordinates $\tilde{x}', \tilde{y}', \tilde{z}'$,

$$\begin{pmatrix}\tilde{x}'\\ \tilde{y}'\\ \tilde{z}'\\ 1\end{pmatrix} = \begin{pmatrix}0 & 1 & 0 & \frac{\bar{1}}{2}\\ \bar{1} & 0 & 0 & 0\\ 0 & 0 & \bar{1} & 0\\ 0 & 0 & 0 & 1\end{pmatrix}\begin{pmatrix}x'\\ y'\\ z'\\ 1\end{pmatrix} = \begin{pmatrix}y' - \frac{1}{2}\\ \bar{x}'\\ \bar{z}'\\ 1\end{pmatrix}.$$

By adding a lattice translation **a**, the transformed coordinates $y + \frac{1}{2}, \bar{x}, \bar{z}$ are obtained as listed in the space-group tables for origin choice 2.

5.2.2. Invariants

A crystal structure and its physical properties are independent of the choice of the unit cell. This implies that invariants occur, *i.e.* quantities which have the same values before and after the transformation. Only some important invariants are considered in this section. Invariants of higher order (tensors) are treated by Altmann & Herzig (1994), second cumulant tensors, *i.e.* anisotropic temperature factors, are given in *International Tables for Crystallography* (2004), Vol. C.

The *orthogonality of the basis vectors* **a**, **b**, **c** of direct space and the basis vectors $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ of reciprocal space,

$$\begin{pmatrix}\mathbf{a}^*\\ \mathbf{b}^*\\ \mathbf{c}^*\end{pmatrix}(\mathbf{a},\mathbf{b},\mathbf{c})=\begin{pmatrix}\mathbf{a}^*\cdot\mathbf{a} & \mathbf{a}^*\cdot\mathbf{b} & \mathbf{a}^*\cdot\mathbf{c}\\ \mathbf{b}^*\cdot\mathbf{a} & \mathbf{b}^*\cdot\mathbf{b} & \mathbf{b}^*\cdot\mathbf{c}\\ \mathbf{c}^*\cdot\mathbf{a} & \mathbf{c}^*\cdot\mathbf{b} & \mathbf{c}^*\cdot\mathbf{c}\end{pmatrix}=\boldsymbol{I},$$

is invariant under a general (affine) transformation. Since both sets of basis vectors are transformed, $\mathbf{a}^*$ is always perpendicular to the plane defined by **b** and **c** and $\mathbf{a}^{*\prime}$ perpendicular to $\mathbf{b}'$ and $\mathbf{c}'$ *etc.*

5.2.2.1. *Position vector*

The position vector **r** in direct space,

$$\mathbf{r}=(\mathbf{a},\mathbf{b},\mathbf{c})\begin{pmatrix}x\\ y\\ z\end{pmatrix}=x\mathbf{a}+y\mathbf{b}+z\mathbf{c},$$

is invariant if the origin of the coordinate system is not changed in the transformation (see example in Section 5.1.3).

5.2.2.2. *Modulus of position vector*

The modulus r of the position vector **r** gives the distance of the point x, y, z from the origin. Its square is obtained by the scalar product

$$\begin{aligned}\mathbf{r}^{t}\cdot\mathbf{r}=r^2&=(x,y,z)\begin{pmatrix}\mathbf{a}\\ \mathbf{b}\\ \mathbf{c}\end{pmatrix}(\mathbf{a},\mathbf{b},\mathbf{c})\begin{pmatrix}x\\ y\\ z\end{pmatrix}\\ &=(x,y,z)\boldsymbol{G}\begin{pmatrix}x\\ y\\ z\end{pmatrix}\\ &=x^2a^2+y^2b^2+z^2c^2+2yzbc\cos\alpha\\ &\quad+2xzac\cos\beta+2xyab\cos\gamma,\end{aligned}$$

with $\mathbf{r}^{t}$ the transposed representation of **r**; a, b, c the moduli of the basis vectors **a**, **b**, **c** (lattice parameters); $\boldsymbol{G}$ the metric matrix of direct space; and α, β, γ the angles of the unit cell.

The same considerations apply to the vector $\mathbf{r}^*$ in reciprocal space and its modulus r^*. Here, $\boldsymbol{G}^*$ is applied. Note that $\mathbf{r}^*$ and r^* are independent of the choice of the origin in direct space.

5.2.2.3. *Metric matrix*

The metric matrix $\boldsymbol{G}$ of the unit cell in the direct lattice

$$\boldsymbol{G}=\begin{pmatrix}\mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c}\\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c}\\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c}\end{pmatrix}=\begin{pmatrix}aa & ab\cos\gamma & ac\cos\beta\\ ba\cos\gamma & bb & bc\cos\alpha\\ ca\cos\beta & cb\cos\alpha & cc\end{pmatrix}$$

changes under a linear transformation, but $\boldsymbol{G}$ is invariant under a symmetry operation of the lattice. The volume of the unit cell V is obtained by

$$V^2=\det(\boldsymbol{G}).$$

The same considerations apply to the metric matrix $\boldsymbol{G}^*$ of the unit cell in the reciprocal lattice and the volume V^* of the reciprocal-lattice unit cell. Thus, there are two invariants under an affine transformation, the product

$$VV^*=1$$

and the product

$$\boldsymbol{G}\boldsymbol{G}^*=\boldsymbol{I}.$$

5.2.2.4. *Scalar product*

The scalar product

$$\mathbf{r}^*\cdot\mathbf{r}=hx+ky+lz$$

of the vector $\mathbf{r}^*$ in reciprocal space with the vector **r** in direct space is invariant under a linear transformation but not under a shift of origin in direct space.

A vector **r** in direct space can also be represented as a product of augmented matrices:

$$\mathbf{r}=(\mathbf{a},\mathbf{b},\mathbf{c},0)\begin{pmatrix}x\\ y\\ z\\ 1\end{pmatrix}=x\mathbf{a}+y\mathbf{b}+z\mathbf{c}.$$

As stated above, the basis vectors are transformed only by the linear part, even in the case of a general affine transformation. Thus, the transformed position vector $\mathbf{r}'$ is obtained by

$$\mathbf{r}'=(\mathbf{a},\mathbf{b},\mathbf{c},0)\begin{pmatrix}\boldsymbol{P} & \boldsymbol{o}^t\\ \boldsymbol{o} & 1\end{pmatrix}\begin{pmatrix}\boldsymbol{Q} & \boldsymbol{q}\\ \boldsymbol{o} & 1\end{pmatrix}\begin{pmatrix}x\\ y\\ z\\ 1\end{pmatrix}.$$

The shift $\boldsymbol{p}$ is set to zero. The shift of origin is contained in the matrix $\mathbb{Q}$ only.

Similarly, a vector in reciprocal space can be represented by

$$\mathbf{r}^*=(h,k,l,1)\begin{pmatrix}\mathbf{a}^*\\ \mathbf{b}^*\\ \mathbf{c}^*\\ 0\end{pmatrix}=h\mathbf{a}^*+k\mathbf{b}^*+l\mathbf{c}^*.$$

The coordinates h, k, l in reciprocal space transform also only linearly. Thus,

$$\mathbf{r}^{*\prime}=(h,k,l,1)\begin{pmatrix}\boldsymbol{P} & \boldsymbol{o}^t\\ \boldsymbol{o} & 1\end{pmatrix}\begin{pmatrix}\boldsymbol{Q} & \boldsymbol{q}\\ \boldsymbol{o} & 1\end{pmatrix}\begin{pmatrix}\mathbf{a}^*\\ \mathbf{b}^*\\ \mathbf{c}^*\\ 0\end{pmatrix}.$$

The reader can see immediately that the scalar product $\mathbf{r}^*\cdot\mathbf{r}$ transforms correctly.

5.2.3. Example: low cristobalite and high cristobalite

The positions of the silicon atoms in the low-cristobalite structure (Nieuwenkamp, 1935) are compared with those of the high-cristobalite structure (Wyckoff, 1925; *cf.* Megaw, 1973). At low temperatures, the space group is $P4_12_12$ (92). The four silicon atoms are located in Wyckoff position 4(*a*) ..2 with the coordinates $x, x, 0$; $\bar{x}, \bar{x}, \frac{1}{2}$; $\frac{1}{2}-x, \frac{1}{2}+x, \frac{1}{4}$; $\frac{1}{2}+x, \frac{1}{2}-x, \frac{3}{4}$; $x=0.300$. During the phase transition, the tetragonal structure is transformed into a cubic one with space group $Fd\bar{3}m$ (227). It is listed in the space-group tables with two different origins. We use 'Origin choice 1' with point symmetry $\bar{4}3m$ at the origin. The silicon atoms occupy the position 8(*a*) $\bar{4}3m$ with the coordinates $0, 0, 0$; $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ and those related by the face-centring translations. In the diamond structure, the carbon atoms occupy the same position.

In order to compare the two structures, the conventional P cell of space group $P4_12_12$ (92) is transformed to an unconventional C cell (*cf.* Section 4.3.4), which corresponds to the F cell of $Fd\bar{3}m$ (227). The P and the C cells are shown in Fig. 5.2.3.1. The coordinate system $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ with origin O' of the C cell is obtained from that of the P cell, origin O, by the linear transformation

$$\mathbf{a}' = \mathbf{a} + \mathbf{b}, \qquad \mathbf{b}' = -\mathbf{a} + \mathbf{b}, \qquad \mathbf{c}' = \mathbf{c}$$

and the shift

$$\boldsymbol{p} = \tfrac{1}{4}\mathbf{a} + \tfrac{1}{4}\mathbf{b}.$$

The matrices $\boldsymbol{P}$, $\boldsymbol{p}$ and $\mathbb{P}$ are thus given by

$$\boldsymbol{P} = \begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{p} = \begin{pmatrix} \frac{1}{4} \\ \frac{1}{4} \\ 0 \end{pmatrix}, \quad \mathbb{P} = \begin{pmatrix} 1 & \bar{1} & 0 & \frac{1}{4} \\ 1 & 1 & 0 & \frac{1}{4} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

From Fig. 5.2.3.1, we derive also the inverse transformation

$$\mathbf{a} = \tfrac{1}{2}\mathbf{a}' - \tfrac{1}{2}\mathbf{b}', \quad \mathbf{b} = \tfrac{1}{2}\mathbf{a}' + \tfrac{1}{2}\mathbf{b}', \quad \mathbf{c} = \mathbf{c}', \quad \mathbf{q} = -\tfrac{1}{4}\mathbf{a}'.$$

Thus, the matrices $\boldsymbol{Q}$, $\boldsymbol{q}$ and $\mathbb{Q}$ are

$$\boldsymbol{Q} = \boldsymbol{P}^{-1} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{\bar{1}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p} = \begin{pmatrix} \frac{\bar{1}}{4} \\ 0 \\ 0 \end{pmatrix},$$

$$\mathbb{Q} = \mathbb{P}^{-1} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & \frac{\bar{1}}{4} \\ \frac{\bar{1}}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The coordinates x, y, z of points in the P cell are transformed by $\mathbb{Q}$:

$$\begin{pmatrix} x' \\ y' \\ z' \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & \frac{\bar{1}}{4} \\ \frac{\bar{1}}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(x+y) - \frac{1}{4} \\ \frac{1}{2}(-x+y) \\ z \\ 1 \end{pmatrix}.$$

The coordinate triplets of the four silicon positions in the P cell are $0.300, 0.300, 0$; $0.700, 0.700, \frac{1}{2}$; $0.200, 0.800, \frac{1}{4}$; $0.800, 0.200, \frac{3}{4}$. Four triplets in the C cell are obtained by inserting these values into the equation just derived. The new coordinates are $0.050, 0, 0$; $0.450, 0, \frac{1}{2}$; $0.250, 0.300, \frac{1}{4}$; $0.250, -0.300, \frac{3}{4}$. A set of four further points is obtained by adding the centring translation $\frac{1}{2}, \frac{1}{2}, 0$ to these coordinates.

The indices h, k, l are transformed by the matrix $\boldsymbol{P}$:

$$(h', k', l') = (h, k, l) \begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = (h + k, \ -h + k, l),$$

i.e. the reflections with the indices h, k, l of the P cell become reflections $h + k, -h + k, l$ of the C cell.

The symmetry operations of space group $P4_12_12$ are listed in the space-group tables for the P cell as follows:

(1)	x, y, z;	(2)	$\bar{x}, \bar{y}, \frac{1}{2} + z$;
(3)	$\frac{1}{2} - y, \frac{1}{2} + x, \frac{1}{4} + z$;	(4)	$\frac{1}{2} + y, \frac{1}{2} - x, \frac{3}{4} + z$;
(5)	$\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{4} - z$;	(6)	$\frac{1}{2} + x, \frac{1}{2} - y, \frac{3}{4} - z$;
(7)	$y, x, \bar{z}$;	(8)	$\bar{y}, \bar{x}, \frac{1}{2} - z$.

The corresponding matrices $\mathbb{W}$ are

$$(1)\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}; \quad (2)\begin{pmatrix} \bar{1} & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ 0 & 0 & 0 & 1 \end{pmatrix}; \quad (3)\begin{pmatrix} 0 & \bar{1} & 0 & \frac{1}{2} \\ 1 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 1 & \frac{1}{4} \\ 0 & 0 & 0 & 1 \end{pmatrix};$$

$$(4)\begin{pmatrix} 0 & 1 & 0 & \frac{1}{2} \\ \bar{1} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 1 & \frac{3}{4} \\ 0 & 0 & 0 & 1 \end{pmatrix}; \quad (5)\begin{pmatrix} \bar{1} & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & \bar{1} & \frac{1}{4} \\ 0 & 0 & 0 & 1 \end{pmatrix}; \quad (6)\begin{pmatrix} 1 & 0 & 0 & \frac{1}{2} \\ 0 & \bar{1} & 0 & \frac{1}{2} \\ 0 & 0 & \bar{1} & \frac{3}{4} \\ 0 & 0 & 0 & 1 \end{pmatrix};$$

$$(7)\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}; \quad (8)\begin{pmatrix} 0 & \bar{1} & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \\ 0 & 0 & \bar{1} & \frac{1}{2} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

These matrices of the P cell are transformed to the matrices $\mathbb{W}'$ of the C cell by

$$\mathbb{W}' = \mathbb{Q}\mathbb{W}\mathbb{P}.$$

For matrix (2), for example, this results in

$$\mathbb{W}' = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & \frac{\bar{1}}{4} \\ \frac{\bar{1}}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \bar{1} & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & \bar{1} & 0 & \frac{1}{4} \\ 1 & 1 & 0 & \frac{1}{4} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} \bar{1} & 0 & 0 & \frac{1}{2} \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The eight transformed matrices $\mathbb{W}'$, derived in this way, are

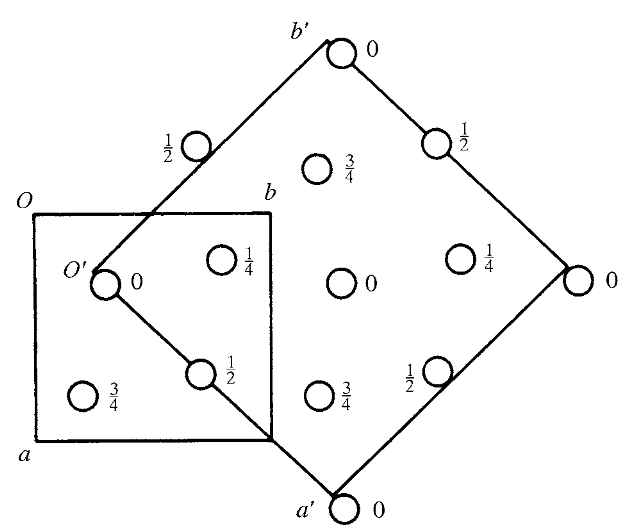

Fig. 5.2.3.1. Positions of silicon atoms in the low-cristobalite structure, projected along $[00\bar{1}]$. Primitive tetragonal cell a, b, c; C-centred tetragonal cell a', b', c'. Shift of origin from O to O' by the vector $\mathbf{p} = \frac{1}{4}\mathbf{a} + \frac{1}{4}\mathbf{b}$.

$$(1)\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix};\quad (2)\begin{pmatrix}\bar{1}&0&0&\frac{\bar{1}}{2}\\0&\bar{1}&0&0\\0&0&1&\frac{1}{2}\\0&0&0&1\end{pmatrix};\quad (3)\begin{pmatrix}0&\bar{1}&0&\frac{1}{4}\\1&0&0&\frac{1}{4}\\0&0&1&\frac{1}{4}\\0&0&0&1\end{pmatrix};$$

$$(4)\begin{pmatrix}0&1&0&\frac{1}{4}\\\bar{1}&0&0&\frac{\bar{1}}{4}\\0&0&1&\frac{3}{4}\\0&0&0&1\end{pmatrix};\quad (5)\begin{pmatrix}0&1&0&\frac{1}{4}\\1&0&0&\frac{1}{4}\\0&0&\bar{1}&\frac{1}{4}\\0&0&0&1\end{pmatrix};\quad (6)\begin{pmatrix}0&\bar{1}&0&\frac{1}{4}\\\bar{1}&0&0&\frac{\bar{1}}{4}\\0&0&\bar{1}&\frac{3}{4}\\0&0&0&1\end{pmatrix};$$

$$(7)\begin{pmatrix}1&0&0&0\\0&\bar{1}&0&0\\0&0&\bar{1}&0\\0&0&0&1\end{pmatrix};\quad (8)\begin{pmatrix}\bar{1}&0&0&\frac{\bar{1}}{2}\\0&1&0&0\\0&0&\bar{1}&\frac{1}{2}\\0&0&0&1\end{pmatrix}.$$

Another set of eight matrices is obtained by adding the C-centring translation $\frac{1}{2}, \frac{1}{2}, 0$ to the $\boldsymbol{w}$'s.

From these matrices, one obtains the coordinates of the general position in the C cell, for instance from matrix (2)

$$\begin{pmatrix}\tilde{x}\\\tilde{y}\\\tilde{z}\\1\end{pmatrix} = \begin{pmatrix}\bar{1}&0&0&\frac{\bar{1}}{2}\\0&\bar{1}&0&0\\0&0&1&\frac{1}{2}\\0&0&0&1\end{pmatrix}\begin{pmatrix}x\\y\\z\\1\end{pmatrix} = \begin{pmatrix}-x-\frac{1}{2}\\-y\\z+\frac{1}{2}\\1\end{pmatrix}.$$

The eight points obtained by the eight matrices $\mathbb{W}'$ are

(1)	$x, y, z;$	(2)	$-\frac{1}{2}-x, \bar{y}, \frac{1}{2}+z;$
(3)	$\frac{1}{4}-y, \frac{1}{4}+x, \frac{1}{4}+z;$	(4)	$\frac{1}{4}+y, -\frac{1}{4}-x, \frac{3}{4}+z;$
(5)	$\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}-z;$	(6)	$\frac{1}{4}-y, -\frac{1}{4}-x, \frac{3}{4}-z;$
(7)	$x, \bar{y}, \bar{z};$	(8)	$-\frac{1}{2}-x, y, \frac{1}{2}-z.$

The other set of eight points is obtained by adding $\frac{1}{2}, \frac{1}{2}, 0$.

In space group $P4_12_12$, the silicon atoms are in special position $4(a)$ ..2 with the coordinates $x, x, 0$. Transformed into the C cell, the position becomes

$$\begin{array}{llll}(0,0,0)+ & (\frac{1}{2},\frac{1}{2},0)+ & & \\ x,0,0; & \frac{1}{2}-x,0,\frac{1}{2}; & \frac{1}{4},\frac{1}{4}+x,\frac{1}{4}; & \frac{1}{4},\frac{3}{4}-x,\frac{3}{4}.\end{array}$$

The parameter $x = 0.300$ of the P cell has changed to $x = 0.050$ in the C cell. For $x = 0$, the special position of the C cell assumes the same coordinate triplets as Wyckoff position $8(a)$ $\bar{4}3m$ in space group $Fd\bar{3}m$ (227), *i.e.* this change of the x parameter reflects the displacement of the silicon atoms in the cubic to tetragonal phase transition.

References

5.2

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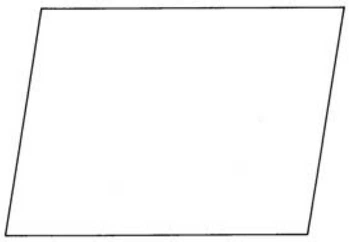
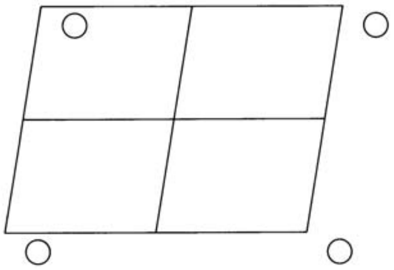
references

$p1$ 1 Oblique

No. 1 $p1$ Patterson symmetry $p2$





Origin arbitrary

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$

Symmetry operations

(1) 1

Generators selected (1); $t(1,0)$; $t(0,1)$

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	Reflection conditions
				General:
1	a	1	(1) x,y	no conditions

Maximal non-isomorphic subgroups

I none
IIa none
IIb none

Maximal isomorphic subgroups of lowest index

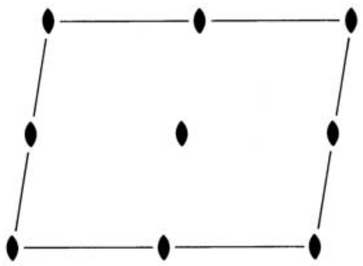
IIc [2] $p1$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a}+\mathbf{b}, \mathbf{b}' = -\mathbf{a}+\mathbf{b}$) (1)

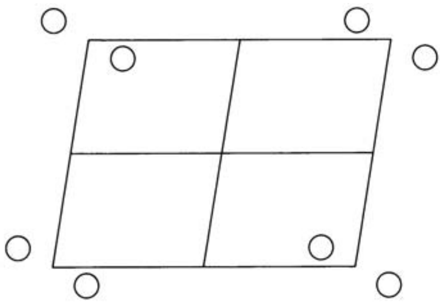
Minimal non-isomorphic supergroups

I [2] $p2$ (2); [2] pm (3); [2] pg (4); [2] cm (5); [3] $p3$ (13)
II none

Oblique | 2 | $p2$

Patterson symmetry $p2$ | $p2$ | No. 2





Origin at 2

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$

Symmetry operations

(1) 1 (2) 2 0,0

Generators selected (1); $t(1,0)$; $t(0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	*e*	1	(1) x,y	(2) $\bar{x},\bar{y}$	no conditions
					Special: no extra conditions
1	*d*	2	$\frac{1}{2},\frac{1}{2}$		
1	*c*	2	$\frac{1}{2},0$		
1	*b*	2	$0,\frac{1}{2}$		
1	*a*	2	$0,0$		

Maximal non-isomorphic subgroups

I [2] $p1$ (1) 1
IIa none
IIb none

Maximal isomorphic subgroups of lowest index

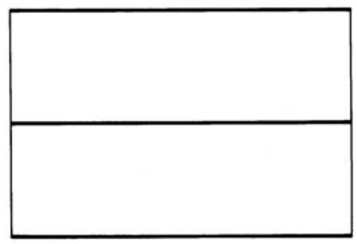
IIc [2] $p2$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a}+\mathbf{b}, \mathbf{b}' = -\mathbf{a}+\mathbf{b}$) (2)

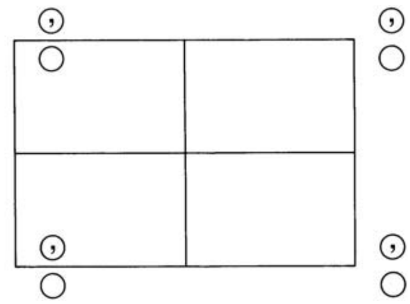
Minimal non-isomorphic supergroups

I [2] $p2mm$ (6); [2] $p2mg$ (7); [2] $p2gg$ (8); [2] $c2mm$ (9); [2] $p4$ (10); [3] $p6$ (16)
II none

pm m Rectangular

No. 3 $p1m1$ Patterson symmetry $p2mm$





Origin on m

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$

Symmetry operations

(1) 1   (2) m $0, y$

Generators selected   (1); $t(1,0)$; $t(0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	c	1	(1) x, y	(2) $\bar{x}, y$	no conditions
					Special: no extra conditions
1	b	$.m.$	$\frac{1}{2}, y$		
1	a	$.m.$	$0, y$		

Maximal non-isomorphic subgroups

I   [2] $p1$ (1)   1

IIa   none

IIb   [2] pg ($\mathbf{b}' = 2\mathbf{b}$) (4); [2] cm ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (5)

Maximal isomorphic subgroups of lowest index

IIc   [2] pm ($\mathbf{a}' = 2\mathbf{a}$) (3); [2] pm ($\mathbf{b}' = 2\mathbf{b}$) (3)

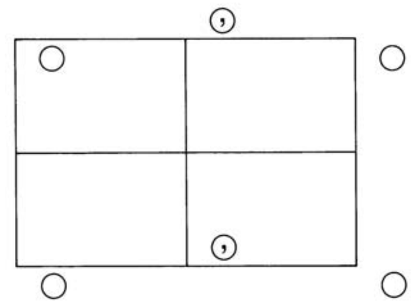
Minimal non-isomorphic supergroups

I   [2] $p2mm$ (6); [2] $p2mg$ (7)

II   [2] cm (5)

Rectangular m pg

Patterson symmetry $p2mm$ $p1g1$ No. 4



Origin on g

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$

Symmetry operations

(1) 1 (2) b $0, y$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	a	1	(1) x, y	(2) $\bar{x}, y+\frac{1}{2}$	$0k$: $k = 2n$

Maximal non-isomorphic subgroups

I [2] $p1$ (1) 1

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] pg ($\mathbf{a}' = 2\mathbf{a}$) (4); [3] pg ($\mathbf{b}' = 3\mathbf{b}$) (4)

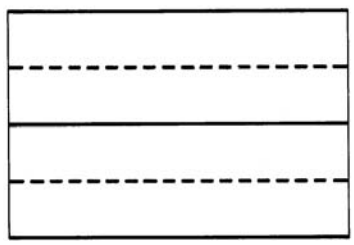
Minimal non-isomorphic supergroups

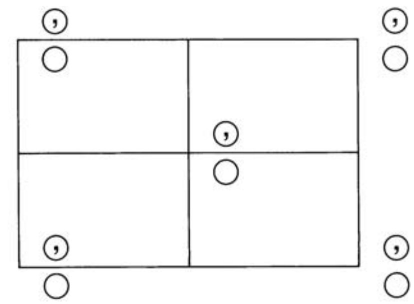
I [2] $p2mg$ (7); [2] $p2gg$ (8)

II [2] cm (5); [2] pm ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (3)

cm m Rectangular

No. 5 $c1m1$ Patterson symmetry $c2mm$





Origin on m

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

For $(0,0)+$ set

(1) 1 (2) $m \;\; 0,y$

For $(\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2})$ (2) $b \;\; \frac{1}{4},y$

Generators selected $\quad (1);\; t(1,0);\; t(0,1);\; t(\frac{1}{2},\frac{1}{2});\; (2)$

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0)+ \quad (\frac{1}{2},\frac{1}{2})+$	Reflection conditions
		General:
4 $\quad b \quad 1$	(1) x,y (2) $\bar{x},y$	hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
		Special: no extra conditions
2 $\quad a \quad .m.$	$0,y$	

Maximal non-isomorphic subgroups

I $\quad$ [2] $c1\,(p1,\,1)$ $\quad 1+$

IIa $\quad$ [2] $pg\,(4)$ $\quad 1;\; 2+(\frac{1}{2},\frac{1}{2})$
$\quad$ [2] $pm\,(3)$ $\quad 1;\; 2$

IIb $\quad$ none

Maximal isomorphic subgroups of lowest index

IIc $\quad$ [3] $cm\,(\mathbf{a}'=3\mathbf{a})\,(5)$; [3] $cm\,(\mathbf{b}'=3\mathbf{b})\,(5)$

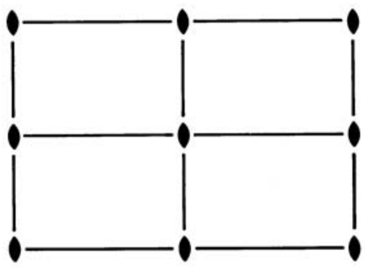
Minimal non-isomorphic supergroups

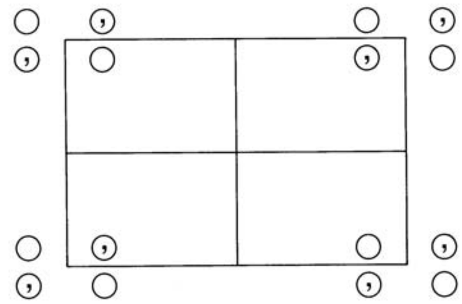
I $\quad$ [2] $c2mm\,(9)$; [3] $p3m1\,(14)$; [3] $p31m\,(15)$

II $\quad$ [2] $pm\,(\mathbf{a}'=\frac{1}{2}\mathbf{a}, \mathbf{b}'=\frac{1}{2}\mathbf{b})\,(3)$

Rectangular $2mm$ $p2mm$

Patterson symmetry $p2mm$ $p2mm$ No. 6





Origin at $2mm$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0$ (3) m $0,y$ (4) m $x,0$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	i	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{x},y$	(4) $x,\bar{y}$	no conditions
							Special: no extra conditions
2	h	$.m.$	$\frac{1}{2},y$	$\frac{1}{2},\bar{y}$			
2	g	$.m.$	$0,y$	$0,\bar{y}$			
2	f	$..m$	$x,\frac{1}{2}$	$\bar{x},\frac{1}{2}$			
2	e	$..m$	$x,0$	$\bar{x},0$			
1	d	$2mm$	$\frac{1}{2},\frac{1}{2}$				
1	c	$2mm$	$\frac{1}{2},0$				
1	b	$2mm$	$0,\frac{1}{2}$				
1	a	$2mm$	$0,0$				

Maximal non-isomorphic subgroups

I [2] $p1m1$ (pm, 3) 1; 3
[2] $p11m$ (pm, 3) 1; 4
[2] $p211$ ($p2$, 2) 1; 2

IIa none

IIb [2] $p2mg$ ($\mathbf{a}' = 2\mathbf{a}$) (7); [2] $p2gm$ ($\mathbf{b}' = 2\mathbf{b}$) ($p2mg$, 7); [2] $c2mm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (9)

Maximal isomorphic subgroups of lowest index

IIc [2] $p2mm$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$) (6)

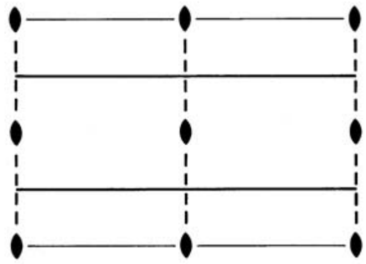
Minimal non-isomorphic supergroups

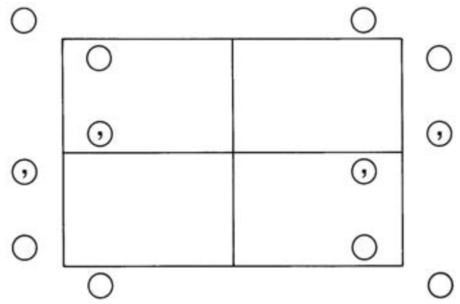
I [2] $p4mm$ (11)

II [2] $c2mm$ (9)

$p2mg$ $\qquad$ $2mm$ $\qquad$ Rectangular

No. 7 $\qquad$ $p2mg$ $\qquad$ Patterson symmetry $p2mm$





Origin at $21g$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1$

Symmetry operations

(1) 1 $\qquad$ (2) $2 \quad 0,0$ $\qquad$ (3) $m \quad \frac{1}{4},y$ $\qquad$ (4) $a \quad x,0$

Generators selected $\quad$ (1); $t(1,0)$; $t(0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	d	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{x}+\frac{1}{2},y$	(4) $x+\frac{1}{2},\bar{y}$	$h0$: $h=2n$
							Special: as above, plus
2	c	$.m.$	$\frac{1}{4},y$	$\frac{3}{4},\bar{y}$			no extra conditions
2	b	$2..$	$0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2}$			hk: $h=2n$
2	a	$2..$	$0,0$	$\frac{1}{2},0$			hk: $h=2n$

Maximal non-isomorphic subgroups

I $\quad$ [2] $p11g$ (pg, 4) $\quad$ 1; 4
$\quad$ [2] $p1m1$ (pm, 3) $\quad$ 1; 3
$\quad$ [2] $p211$ ($p2$, 2) $\quad$ 1; 2

IIa $\quad$ none

IIb $\quad$ [2] $p2gg$ ($\mathbf{b}'=2\mathbf{b}$) (8)

Maximal isomorphic subgroups of lowest index

IIc $\quad$ [2] $p2mg$ ($\mathbf{b}'=2\mathbf{b}$) (7); [3] $p2mg$ ($\mathbf{a}'=3\mathbf{a}$) (7)

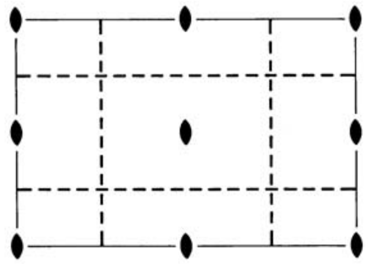
Minimal non-isomorphic supergroups

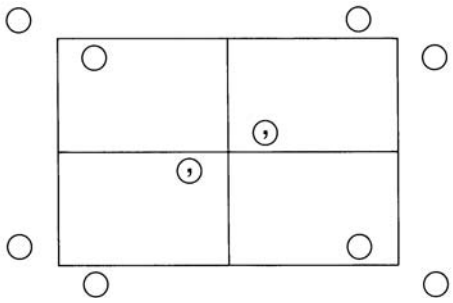
I $\quad$ none

II $\quad$ [2] $c2mm$ (9); [2] $p2mm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (6)

Rectangular $2mm$ $p2gg$

Patterson symmetry $p2mm$ $p2gg$ No. 8





Origin at 2

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0$ (3) b $\frac{1}{4},y$ (4) a $x,\frac{1}{4}$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2}$	$h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
2	b	2 . .	$\frac{1}{2},0$	$0,\frac{1}{2}$			hk: $h+k=2n$
2	a	2 . .	$0,0$	$\frac{1}{2},\frac{1}{2}$			hk: $h+k=2n$

Maximal non-isomorphic subgroups

I [2] $p1g1$ (pg, 4) 1; 3
[2] $p11g$ (pg, 4) 1; 4
[2] $p211$ ($p2$, 2) 1; 2

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $p2gg$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (8)

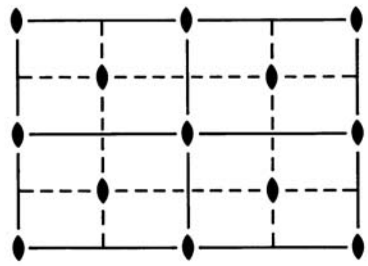
Minimal non-isomorphic supergroups

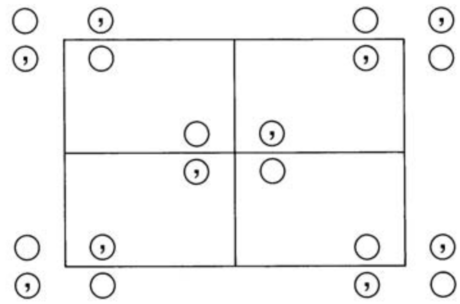
I [2] $p4gm$ (12)

II [2] $c2mm$ (9); [2] $p2mg$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (7); [2] $p2gm$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($p2mg$, 7)

$c2mm$ $2mm$ Rectangular

No. 9 $c2mm$ Patterson symmetry $c2mm$





Origin at $2mm$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

For $(0,0)+$ set

(1) 1 (2) $2\ \ 0,0$ (3) $m\ \ 0,y$ (4) $m\ \ x,0$

For $(\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2})$ (2) $2\ \ \frac{1}{4},\frac{1}{4}$ (3) $b\ \ \frac{1}{4},y$ (4) $a\ \ x,\frac{1}{4}$

Generators selected $\quad (1);\ t(1,0);\ t(0,1);\ t(\frac{1}{2},\frac{1}{2});\ (2);\ (3)$

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0)+\ \ (\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
8	f	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{x},y$	(4) $x,\bar{y}$	hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
4	e	$.m.$	$0,y$	$0,\bar{y}$			no extra conditions
4	d	$..m$	$x,0$	$\bar{x},0$			no extra conditions
4	c	$2..$	$\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4}$			hk: $h=2n$
2	b	$2mm$	$0,\frac{1}{2}$				no extra conditions
2	a	$2mm$	$0,0$				no extra conditions

Maximal non-isomorphic subgroups

I	[2] $c1m1$ (cm, 5)	$(1;\ 3)+$
	[2] $c11m$ (cm, 5)	$(1;\ 4)+$
	[2] $c211$ ($p2$, 2)	$(1;\ 2)+$
IIa	[2] $p2gg$ (8)	$1;\ 2;\ (3;\ 4)+(\frac{1}{2},\frac{1}{2})$
	[2] $p2gm$ ($p2mg$, 7)	$1;\ 4;\ (2;\ 3)+(\frac{1}{2},\frac{1}{2})$
	[2] $p2mg$ (7)	$1;\ 3;\ (2;\ 4)+(\frac{1}{2},\frac{1}{2})$
	[2] $p2mm$ (6)	$1;\ 2;\ 3;\ 4$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $c2mm$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (9)

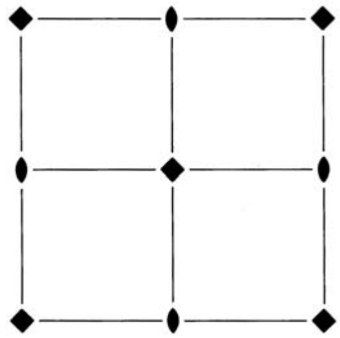
Minimal non-isomorphic supergroups

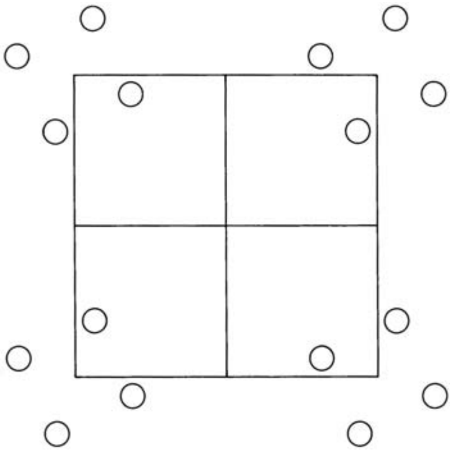
I [2] $p4mm$ (11); [2] $p4gm$ (12); [3] $p6mm$ (17)

II [2] $p2mm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) (6)

Square | 4 | $p4$

Patterson symmetry $p4$ | $p4$ | No. 10





Origin at 4

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 0,0 (3) 4^{+} 0,0 (4) 4^{-} 0,0

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	*d*	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{y},x$	(4) $y,\bar{x}$	no conditions
							Special:
2	*c*	2 . .	$\frac{1}{2},0$	$0,\frac{1}{2}$			hk: $h+k=2n$
1	*b*	4 . .	$\frac{1}{2},\frac{1}{2}$				no extra conditions
1	*a*	4 . .	$0,0$				no extra conditions

Maximal non-isomorphic subgroups

I [2] $p2$ (2) 1; 2

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $c4$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p4$, 10)

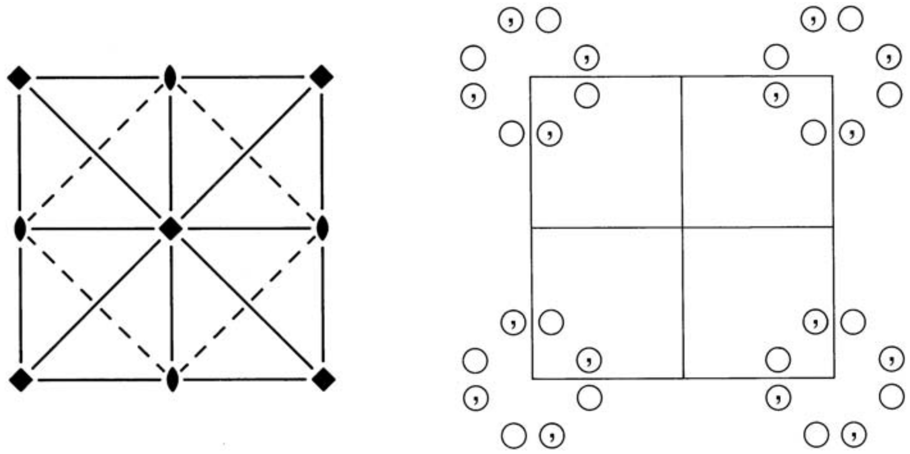
Minimal non-isomorphic supergroups

I [2] $p4mm$ (11); [2] $p4gm$ (12)

II none

$p4mm$ $4mm$ Square

No. 11 $p4mm$ Patterson symmetry $p4mm$



Origin at $4mm$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $x \le y$

Symmetry operations

(1) 1	(2) 2 0,0	(3) 4^+ 0,0	(4) 4^- 0,0
(5) m 0,y	(6) m x,0	(7) m x,x	(8) m $x,\bar{x}$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y (5) $\bar{x},y$	(2) $\bar{x},\bar{y}$ (6) $x,\bar{y}$	(3) $\bar{y},x$ (7) y,x	(4) $y,\bar{x}$ (8) $\bar{y},\bar{x}$	no conditions
							Special:
4	f	$..m$	x,x	$\bar{x},\bar{x}$	$\bar{x},x$	$x,\bar{x}$	no extra conditions
4	e	$.m.$	$x,\frac{1}{2}$	$\bar{x},\frac{1}{2}$	$\frac{1}{2},x$	$\frac{1}{2},\bar{x}$	no extra conditions
4	d	$.m.$	$x,0$	$\bar{x},0$	$0,x$	$0,\bar{x}$	no extra conditions
2	c	$2mm.$	$\frac{1}{2},0$	$0,\frac{1}{2}$			hk: $h+k=2n$
1	b	$4mm$	$\frac{1}{2},\frac{1}{2}$				no extra conditions
1	a	$4mm$	$0,0$				no extra conditions

Maximal non-isomorphic subgroups

I [2] $p411$ ($p4$, 10) 1; 2; 3; 4
[2] $p21m$ ($c2mm$, 9) 1; 2; 7; 8
[2] $p2m1$ ($p2mm$, 6) 1; 2; 5; 6

IIa none

IIb [2] $c4mg$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p4gm$, 12)

Maximal isomorphic subgroups of lowest index

IIc [2] $c4mm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p4mm$, 11)

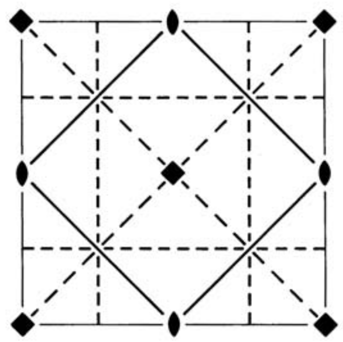
Minimal non-isomorphic supergroups

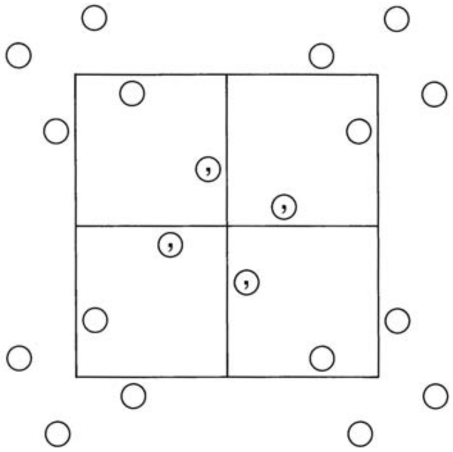
I none

II none

Square $4mm$ $p4gm$

Patterson symmetry $p4mm$ $p4gm$ No. 12





Origin at $41g$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $y \le \frac{1}{2} - x$

Symmetry operations

(1) 1	(2) 2 $0,0$	(3) 4^+ $0,0$	(4) 4^- $0,0$
(5) b $\frac{1}{4},y$	(6) a $x,\frac{1}{4}$	(7) $g(\frac{1}{2},\frac{1}{2})$ x,x	(8) m $x+\frac{1}{2},\bar{x}$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{y},x$	(4) $y,\bar{x}$	$h0$: $h=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$0k$: $k=2n$
							Special: as above, plus
4	c	$..m$	$x,x+\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x$	$x+\frac{1}{2},\bar{x}$	no extra conditions
2	b	$2.mm$	$\frac{1}{2},0$	$0,\frac{1}{2}$			hk: $h+k=2n$
2	a	$4..$	$0,0$	$\frac{1}{2},\frac{1}{2}$			hk: $h+k=2n$

Maximal non-isomorphic subgroups

I [2] $p411$ ($p4$, 10) 1; 2; 3; 4
[2] $p21m$ ($c2mm$, 9) 1; 2; 7; 8
[2] $p2g1$ ($p2gg$, 8) 1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [9] $p4gm$ ($\mathbf{a}'=3\mathbf{a}, \mathbf{b}'=3\mathbf{b}$) (12)

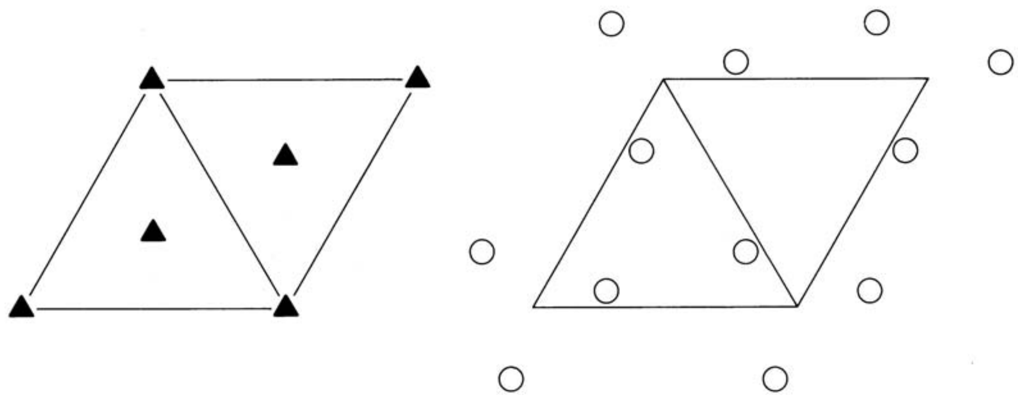
Minimal non-isomorphic supergroups

I none

II [2] $c4gm$ ($p4mm$, 11)

$p3$ 3   Hexagonal

No. 13 $p3$ Patterson symmetry $p6$



Origin at 3

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $x \le (1+y)/2$; $y \le \min(1-x, (1+x)/2)$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{3},\frac{2}{3}$ $0,\frac{1}{2}$

Symmetry operations

(1) 1   (2) 3^+ $0,0$ (3) 3^- $0,0$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
3	*d*	1	(1) x,y	(2) $\bar{y},x-y$	(3) $\bar{x}+y,\bar{x}$	no conditions
						Special: no extra conditions
1	*c*	3 . .	$\frac{2}{3},\frac{1}{3}$			
1	*b*	3 . .	$\frac{1}{3},\frac{2}{3}$			
1	*a*	3 . .	$0,0$			

Maximal non-isomorphic subgroups

I [3] $p1$ (1) 1

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $h3$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($p3$, 13)

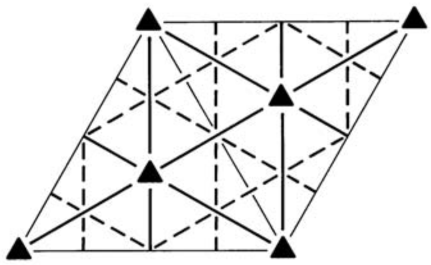
Minimal non-isomorphic supergroups

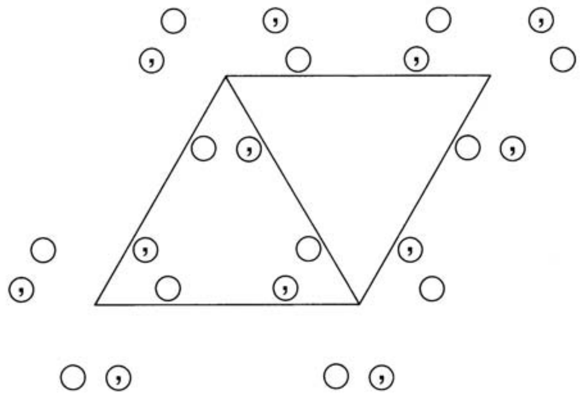
I [2] $p3m1$ (14); [2] $p31m$ (15); [2] $p6$ (16)

II none

Hexagonal $3m$ $p3m1$

Patterson symmetry $p6mm$ $p3m1$ No. 14





Origin at $3m1$

Asymmetric unit $0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{2}{3};\quad x \le 2y;\quad y \le \min(1-x, 2x)$

Vertices $0,0 \quad \frac{2}{3},\frac{1}{3} \quad \frac{1}{3},\frac{2}{3}$

Symmetry operations

(1) 1	(2) 3^{+} 0,0	(3) 3^{-} 0,0
(4) $m\ \ x,\bar{x}$	(5) $m\ \ x,2x$	(6) $m\ \ 2x,x$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	e	1	(1) x,y (4) $\bar{y},\bar{x}$	(2) $\bar{y},x-y$ (5) $\bar{x}+y,y$	(3) $\bar{x}+y,\bar{x}$ (6) $x,x-y$	no conditions
						Special: no extra conditions
3	d	$.m.$	$x,\bar{x}$	$x,2x$	$2\bar{x},\bar{x}$	
1	c	$3m.$	$\frac{2}{3},\frac{1}{3}$			
1	b	$3m.$	$\frac{1}{3},\frac{2}{3}$			
1	a	$3m.$	$0,0$			

Maximal non-isomorphic subgroups

I [2] $p311$ ($p3$, 13) 1; 2; 3
[3] $p1m1$ (cm, 5) 1; 4
[3] $p1m1$ (cm, 5) 1; 5
[3] $p1m1$ (cm, 5) 1; 6

IIa none

IIb [3] $h3m1$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($p31m$, 15)

Maximal isomorphic subgroups of lowest index

IIc [4] $p3m1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (14)

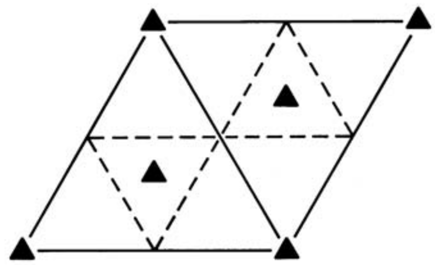
Minimal non-isomorphic supergroups

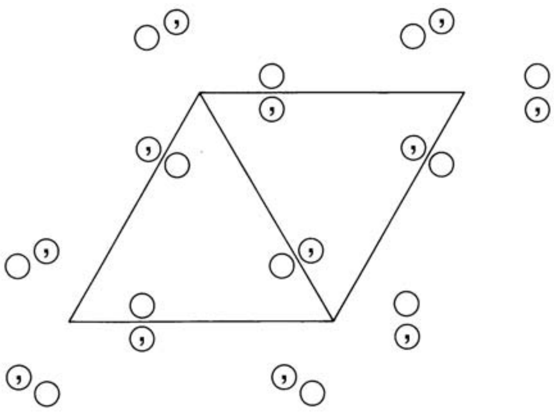
I [2] $p6mm$ (17)

II [3] $h3m1$ ($p31m$, 15)

$p31m$ $3m$ Hexagonal

No. 15 $p31m$ Patterson symmetry $p6mm$





Origin at $31m$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x, x)$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^{+} $0,0$	(3) 3^{-} $0,0$
(4) m x,x	(5) m $x,0$	(6) m $0,y$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	d	1	(1) x,y (4) y,x	(2) $\bar{y},x-y$ (5) $x-y,\bar{y}$	(3) $\bar{x}+y,\bar{x}$ (6) $\bar{x},\bar{x}+y$	no conditions
						Special: no extra conditions
3	c	$..m$	$x,0$	$0,x$	$\bar{x},\bar{x}$	
2	b	$3..$	$\frac{1}{3},\frac{2}{3}$	$\frac{2}{3},\frac{1}{3}$		
1	a	$3.m$	$0,0$			

Maximal non-isomorphic subgroups

I [2] $p311$ ($p3$, 13) 1; 2; 3

$\left\{\begin{array}{ll} [3]\ p11m\ (cm, 5) & 1;\ 4 \\ [3]\ p11m\ (cm, 5) & 1;\ 5 \\ [3]\ p11m\ (cm, 5) & 1;\ 6 \end{array}\right.$

IIa none

IIb [3] $h31m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($p3m1$, 14)

Maximal isomorphic subgroups of lowest index

IIc [4] $p31m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (15)

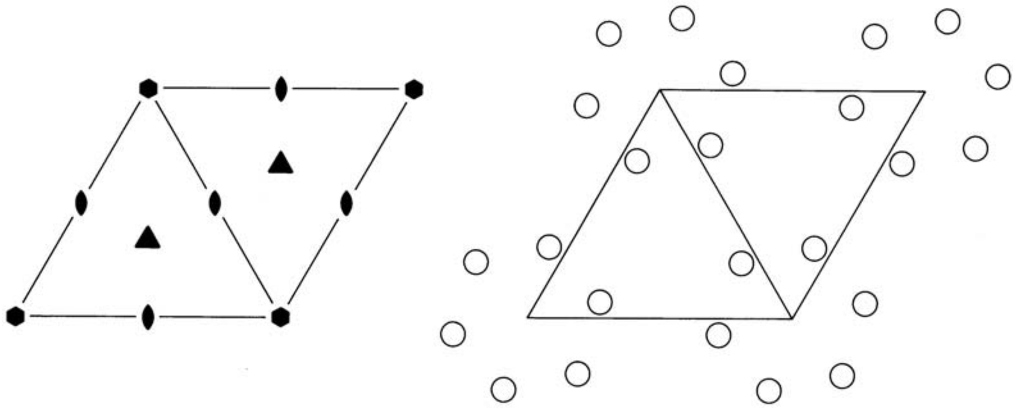
Minimal non-isomorphic supergroups

I [2] $p6mm$ (17)

II [3] $h31m$ ($p3m1$, 14)

Hexagonal 6 *p*6

Patterson symmetry *p*6 — *p*6 — No. 16



Origin at 6

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x, x)$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^+ 0,0	(3) 3^- 0,0
(4) 2 0,0	(5) 6^- 0,0	(6) 6^+ 0,0

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	*d*	1	(1) x,y	(2) $\bar{y},x-y$	(3) $\bar{x}+y,\bar{x}$	no conditions
			(4) $\bar{x},\bar{y}$	(5) $y,\bar{x}+y$	(6) $x-y,x$	
						Special: no extra conditions
3	*c*	2 . .	$\frac{1}{2},0$	$0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2}$	
2	*b*	3 . .	$\frac{1}{3},\frac{2}{3}$	$\frac{2}{3},\frac{1}{3}$		
1	*a*	6 . .	$0,0$			

Maximal non-isomorphic subgroups

I [2] *p*3 (13) 1; 2; 3
[3] *p*2 (2) 1; 4

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] *h*6 ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (*p*6, 16)

Minimal non-isomorphic supergroups

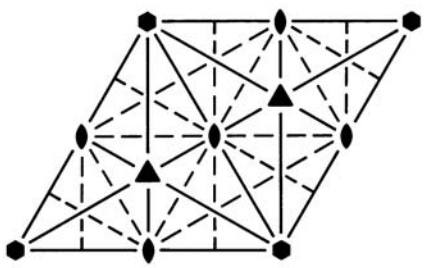
I [2] *p*6*mm* (17)

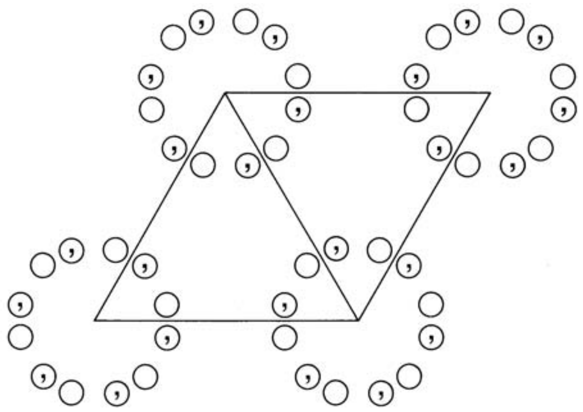
II none

International Tables for Crystallography (2006). Vol. A, Plane group 17, pp. 108–109.

$p6mm$ $6mm$ Hexagonal

No. 17 $p6mm$ Patterson symmetry $p6mm$





Origin at $6mm$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{3}$; $x \le (1+y)/2$; $y \le x/2$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$

Symmetry operations

(1) 1	(2) 3^{+} $0,0$	(3) 3^{-} $0,0$
(4) 2 $0,0$	(5) 6^{-} $0,0$	(6) 6^{+} $0,0$
(7) m $x,\bar{x}$	(8) m $x,2x$	(9) m $2x,x$
(10) m x,x	(11) m $x,0$	(12) m $0,y$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	f	1	(1) x,y	(2) $\bar{y},x-y$	(3) $\bar{x}+y,\bar{x}$				no conditions
			(4) $\bar{x},\bar{y}$	(5) $y,\bar{x}+y$	(6) $x-y,x$				
			(7) $\bar{y},\bar{x}$	(8) $\bar{x}+y,y$	(9) $x,x-y$				
			(10) y,x	(11) $x-y,\bar{y}$	(12) $\bar{x},\bar{x}+y$				
									Special: no extra conditions
6	e	$.m.$	$x,\bar{x}$	$x,2x$	$2\bar{x},\bar{x}$	$\bar{x},x$	$\bar{x},2\bar{x}$	$2x,x$	
6	d	$..m$	$x,0$	$0,x$	$\bar{x},\bar{x}$	$\bar{x},0$	$0,\bar{x}$	x,x	
3	c	$2mm$	$\frac{1}{2},0$	$0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2}$				
2	b	$3m.$	$\frac{1}{3},\frac{2}{3}$	$\frac{2}{3},\frac{1}{3}$					
1	a	$6mm$	$0,0$						

Maximal non-isomorphic subgroups

I	[2] $p611$ ($p6$, 16)	1; 2; 3; 4; 5; 6
	[2] $p31m$ (15)	1; 2; 3; 10; 11; 12
	[2] $p3m1$ (14)	1; 2; 3; 7; 8; 9
	{ [3] $p2mm$ ($c2mm$, 9)	1; 4; 7; 10
	{ [3] $p2mm$ ($c2mm$, 9)	1; 4; 8; 11
	{ [3] $p2mm$ ($c2mm$, 9)	1; 4; 9; 12
IIa	none	
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $h6mm$ ($\mathbf{a}'=3\mathbf{a}, \mathbf{b}'=3\mathbf{b}$) ($p6mm$, 17)

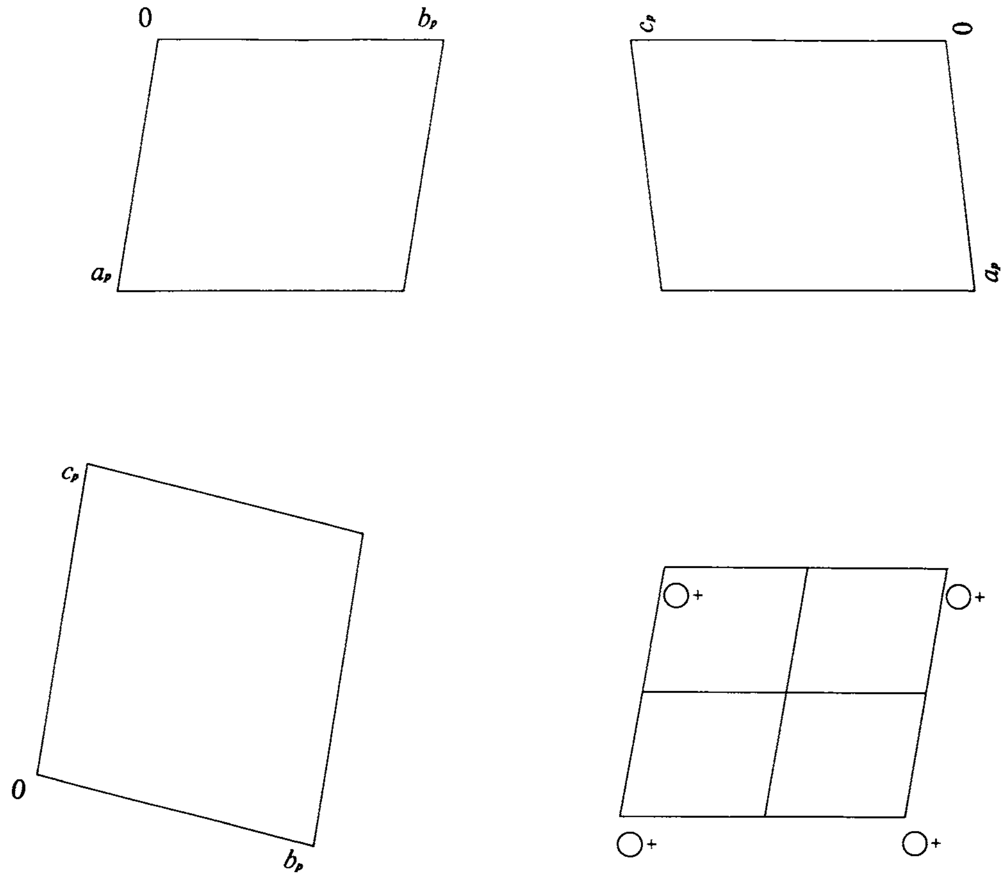
Minimal non-isomorphic supergroups

I none

II none

$P1$ C_1^1 1 Triclinic

No. 1 $P1$ Patterson symmetry $P\bar{1}$



Drawings for type II cell. Proper cell reduction (Chapter 9.2) gives either a type I (α, β, γ acute) or a type II (α, β, γ non-acute) cell.

Origin arbitrary

Asymmetric unit $0 \leq x \leq 1;\quad 0 \leq y \leq 1;\quad 0 \leq z \leq 1$

Symmetry operations

(1) 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
1 a 1	(1) x, y, z	no conditions

Symmetry of special projections

Along [001] $p1$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}_p$
Origin at $0, 0, z$

Along [100] $p1$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x, 0, 0$

Along [010] $p1$
$\mathbf{a}' = \mathbf{c}_p$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I none
IIa none
IIb none

Maximal isomorphic subgroups of lowest index

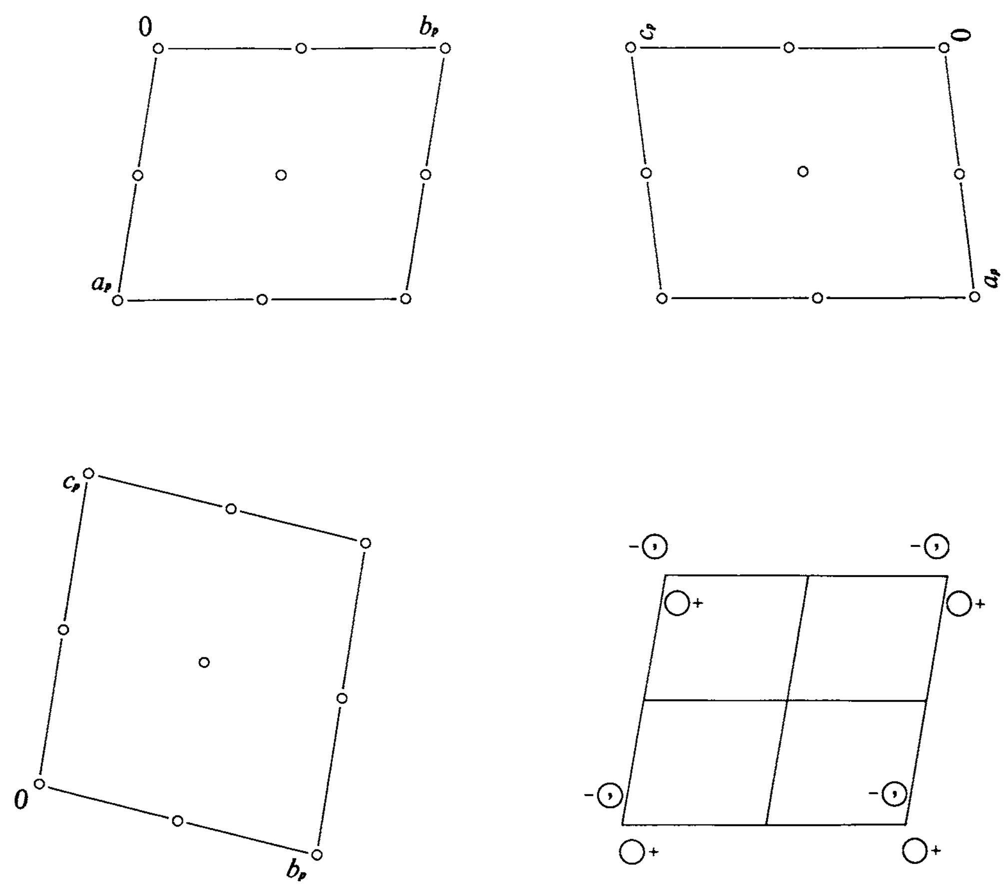
IIc [2] $P1$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{c}' = 2\mathbf{c}$ or $\mathbf{b}' = \mathbf{b}+\mathbf{c}, \mathbf{c}' = -\mathbf{b}+\mathbf{c}$ or $\mathbf{a}' = \mathbf{a}-\mathbf{c}, \mathbf{c}' = \mathbf{a}+\mathbf{c}$ or $\mathbf{a}' = \mathbf{a}+\mathbf{b}, \mathbf{b}' = -\mathbf{a}+\mathbf{b}$ or $\mathbf{a}' = \mathbf{b}+\mathbf{c}, \mathbf{b}' = \mathbf{a}+\mathbf{c}, \mathbf{c}' = \mathbf{a}+\mathbf{b}$) (1)

Minimal non-isomorphic supergroups

I [2] $P\bar{1}$ (2); [2] $P2$ (3); [2] $P2_1$ (4); [2] $C2$ (5); [2] Pm (6); [2] Pc (7); [2] Cm (8); [2] Cc (9); [3] $P3$ (143); [3] $P3_1$ (144); [3] $P3_2$ (145); [3] $R3$ (146)
II none

International Tables for Crystallography (2006). Vol. A, Space group 2, pp. 114–115.

$P\bar{1}$	C_i^1	$\bar{1}$	Triclinic
No. 2	$P\bar{1}$		Patterson symmetry $P\bar{1}$



Drawings for type II cell. Proper cell reduction (Chapter 9.2) gives either a type I (α, β, γ acute) or a type II (α, β, γ non-acute) cell.

Origin at $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) $\bar{1}$ $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},\bar{z}$	no conditions
					Special: no extra conditions
1	h	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		
1	g	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$		
1	f	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$		
1	e	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$		
1	d	$\bar{1}$	$\frac{1}{2},0,0$		
1	c	$\bar{1}$	$0,\frac{1}{2},0$		
1	b	$\bar{1}$	$0,0,\frac{1}{2}$		
1	a	$\bar{1}$	$0,0,0$		

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}_p$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\mathbf{c}_p$ $\mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1$ (1) 1

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{1}$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{b}'=2\mathbf{b}$ or $\mathbf{c}'=2\mathbf{c}$ or $\mathbf{b}'=\mathbf{b}+\mathbf{c},\mathbf{c}'=-\mathbf{b}+\mathbf{c}$ or $\mathbf{a}'=\mathbf{a}-\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{c}$ or $\mathbf{a}'=\mathbf{a}+\mathbf{b},\mathbf{b}'=-\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{b}+\mathbf{c},\mathbf{b}'=\mathbf{a}+\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}$) (2)

Minimal non-isomorphic supergroups

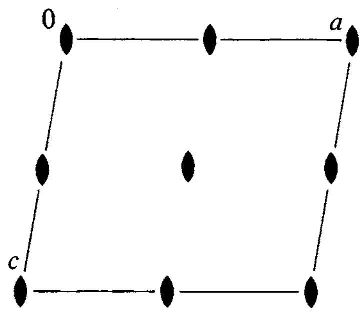
I [2] $P2/m$ (10); [2] $P2_1/m$ (11); [2] $C2/m$ (12); [2] $P2/c$ (13); [2] $P2_1/c$ (14); [2] $C2/c$ (15); [3] $P\bar{3}$ (147); [3] $R\bar{3}$ (148)

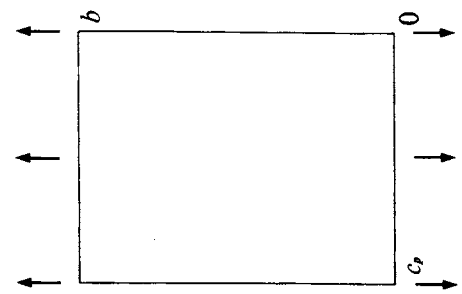
II none

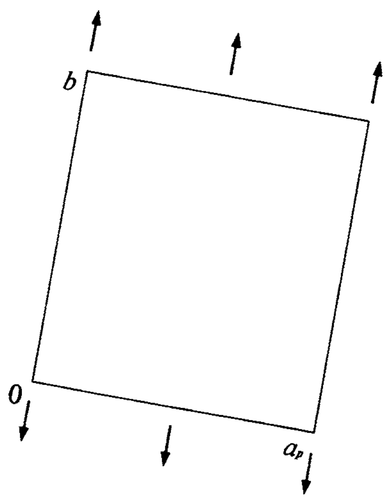
$P2$ $\qquad$ C_2^1 $\qquad$ 2 $\qquad$ Monoclinic

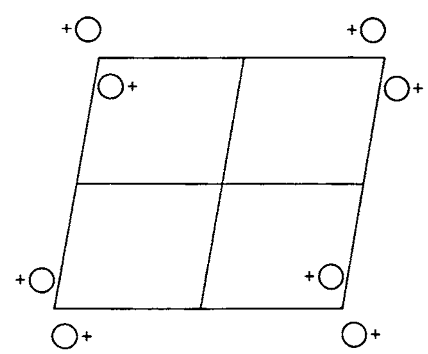
No. 3 $\qquad$ $P121$ $\qquad$ Patterson symmetry $P12/m1$

UNIQUE AXIS *b*









Origin on 2

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 $\qquad$ (2) 2 $\;0, y, 0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	e	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	no conditions
					Special: no extra conditions
1	d	2	$\frac{1}{2},y,\frac{1}{2}$		
1	c	2	$\frac{1}{2},y,0$		
1	b	2	$0,y,\frac{1}{2}$		
1	a	2	$0,y,0$		

Symmetry of special projections

Along [001] $p1m1$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p11m$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1$ (1) 1

IIa none

IIb [2] $P12_11$ ($\mathbf{b}'=2\mathbf{b}$) ($P2_1$, 4); [2] $C121$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($C2$, 5); [2] $A121$ ($\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($C2$, 5); [2] $F121$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($C2$, 5)

Maximal isomorphic subgroups of lowest index

IIc [2] $P121$ ($\mathbf{b}'=2\mathbf{b}$) ($P2$, 3); [2] $P121$ ($\mathbf{c}'=2\mathbf{c}$ or $\mathbf{a}'=2\mathbf{a}$ or $\mathbf{a}'=\mathbf{a}+\mathbf{c},\mathbf{c}'=-\mathbf{a}+\mathbf{c}$) ($P2$, 3)

Minimal non-isomorphic supergroups

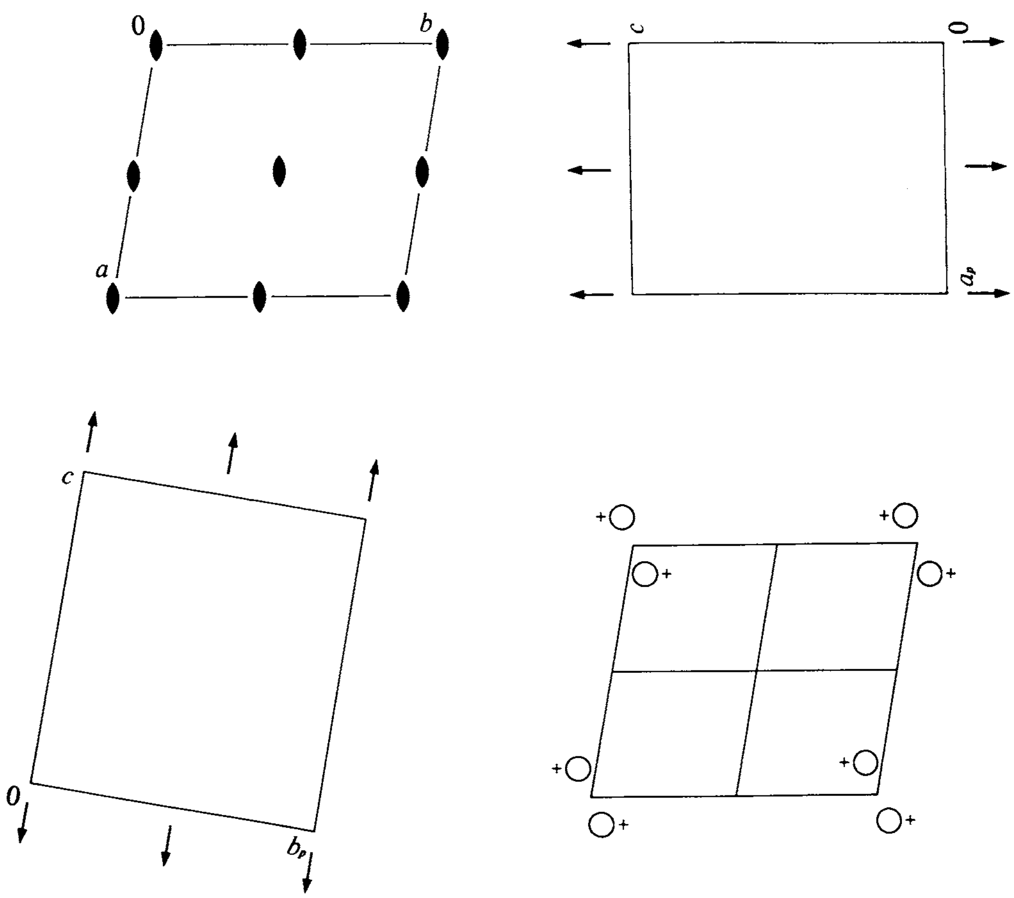
I [2] $P2/m$ (10); [2] $P2/c$ (13); [2] $P222$ (16); [2] $P222_1$ (17); [2] $P2_12_12$ (18); [2] $C222$ (21); [2] $Pmm2$ (25); [2] $Pcc2$ (27); [2] $Pma2$ (28); [2] $Pnc2$ (30); [2] $Pba2$ (32); [2] $Pnn2$ (34); [2] $Cmm2$ (35); [2] $Ccc2$ (37); [2] $P4$ (75); [2] $P4_2$ (77); [2] $P\bar{4}$ (81); [3] $P6$ (168); [3] $P6_2$ (171); [3] $P6_4$ (172)

II [2] $C121$ ($C2$, 5); [2] $A121$ ($C2$, 5); [2] $I121$ ($C2$, 5)

$P2$ C_2^1 2 Monoclinic

No. 3 $P112$ Patterson symmetry $P112/m$

UNIQUE AXIS c



Origin on 2

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	no conditions
					Special: no extra conditions
1	d	2	$\frac{1}{2},\frac{1}{2},z$		
1	c	2	$0,\frac{1}{2},z$		
1	b	2	$\frac{1}{2},0,z$		
1	a	2	$0,0,z$		

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1$ (1) 1

IIa none

IIb [2] $P112_1$ ($\mathbf{c}' = 2\mathbf{c}$) ($P2_1$, 4); [2] $A112$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2$, 5); [2] $B112$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($C2$, 5); [2] $F112$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2$, 5)

Maximal isomorphic subgroups of lowest index

IIc [2] $P112$ ($\mathbf{c}' = 2\mathbf{c}$) ($P2$, 3); [2] $P112$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b}$) ($P2$, 3)

Minimal non-isomorphic supergroups

I [2] $P2/m$ (10); [2] $P2/c$ (13); [2] $P222$ (16); [2] $P222_1$ (17); [2] $P2_12_12$ (18); [2] $C222$ (21); [2] $Pmm2$ (25); [2] $Pcc2$ (27); [2] $Pma2$ (28); [2] $Pnc2$ (30); [2] $Pba2$ (32); [2] $Pnn2$ (34); [2] $Cmm2$ (35); [2] $Ccc2$ (37); [2] $P4$ (75); [2] $P4_2$ (77); [2] $P\bar{4}$ (81); [3] $P6$ (168); [3] $P6_2$ (171); [3] $P6_4$ (172)

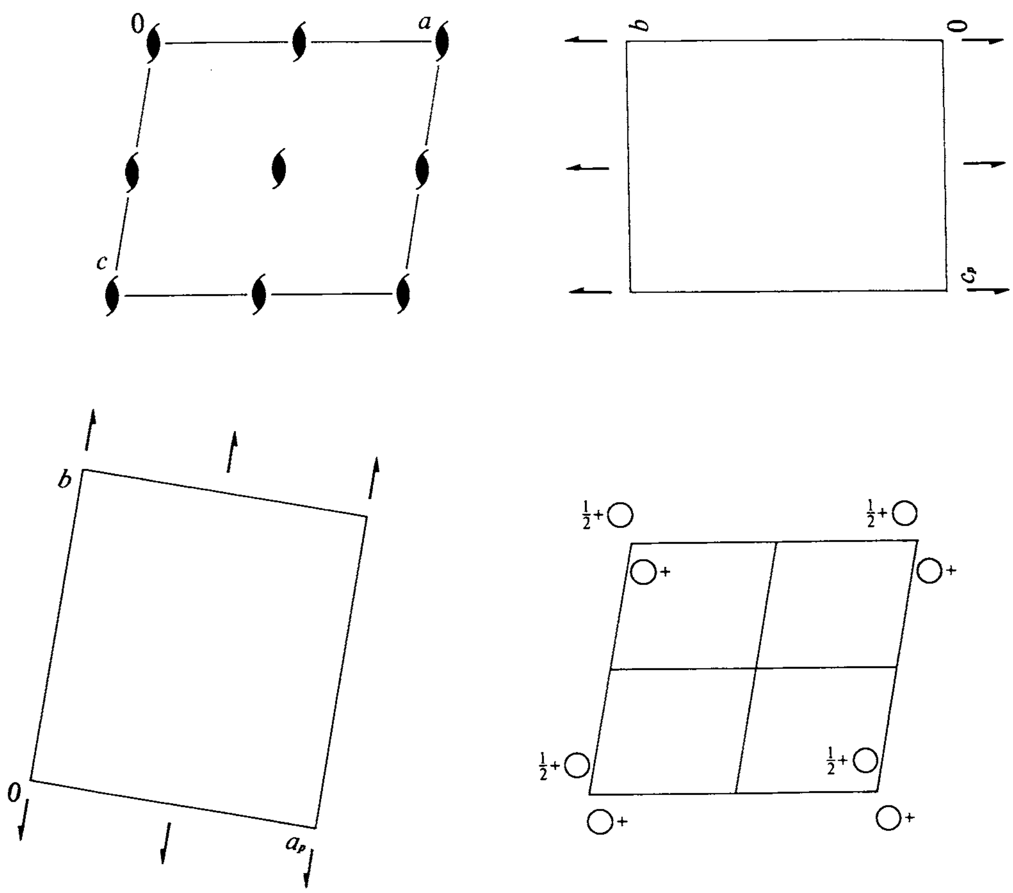
II [2] $A112$ ($C2$, 5); [2] $B112$ ($C2$, 5); [2] $I112$ ($C2$, 5)

International Tables for Crystallography (2006). Vol. A, Space group 4, pp. 120–123.

$P2_1$ C_2^2 2   Monoclinic

No. 4 $P\,1\,2_1\,1$ Patterson symmetry $P\,1\,2/m\,1$

UNIQUE AXIS b



Origin on 2_1

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1   (2) $2(0,\frac{1}{2},0)\quad 0,y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
2 a 1	(1) x,y,z (2) $\bar{x},y+\frac{1}{2},\bar{z}$	$0k0: k=2n$

Symmetry of special projections

Along [001] $p\,1\,g\,1$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,1\,g$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p\,2$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P\,1$ (1) 1
IIa none
IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $P\,1\,2_1\,1$ ($\mathbf{c}'=2\mathbf{c}$ or $\mathbf{a}'=2\mathbf{a}$ or $\mathbf{a}'=\mathbf{a}+\mathbf{c}, \mathbf{c}'=-\mathbf{a}+\mathbf{c}$) ($P2_1$, 4); [3] $P\,1\,2_1\,1$ ($\mathbf{b}'=3\mathbf{b}$) ($P2_1$, 4)

Minimal non-isomorphic supergroups

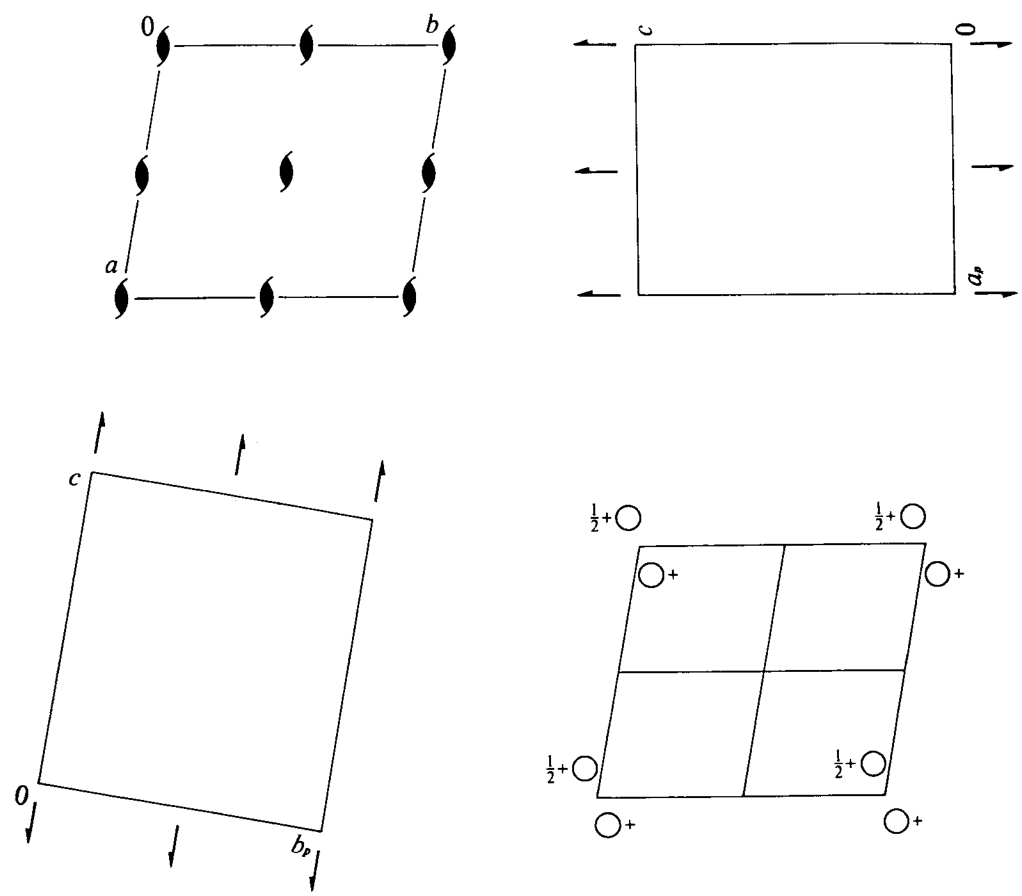
I [2] $P\,2_1/m$ (11); [2] $P\,2_1/c$ (14); [2] $P\,2\,2\,2_1$ (17); [2] $P\,2_1\,2_1\,2$ (18); [2] $P\,2_1\,2_1\,2_1$ (19); [2] $C\,2\,2\,2_1$ (20); [2] $P\,m\,c\,2_1$ (26); [2] $P\,c\,a\,2_1$ (29); [2] $P\,m\,n\,2_1$ (31); [2] $P\,n\,a\,2_1$ (33); [2] $C\,m\,c\,2_1$ (36); [2] $P\,4_1$ (76); [2] $P\,4_3$ (78); [3] $P\,6_1$ (169); [3] $P\,6_5$ (170); [3] $P\,6_3$ (173)

II [2] $C\,1\,2\,1$ ($C2$, 5); [2] $A\,1\,2\,1$ ($C2$, 5); [2] $I\,1\,2\,1$ ($C2$, 5); [2] $P\,1\,2\,1$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($P2$, 3)

$P2_1$ $\qquad C_2^2$ $\qquad 2$ $\qquad$ Monoclinic

No. 4 $\qquad P112_1$ $\qquad$ Patterson symmetry $P112/m$

UNIQUE AXIS c



Origin on 2_1

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $\qquad$ (2) $2(0,0,\frac{1}{2})$ $\quad 0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
2 a 1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$	$00l$: $l=2n$

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11g$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1$ (1) 1
IIa none
IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $P112_1$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{b}'=2\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{a}+\mathbf{b}$) ($P2_1$, 4); [3] $P112_1$ ($\mathbf{c}'=3\mathbf{c}$) ($P2_1$, 4)

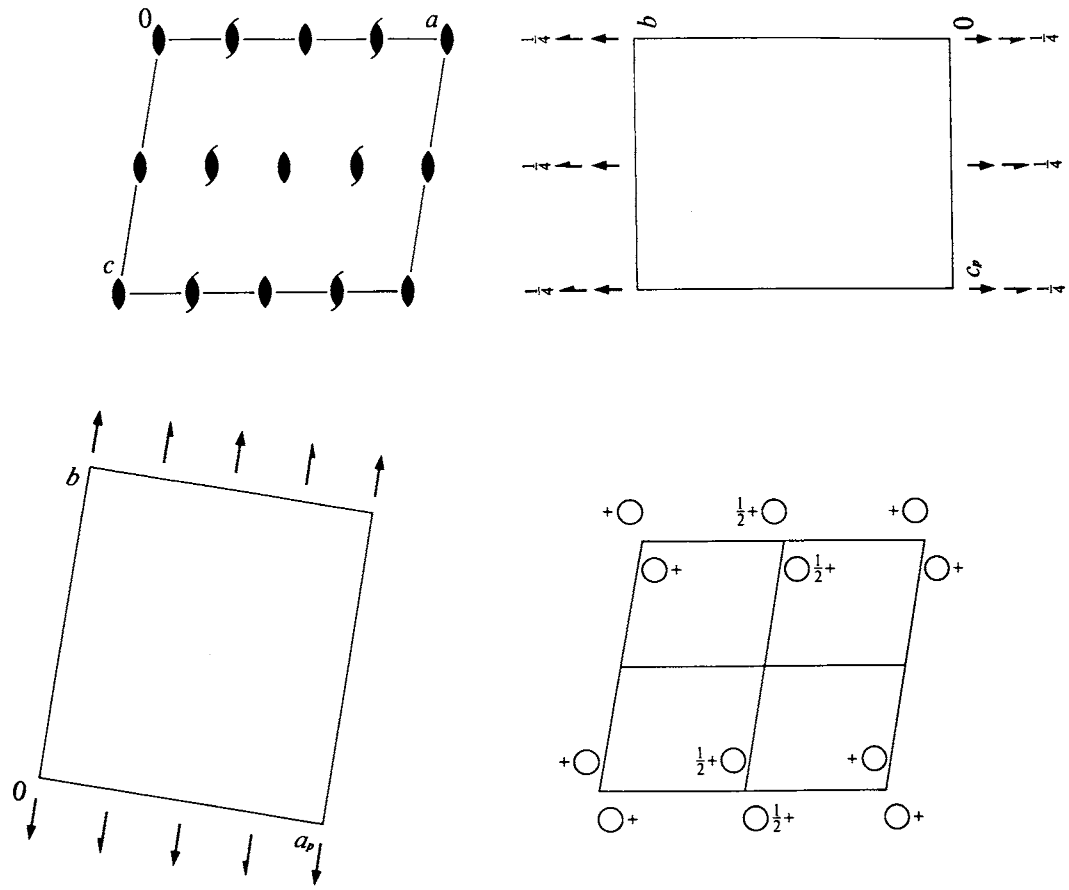
Minimal non-isomorphic supergroups

I [2] $P2_1/m$ (11); [2] $P2_1/c$ (14); [2] $P222_1$ (17); [2] $P2_12_12$ (18); [2] $P2_12_12_1$ (19); [2] $C222_1$ (20); [2] $Pmc2_1$ (26); [2] $Pca2_1$ (29); [2] $Pmn2_1$ (31); [2] $Pna2_1$ (33); [2] $Cmc2_1$ (36); [2] $P4_1$ (76); [2] $P4_3$ (78); [3] $P6_1$ (169); [3] $P6_5$ (170); [3] $P6_3$ (173)
II [2] $A112$ ($C2$, 5); [2] $B112$ ($C2$, 5); [2] $I112$ ($C2$, 5); [2] $P112$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P2$, 3)

International Tables for Crystallography (2006). Vol. A, Space group 5, pp. 124–131.

$C2$	C_2^3	2	Monoclinic
No. 5	$C121$		Patterson symmetry $C12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin on 2

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,y,0$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$	General:
4	c	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	$hkl: h+k=2n$ $h0l: h=2n$ $0kl: k=2n$ $hk0: h+k=2n$ $0k0: k=2n$ $h00: h=2n$
					Special: no extra conditions
2	b	2	$0,y,\frac{1}{2}$		
2	a	2	$0,y,0$		

Symmetry of special projections

Along [001] $c1m1$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $C1$ ($P1$, 1) 1+

IIa [2] $P12_11$ ($P2_1$, 4) 1; $2+(\frac{1}{2},\frac{1}{2},0)$
[2] $P121$ ($P2$, 3) 1; 2

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $C121$ ($\mathbf{c}'=2\mathbf{c}$ or $\mathbf{a}'=\mathbf{a}+2\mathbf{c},\mathbf{c}'=2\mathbf{c}$) ($C2$, 5); [3] $C121$ ($\mathbf{b}'=3\mathbf{b}$) ($C2$, 5)

Minimal non-isomorphic supergroups

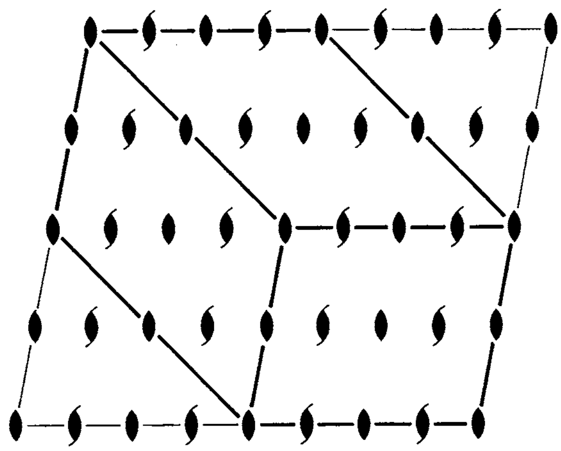
I [2] $C2/m$ (12); [2] $C2/c$ (15); [2] $C222_1$ (20); [2] $C222$ (21); [2] $F222$ (22); [2] $I222$ (23); [2] $I2_12_12_1$ (24); [2] $Amm2$ (38); [2] $Aem2$ (39); [2] $Ama2$ (40); [2] $Aea2$ (41); [2] $Fmm2$ (42); [2] $Fdd2$ (43); [2] $Imm2$ (44); [2] $Iba2$ (45); [2] $Ima2$ (46); [2] $I4$ (79); [2] $I4_1$ (80); [2] $I\bar{4}$ (82); [3] $P312$ (149); [3] $P321$ (150); [3] $P3_112$ (151); [3] $P3_121$ (152); [3] $P3_212$ (153); [3] $P3_221$ (154); [3] $R32$ (155)

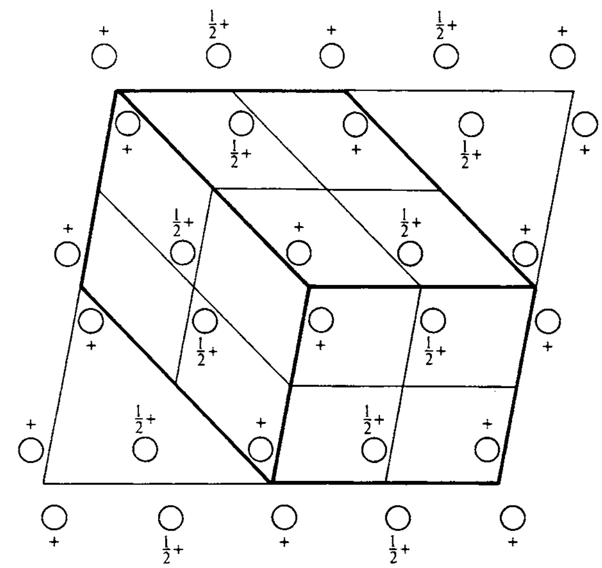
II [2] $P121$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($P2$, 3)

$C2$ $\qquad$ C_2^3 $\qquad$ 2 $\qquad$ Monoclinic

No. 5

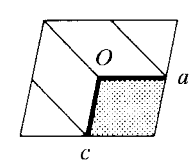
UNIQUE AXIS b, DIFFERENT CELL CHOICES





$C121$

UNIQUE AXIS b, CELL CHOICE 1



Origin on 2

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

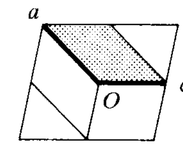
Generators selected $\quad$ (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},0)+$		General:
4	c	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	$hkl: h+k=2n$ $h0l: h=2n$ $0kl: k=2n$ $hk0: h+k=2n$ $0k0: k=2n$ $h00: h=2n$
					Special: no extra conditions
2	b	2	$0,y,\frac{1}{2}$		
2	a	2	$0,y,0$		

$A121$

UNIQUE AXIS b, CELL CHOICE 2



Origin on 2

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

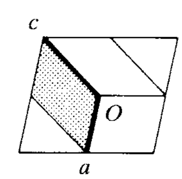
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$		Reflection conditions
					General:
4	c	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	hkl : $k+l=2n$ $h0l$: $l=2n$ $0kl$: $k+l=2n$ $hk0$: $k=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
					Special: no extra conditions
2	b	2	$\frac{1}{2},y,\frac{1}{2}$		
2	a	2	$0,y,0$		

$I121$

UNIQUE AXIS b, CELL CHOICE 3



Origin on 2

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)

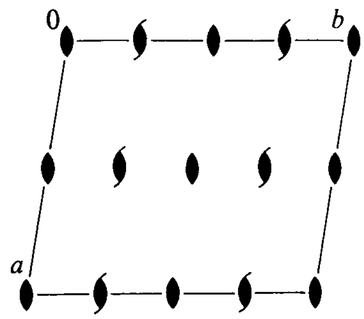
Positions

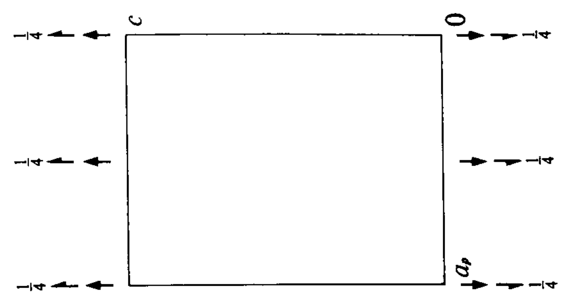
Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$		Reflection conditions
					General:
4	c	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	hkl : $h+k+l=2n$ $h0l$: $h+l=2n$ $0kl$: $k+l=2n$ $hk0$: $h+k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$
					Special: no extra conditions
2	b	2	$\frac{1}{2},y,0$		
2	a	2	$0,y,0$		

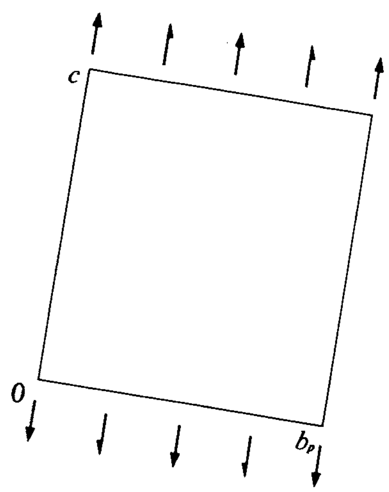
$C2$ $\quad$ C_2^3 $\quad$ 2 $\quad$ Monoclinic

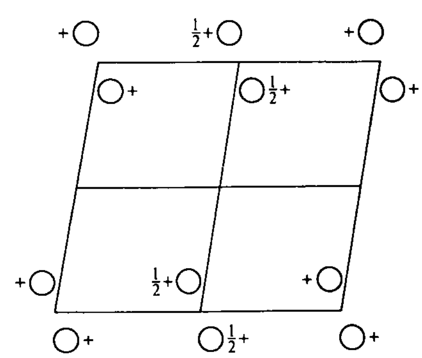
No. 5 $\quad$ $A112$ $\quad$ Patterson symmetry $A112/m$

UNIQUE AXIS c, CELL CHOICE 1









Origin on 2

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 $\qquad$ (2) $2 \quad 0,0,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ $\qquad$ (2) $2(0,0,\frac{1}{2}) \quad 0,\frac{1}{4},z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	hkl : $k+l=2n$ $hk0$: $k=2n$ $0kl$: $k+l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$ $0k0$: $k=2n$
					Special: no extra conditions
2	b	2	$\frac{1}{2},0,z$		
2	a	2	$0,0,z$		

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $A1$ ($P1$, 1) 1+

IIa [2] $P112_1$ ($P2_1$, 4) 1; $2+(0,\frac{1}{2},\frac{1}{2})$
[2] $P112$ ($P2$, 3) 1; 2

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $A112$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) ($C2$, 5); [3] $A112$ ($\mathbf{c}'=3\mathbf{c}$) ($C2$, 5)

Minimal non-isomorphic supergroups

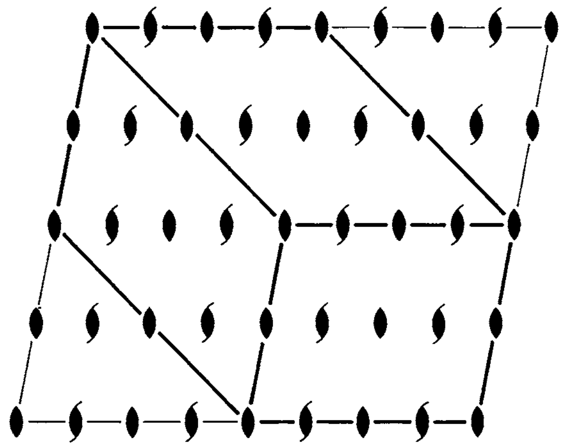
I [2] $C2/m$ (12); [2] $C2/c$ (15); [2] $C222_1$ (20); [2] $C222$ (21); [2] $F222$ (22); [2] $I222$ (23); [2] $I2_12_12_1$ (24); [2] $Amm2$ (38); [2] $Aem2$ (39); [2] $Ama2$ (40); [2] $Aea2$ (41); [2] $Fmm2$ (42); [2] $Fdd2$ (43); [2] $Imm2$ (44); [2] $Iba2$ (45); [2] $Ima2$ (46); [2] $I4$ (79); [2] $I4_1$ (80); [2] $I\bar{4}$ (82); [3] $P312$ (149); [3] $P321$ (150); [3] $P3_112$ (151); [3] $P3_121$ (152); [3] $P3_212$ (153); [3] $P3_221$ (154); [3] $R32$ (155)

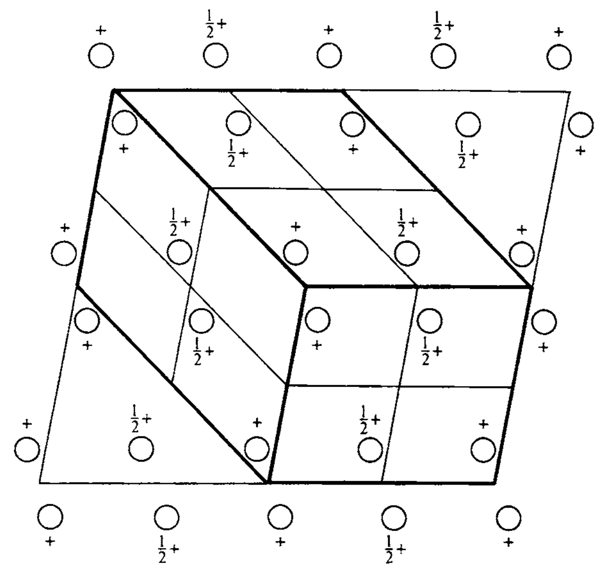
II [2] $P112$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P2$, 3)

$C2$ $\quad C_2^3$ $\quad 2$ $\quad$ Monoclinic

No. 5

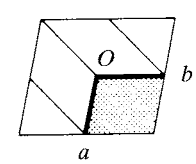
UNIQUE AXIS c, DIFFERENT CELL CHOICES





$A112$

UNIQUE AXIS c, CELL CHOICE 1



Origin on 2

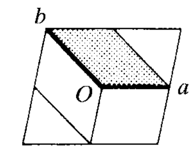
Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Generators selected $\quad (1);\ t(1,0,0);\ t(0,1,0);\ t(0,0,1);\ t(0,\frac{1}{2},\frac{1}{2});\ (2)$

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+\quad (0,\frac{1}{2},\frac{1}{2})+$		General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	hkl : $k+l=2n$ $hk0$: $k=2n$ $0kl$: $k+l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$ $0k0$: $k=2n$
					Special: no extra conditions
2	b	2	$\frac{1}{2},0,z$		
2	a	2	$0,0,z$		

$B112$



UNIQUE AXIS c, CELL CHOICE 2

Origin on 2

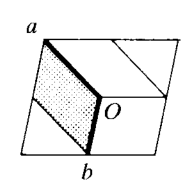
Asymmetric unit $0 \le x \le 1$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},0,\frac{1}{2})+$		Reflection conditions
					General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	hkl : $h+l=2n$ $hk0$: $h=2n$ $0kl$: $l=2n$ $h0l$: $h+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
					Special: no extra conditions
2	b	2	$\frac{1}{2},\frac{1}{2},z$		
2	a	2	$0,0,z$		

$I112$



UNIQUE AXIS c, CELL CHOICE 3

Origin on 2

Asymmetric unit $0 \le x \le 1$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)

Positions

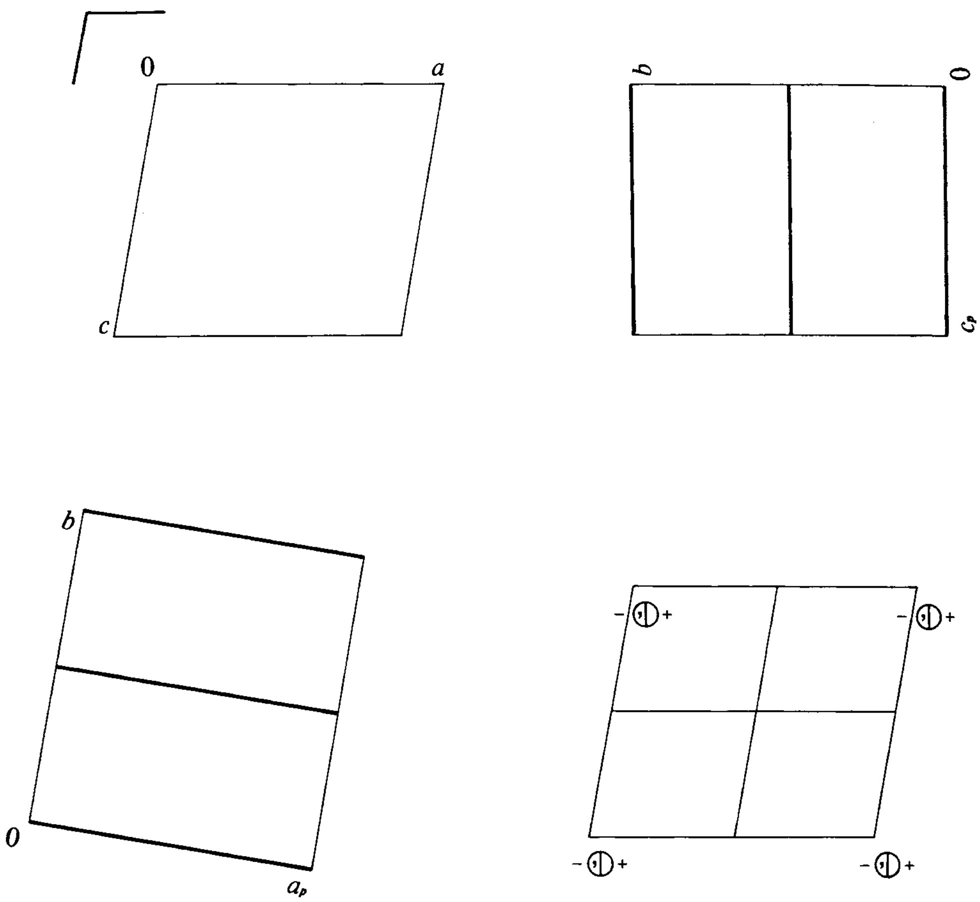
Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$		Reflection conditions
					General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
					Special: no extra conditions
2	b	2	$0,\frac{1}{2},z$		
2	a	2	$0,0,z$		

International Tables for Crystallography (2006). Vol. A, Space group 6, pp. 132–135.

Pm $\quad C_s^1$ $\quad m$ $\quad$ Monoclinic

No. 6 $\quad P1m1$ $\quad$ Patterson symmetry $P12/m1$

UNIQUE AXIS b



Origin on mirror plane m

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $\qquad$ (2) $m \;\; x,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	c	1	(1) x,y,z	(2) $x,\bar{y},z$	no conditions
					Special: no extra conditions
1	b	m	$x,\frac{1}{2},z$		
1	a	m	$x,0,z$		

Symmetry of special projections

Along [001] $p\,1\,1\,m$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,m\,1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p\,1$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P\,1$ (1) 1

IIa none

IIb [2] $P\,1\,c\,1$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pc$, 7); [2] $P\,1\,a\,1$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pc$, 7); [2] $B\,1\,e\,1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Pc$, 7); [2] $C\,1\,m\,1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($Cm$, 8); [2] $A\,1\,m\,1$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($Cm$, 8); [2] $F\,1\,m\,1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($Cm$, 8)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\,1\,m\,1$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pm$, 6); [2] $P\,1\,m\,1$ ($\mathbf{c}' = 2\mathbf{c}$ or $\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{a}' = \mathbf{a}+\mathbf{c}, \mathbf{c}' = -\mathbf{a}+\mathbf{c}$) ($Pm$, 6)

Minimal non-isomorphic supergroups

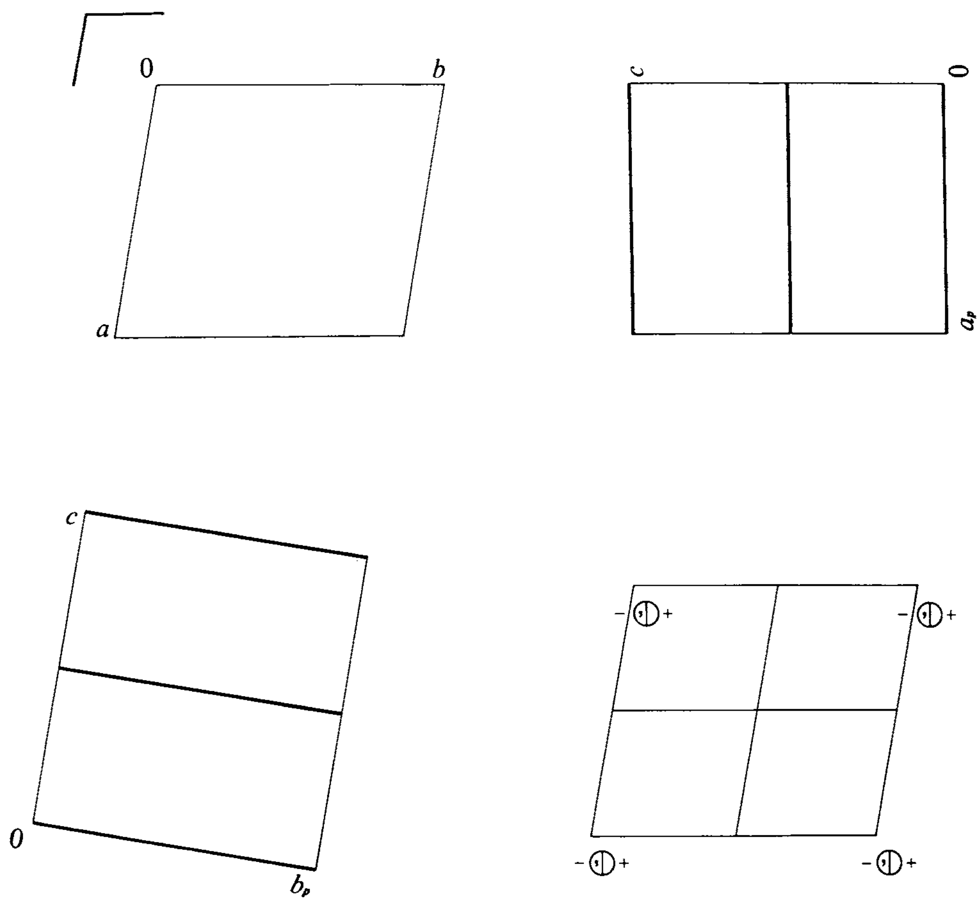
I [2] $P\,2/m$ (10); [2] $P\,2_1/m$ (11); [2] $P\,m\,m\,2$ (25); [2] $P\,m\,c\,2_1$ (26); [2] $P\,m\,a\,2$ (28); [2] $P\,m\,n\,2_1$ (31); [2] $A\,m\,m\,2$ (38); [2] $A\,m\,a\,2$ (40); [3] $P\,\bar{6}$ (174)

II [2] $C\,1\,m\,1$ (Cm, 8); [2] $A\,1\,m\,1$ (Cm, 8); [2] $I\,1\,m\,1$ (Cm, 8)

Pm C_s^1 m Monoclinic

No. 6 $P\,1\,1\,m$ Patterson symmetry $P\,1\,1\,2/m$

UNIQUE AXIS c



Origin on mirror plane m

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) $m\ \ x,y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	c	1	(1) x,y,z	(2) $x,y,\bar{z}$	no conditions
					Special: no extra conditions
1	b	m	$x,y,\frac{1}{2}$		
1	a	m	$x,y,0$		

Symmetry of special projections

Along [001] $p1$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p11m$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p1m1$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1$ (1) 1

IIa none

IIb [2] $P11a$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pc$, 7); [2] $P11b$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pc$, 7); [2] $C11e$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($Pc$, 7); [2] $A11m$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($Cm$, 8); [2] $B11m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Cm$, 8); [2] $F11m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($Cm$, 8)

Maximal isomorphic subgroups of lowest index

IIc [2] $P11m$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pm$, 6); [2] $P11m$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b}$) ($Pm$, 6)

Minimal non-isomorphic supergroups

I [2] $P2/m$ (10); [2] $P2_1/m$ (11); [2] $Pmm2$ (25); [2] $Pmc2_1$ (26); [2] $Pma2$ (28); [2] $Pmn2_1$ (31); [2] $Amm2$ (38); [2] $Ama2$ (40); [3] $P\bar{6}$ (174)

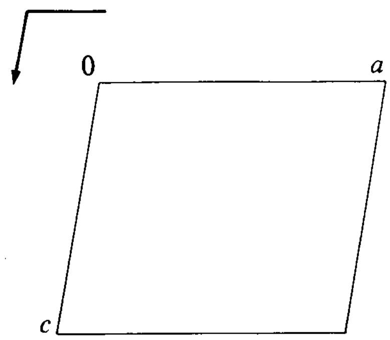
II [2] $A11m$ (Cm, 8); [2] $B11m$ (Cm, 8); [2] $I11m$ (Cm, 8)

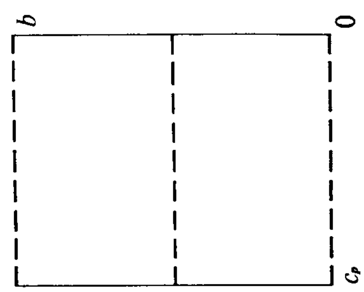
International Tables for Crystallography (2006). Vol. A, Space group 7, pp. 136–143.

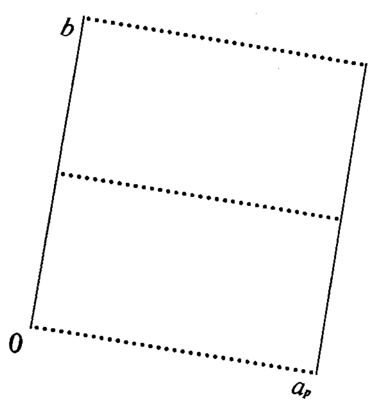
Pc C_s^2 m Monoclinic

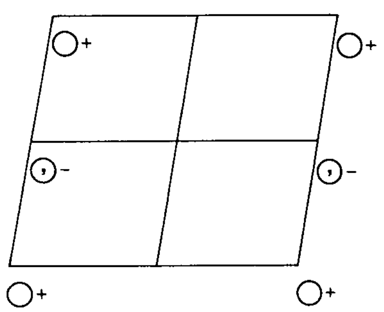
No. 7 $P1c1$ Patterson symmetry $P12/m1$

UNIQUE AXIS b, CELL CHOICE 1









Origin on glide plane c

Asymmetric unit $0 \le x \le 1$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) c $x,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		Reflection conditions
			General:
2 a 1	(1) x,y,z	(2) $x,\bar{y},z+\frac{1}{2}$	$h0l$: $l=2n$ $00l$: $l=2n$

Symmetry of special projections

Along [001] $p\,1\,1\,m$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,g\,1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p\,1$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P\,1$ (1) 1

IIa none

IIb [2] $C\,1\,c\,1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($Cc$, 9)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\,1\,c\,1$ ($\mathbf{b}'=2\mathbf{b}$) (Pc, 7); [2] $P\,1\,c\,1$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{a}'=2\mathbf{a},\mathbf{c}'=2\mathbf{a}+\mathbf{c}$) ($Pc$, 7)

Minimal non-isomorphic supergroups

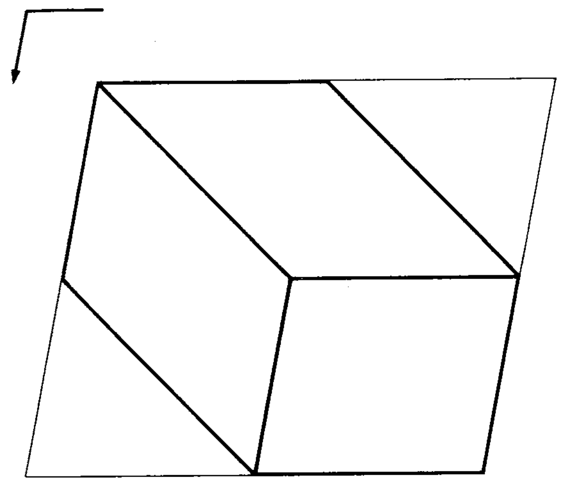
I [2] $P\,2/c$ (13); [2] $P\,2_1/c$ (14); [2] $P\,m\,c\,2_1$ (26); [2] $P\,c\,c\,2$ (27); [2] $P\,m\,a\,2$ (28); [2] $P\,c\,a\,2_1$ (29); [2] $P\,n\,c\,2$ (30); [2] $P\,m\,n\,2_1$ (31); [2] $P\,b\,a\,2$ (32); [2] $P\,n\,a\,2_1$ (33); [2] $P\,n\,n\,2$ (34); [2] $A\,e\,m\,2$ (39); [2] $A\,e\,a\,2$ (41)

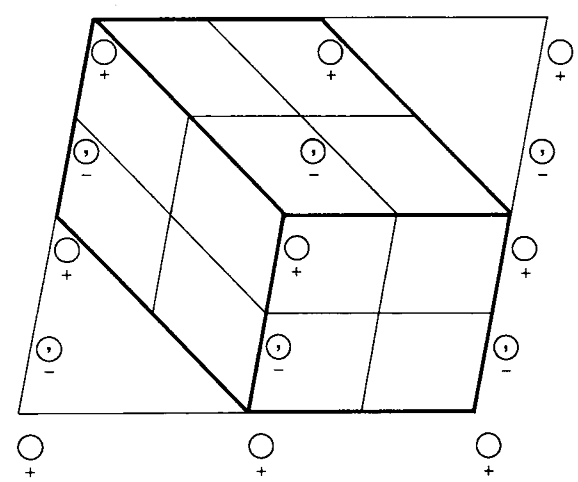
II [2] $C\,1\,c\,1$ (Cc, 9); [2] $A\,1\,m\,1$ (Cm, 8); [2] $I\,1\,c\,1$ (Cc, 9); [2] $P\,1\,m\,1$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($Pm$, 6)

Pc $\quad C_s^2$ $\quad m$ $\quad$ Monoclinic

No. 7

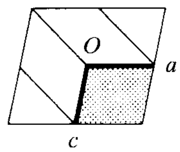
UNIQUE AXIS b, DIFFERENT CELL CHOICES





$P1c1$

UNIQUE AXIS b, CELL CHOICE 1



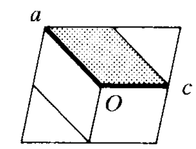
Origin on glide plane c

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Generators selected $\quad (1);\ t(1,0,0);\ t(0,1,0);\ t(0,0,1);\ (2)$

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		Reflection conditions
			General:
2 a 1	(1) x,y,z	(2) $x,\bar{y},z+\frac{1}{2}$	$h0l:\ l=2n$ $00l:\ l=2n$



$P1n1$

UNIQUE AXIS b, CELL CHOICE 2

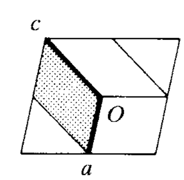
Origin on glide plane n

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		Reflection conditions
			General:
2 a 1	(1) x,y,z	(2) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	$h0l$: $h+l=2n$ $h00$: $h=2n$ $00l$: $l=2n$



$P1a1$

UNIQUE AXIS b, CELL CHOICE 3

Origin on glide plane a

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

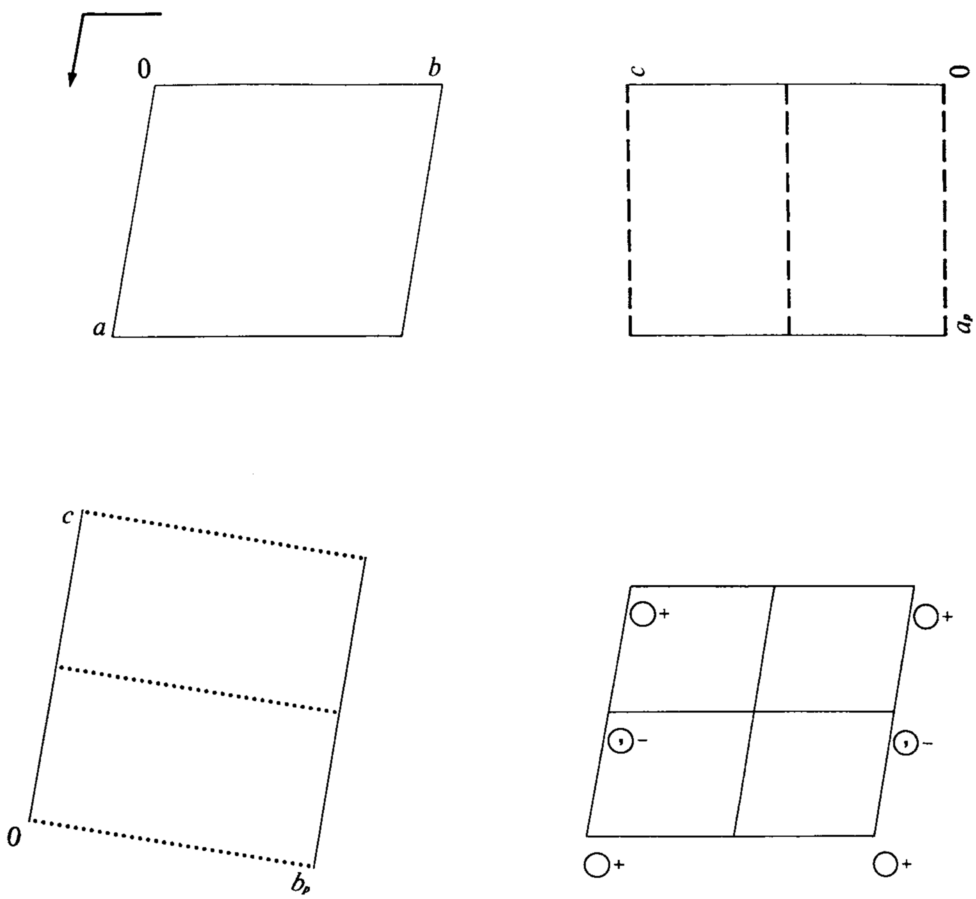
Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		Reflection conditions
			General:
2 a 1	(1) x,y,z	(2) $x+\frac{1}{2},\bar{y},z$	$h0l$: $h=2n$ $h00$: $h=2n$

Pc C_s^2 m Monoclinic

No. 7 $P\,1\,1\,a$ Patterson symmetry $P\,1\,1\,2/m$

UNIQUE AXIS c, CELL CHOICE 1



Origin on glide plane a

Asymmetric unit $0 \leq x \leq 1;\quad 0 \leq y \leq 1;\quad 0 \leq z \leq \frac{1}{2}$

Symmetry operations

(1) 1 (2) $a\quad x,y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
2 a 1	(1) x,y,z (2) $x+\frac{1}{2},y,\bar{z}$	$hk0: h=2n$ $h00: h=2n$

Symmetry of special projections

Along [001] $p\,1$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,1\,m$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p\,1\,g\,1$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P\,1$ (1) 1
IIa none
IIb [2] $A\,1\,1\,a$ ($\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($Cc$, 9)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\,1\,1\,a$ ($\mathbf{c}'=2\mathbf{c}$) (Pc, 7); [2] $P\,1\,1\,a$ ($\mathbf{b}'=2\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=2\mathbf{b}$) ($Pc$, 7)

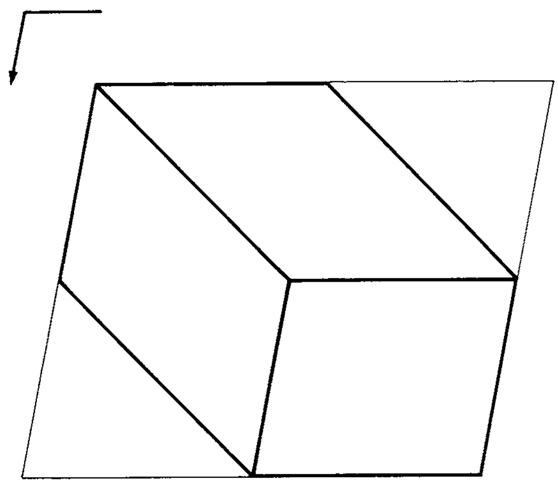
Minimal non-isomorphic supergroups

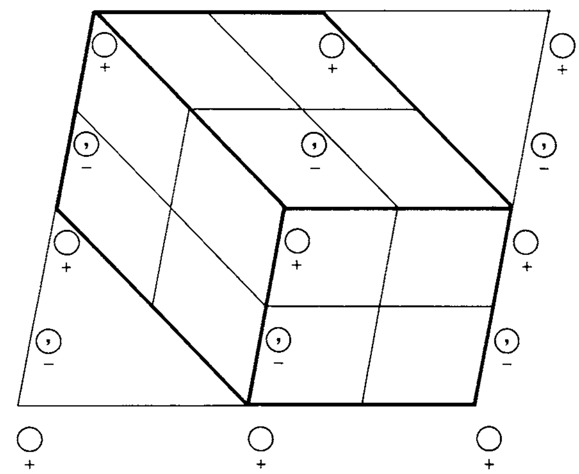
I [2] $P2/c$ (13); [2] $P2_1/c$ (14); [2] $Pmc2_1$ (26); [2] $Pcc2$ (27); [2] $Pma2$ (28); [2] $Pca2_1$ (29); [2] $Pnc2$ (30); [2] $Pmn2_1$ (31); [2] $Pba2$ (32); [2] $Pna2_1$ (33); [2] $Pnn2$ (34); [2] $Aem2$ (39); [2] $Aea2$ (41)
II [2] $A\,1\,1\,a$ (Cc, 9); [2] $B\,1\,1\,m$ (Cm, 8); [2] $I\,1\,1\,a$ (Cc, 9); [2] $P\,1\,1\,m$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Pm$, 6)

Pc $\quad C_s^2 \quad m \quad$ Monoclinic

No. 7

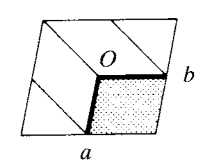
UNIQUE AXIS c, DIFFERENT CELL CHOICES





$P11a$

UNIQUE AXIS c, CELL CHOICE 1



Origin on glide plane a

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

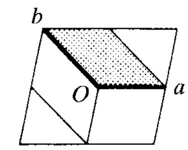
Generators selected $\quad (1);\ t(1,0,0);\ t(0,1,0);\ t(0,0,1);\ (2)$

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		Reflection conditions
			General:
2 a 1	(1) x,y,z	(2) $x+\frac{1}{2},y,\bar{z}$	$hk0:\ h=2n$ $h00:\ h=2n$

$P\,1\,1\,n$

UNIQUE AXIS c, CELL CHOICE 2



Origin on glide plane n

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

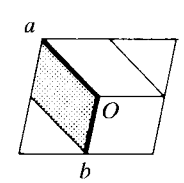
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	a	1	(1) x,y,z	(2) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	$hk0: h+k=2n$ $h00: h=2n$ $0k0: k=2n$

$P\,1\,1\,b$

UNIQUE AXIS c, CELL CHOICE 3



Origin on glide plane b

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

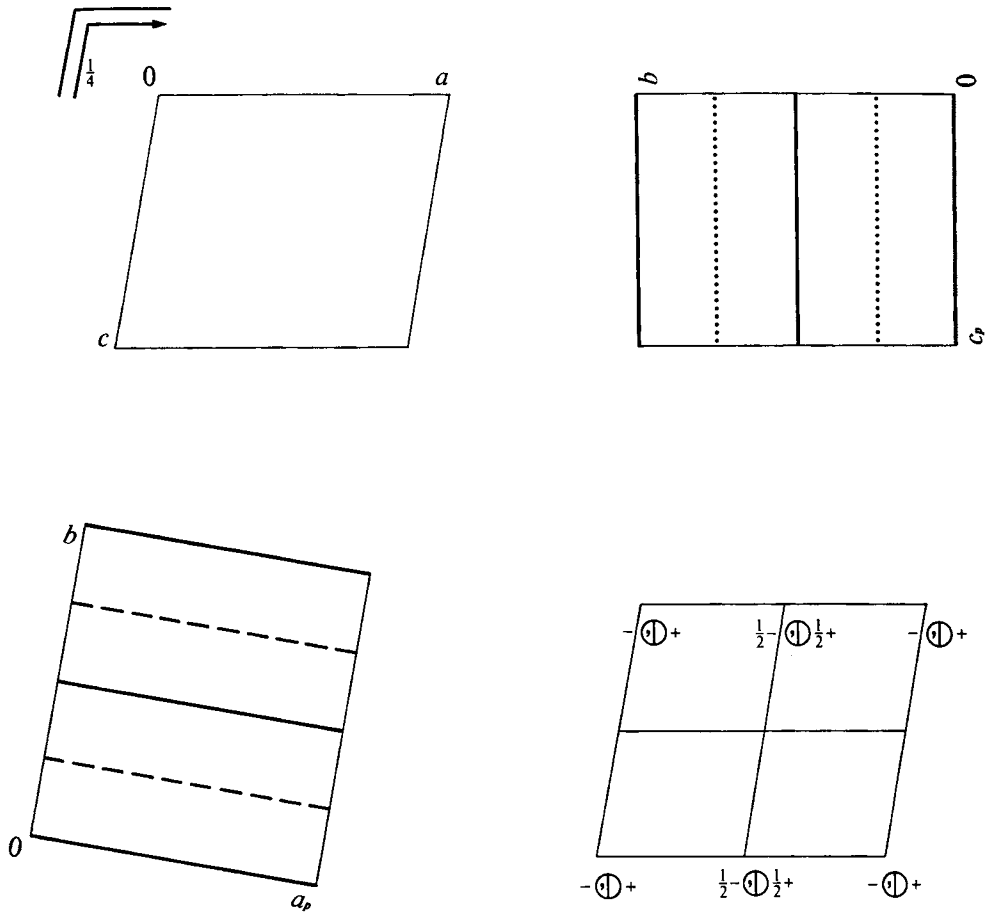
Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	a	1	(1) x,y,z	(2) $x,y+\frac{1}{2},\bar{z}$	$hk0: k=2n$ $0k0: k=2n$

International Tables for Crystallography (2006). Vol. A, Space group 8, pp. 144–151.

Cm $\quad C_s^3 \quad$ m $\quad$ Monoclinic

No. 8 $\quad C1m1 \quad$ Patterson symmetry $C12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin on mirror plane m

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 $\qquad$ (2) $m \quad x,0,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ $\qquad$ (2) $a \quad x,\frac{1}{4},z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$	General:
4	b	1	(1) x,y,z	(2) $x,\bar{y},z$	$hkl: h+k=2n$ $h0l: h=2n$ $0kl: k=2n$ $hk0: h+k=2n$ $0k0: k=2n$ $h00: h=2n$
					Special: no extra conditions
2	a	m	$x,0,z$		

Symmetry of special projections

Along [001] $c\,1\,1\,m$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,m\,1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p\,1$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $C1$ ($P1$, 1) 1+

IIa [2] $P\,1\,a\,1$ (Pc, 7) 1; $2+(\frac{1}{2},\frac{1}{2},0)$
[2] $P\,1\,m\,1$ (Pm, 6) 1; 2

IIb [2] $C\,1\,c\,1$ ($\mathbf{c}'=2\mathbf{c}$) (Cc, 9); [2] $I\,1\,c\,1$ ($\mathbf{c}'=2\mathbf{c}$) (Cc, 9)

Maximal isomorphic subgroups of lowest index

IIc [2] $C\,1\,m\,1$ ($\mathbf{c}'=2\mathbf{c}$ or $\mathbf{a}'=\mathbf{a}+2\mathbf{c},\mathbf{c}'=2\mathbf{c}$) ($Cm$, 8); [3] $C\,1\,m\,1$ ($\mathbf{b}'=3\mathbf{b}$) (Cm, 8)

Minimal non-isomorphic supergroups

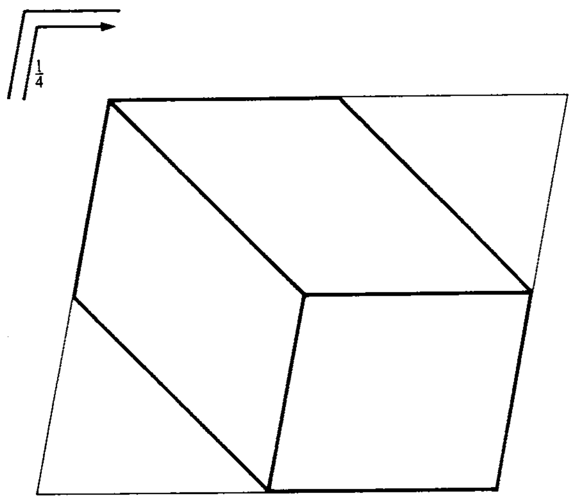
I [2] $C2/m$ (12); [2] $Cmm2$ (35); [2] $Cmc2_1$ (36); [2] $Amm2$ (38); [2] $Aem2$ (39); [2] $Fmm2$ (42); [2] $Imm2$ (44); [2] $Ima2$ (46); [3] $P3m1$ (156); [3] $P31m$ (157); [3] $R3m$ (160)

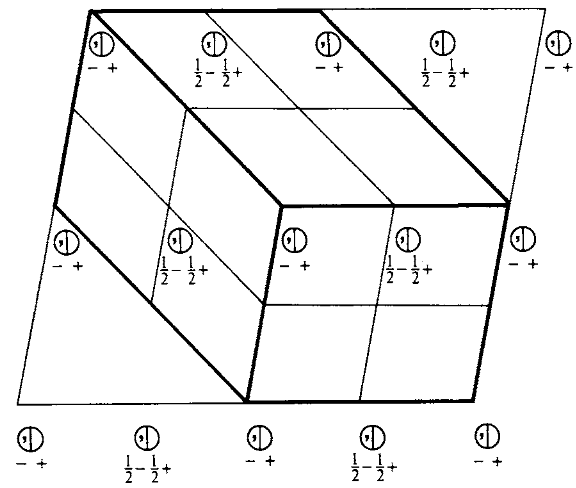
II [2] $P\,1\,m\,1$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Pm$, 6)

Cm $\quad C_s^3 \quad$ m $\quad$ Monoclinic

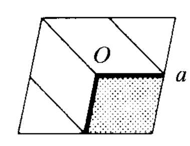
No. 8

UNIQUE AXIS b, DIFFERENT CELL CHOICES





$C1m1$



UNIQUE AXIS b, CELL CHOICE 1

Origin on mirror plane m

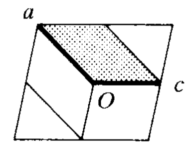
Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Generators selected $\quad (1);\ t(1,0,0);\ t(0,1,0);\ t(0,0,1);\ t(\frac{1}{2},\frac{1}{2},0);\ (2)$

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},0)+$		General:
4	b	1	(1) x,y,z	(2) $x,\bar{y},z$	$hkl: h+k=2n$ $h0l: h=2n$ $0kl: k=2n$ $hk0: h+k=2n$ $0k0: k=2n$ $h00: h=2n$
					Special: no extra conditions
2	a	m	$x,0,z$		

$A\,1\,m\,1$



UNIQUE AXIS b, CELL CHOICE 2

Origin on mirror plane m

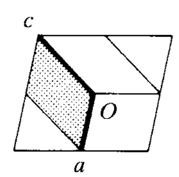
Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+\quad(0,\frac{1}{2},\frac{1}{2})+$		General:
4	b	1	(1) x,y,z	(2) $x,\bar{y},z$	$hkl: k+l=2n$ $h0l: l=2n$ $0kl: k+l=2n$ $hk0: k=2n$ $0k0: k=2n$ $00l: l=2n$
					Special: no extra conditions
2	a	m	$x,0,z$		

$I\,1\,m\,1$



UNIQUE AXIS b, CELL CHOICE 3

Origin on mirror plane m

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)

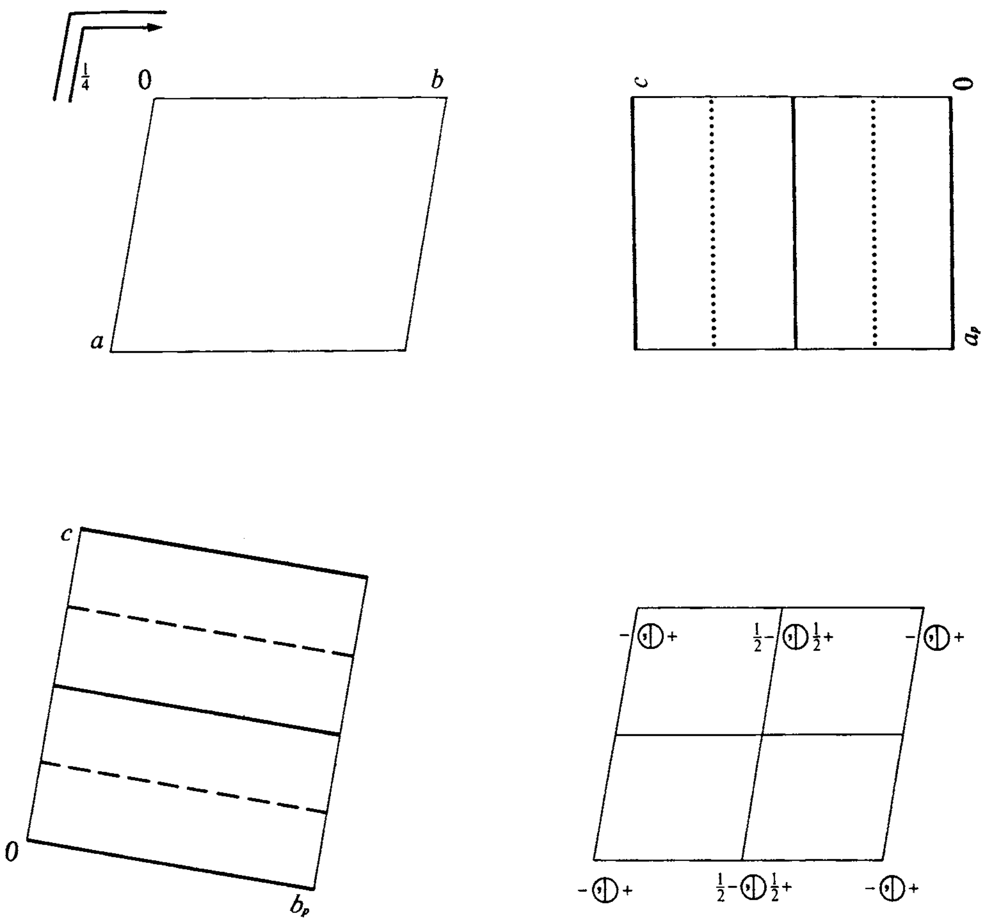
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$		General:
4	b	1	(1) x,y,z	(2) $x,\bar{y},z$	$hkl: h+k+l=2n$ $h0l: h+l=2n$ $0kl: k+l=2n$ $hk0: h+k=2n$ $0k0: k=2n$ $h00: h=2n$ $00l: l=2n$
					Special: no extra conditions
2	a	m	$x,0,z$		

Cm C_s^3 m Monoclinic

No. 8 $A\,1\,1\,m$ Patterson symmetry $A\,1\,1\,2/m$

UNIQUE AXIS c, CELL CHOICE 1



Origin on mirror plane m

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) $m\;\; x,y,0$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $b\;\; x,y,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	General:
4	b	1	(1) x,y,z	(2) $x,y,\bar{z}$	hkl : $k+l=2n$ $hk0$: $k=2n$ $0kl$: $k+l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$ $0k0$: $k=2n$
					Special: no extra conditions
2	a	m	$x,y,0$		

Symmetry of special projections

Along [001] $p1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $c11m$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $A1$ ($P1$, 1) 1+

IIa [2] $P11b$ (Pc, 7) 1; $2+(0,\frac{1}{2},\frac{1}{2})$
[2] $P11m$ (Pm, 6) 1; 2

IIb [2] $A11a$ ($\mathbf{a}'=2\mathbf{a}$) (Cc, 9); [2] $I11a$ ($\mathbf{a}'=2\mathbf{a}$) (Cc, 9)

Maximal isomorphic subgroups of lowest index

IIc [2] $A11m$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) ($Cm$, 8); [3] $A11m$ ($\mathbf{c}'=3\mathbf{c}$) (Cm, 8)

Minimal non-isomorphic supergroups

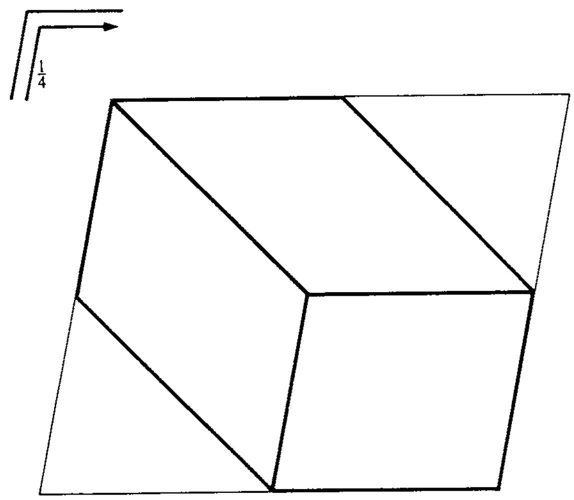
I [2] $C2/m$ (12); [2] $Cmm2$ (35); [2] $Cmc2_1$ (36); [2] $Amm2$ (38); [2] $Aem2$ (39); [2] $Fmm2$ (42); [2] $Imm2$ (44); [2] $Ima2$ (46); [3] $P3m1$ (156); [3] $P31m$ (157); [3] $R3m$ (160)

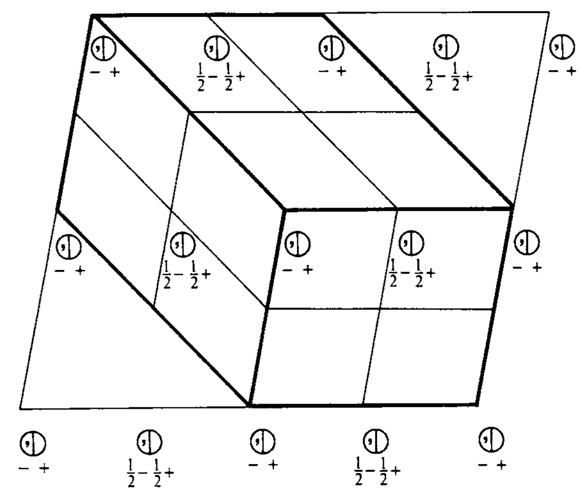
II [2] $P11m$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($Pm$, 6)

Cm $\quad C_s^3 \quad$ m $\quad$ Monoclinic

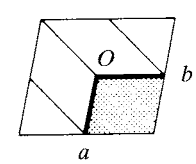
No. 8

UNIQUE AXIS c, DIFFERENT CELL CHOICES





$A11m$



UNIQUE AXIS c, CELL CHOICE 1

Origin on mirror plane m

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

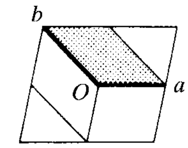
Generators selected $\quad (1);\ t(1,0,0);\ t(0,1,0);\ t(0,0,1);\ t(0,\frac{1}{2},\frac{1}{2});\ (2)$

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+$		Reflection conditions
			General:
4 b 1	(1) x,y,z	(2) $x,y,\bar{z}$	hkl : $k+l=2n$ $hk0$: $k=2n$ $0kl$: $k+l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$ $0k0$: $k=2n$
			Special: no extra conditions
2 a m	$x,y,0$		

$B11m$

UNIQUE AXIS c, CELL CHOICE 2



Origin on mirror plane m

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{4}$

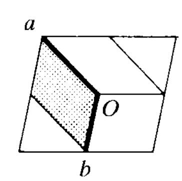
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},0,\frac{1}{2})+$		Reflection conditions
					General:
4	b	1	(1) x,y,z	(2) $x,y,\bar{z}$	hkl : $h+l=2n$ $hk0$: $h=2n$ $0kl$: $l=2n$ $h0l$: $h+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
					Special: no extra conditions
2	a	m	$x,y,0$		

$I11m$

UNIQUE AXIS c, CELL CHOICE 3



Origin on mirror plane m

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)

Positions

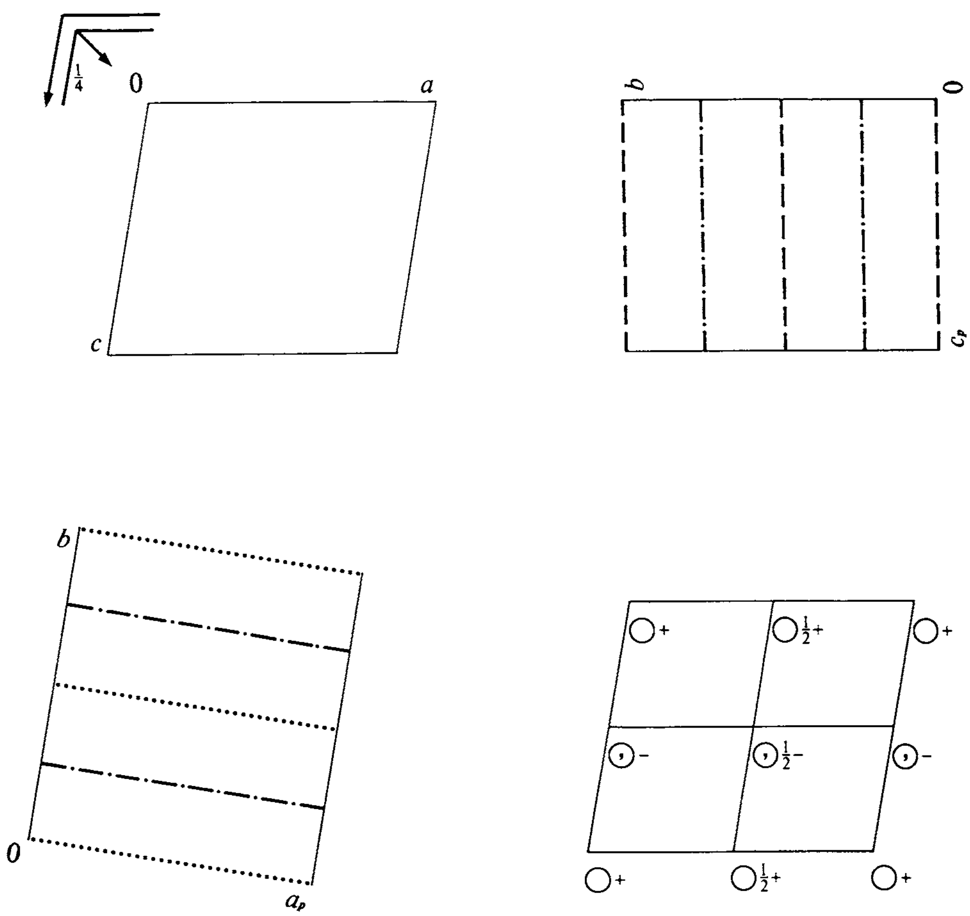
Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$		Reflection conditions
					General:
4	b	1	(1) x,y,z	(2) $x,y,\bar{z}$	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
					Special: no extra conditions
2	a	m	$x,y,0$		

International Tables for Crystallography (2006). Vol. A, Space group 9, pp. 152–159.

Cc $\qquad$ C_s^4 $\qquad$ m $\qquad$ Monoclinic

No. 9 $\qquad$ $C1c1$ $\qquad$ Patterson symmetry $C12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin on glide plane c

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 $\qquad$ (2) $c \quad x,0,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ $\qquad$ (2) $n(\frac{1}{2},0,\frac{1}{2}) \quad x,\frac{1}{4},z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
	$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$	General:
4 a 1	(1) x,y,z (2) $x,\bar{y},z+\frac{1}{2}$	$hkl: h+k=2n$ $h0l: h,l=2n$ $0kl: k=2n$ $hk0: h+k=2n$ $0k0: k=2n$ $h00: h=2n$ $00l: l=2n$

Symmetry of special projections

Along [001] $c11m$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p1$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $C1$ ($P1$, 1) 1+

IIa [2] $P1c1$ (Pc, 7) 1; 2
[2] $P1n1$ (Pc, 7) 1; $2+(\frac{1}{2},\frac{1}{2},0)$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $C1c1$ ($\mathbf{b}'=3\mathbf{b}$) (Cc, 9); [3] $C1c1$ ($\mathbf{c}'=3\mathbf{c}$) (Cc, 9); [3] $C1c1$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{a}'=3\mathbf{a},\mathbf{c}'=-\mathbf{a}+\mathbf{c}$ or $\mathbf{a}'=3\mathbf{a},\mathbf{c}'=\mathbf{a}+\mathbf{c}$) ($Cc$, 9)

Minimal non-isomorphic supergroups

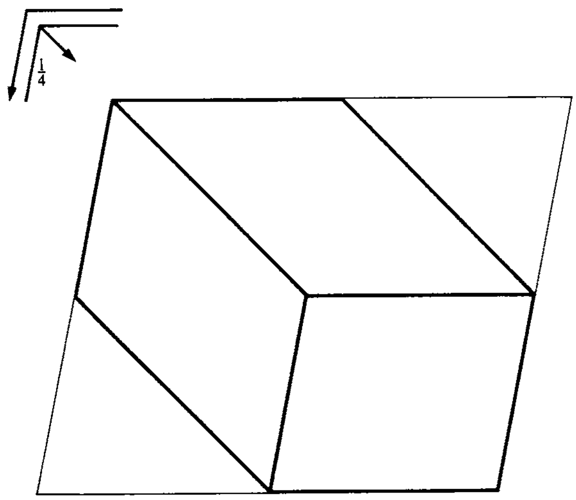
I [2] $C2/c$ (15); [2] $Cmc2_1$ (36); [2] $Ccc2$ (37); [2] $Ama2$ (40); [2] $Aea2$ (41); [2] $Fdd2$ (43); [2] $Iba2$ (45); [2] $Ima2$ (46); [3] $P3c1$ (158); [3] $P31c$ (159); [3] $R3c$ (161)

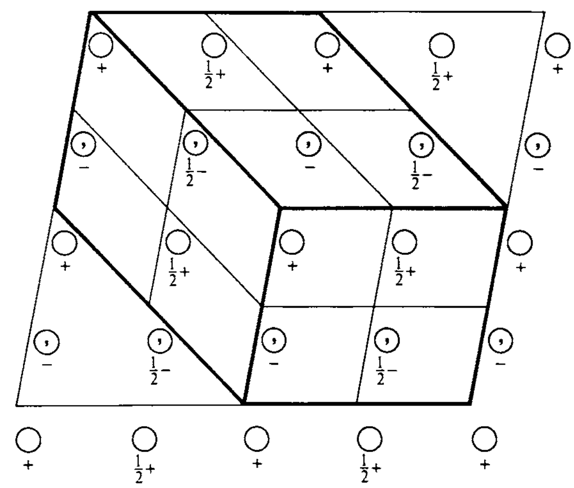
II [2] $F1m1$ (Cm, 8); [2] $C1m1$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($Cm$, 8); [2] $P1c1$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Pc$, 7)

Cc $\quad$ C_s^4 $\quad$ m $\quad$ Monoclinic

No. 9

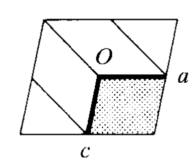
UNIQUE AXIS b, DIFFERENT CELL CHOICES





$C1c1$

UNIQUE AXIS b, CELL CHOICE 1



Origin on glide plane c

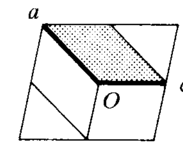
Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Generators selected $\quad (1);\ t(1,0,0);\ t(0,1,0);\ t(0,0,1);\ t(\frac{1}{2},\frac{1}{2},0);\ (2)$

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},0)+$		Reflection conditions
					General:
4	a	1	(1) x,y,z	(2) $x,\bar{y},z+\frac{1}{2}$	hkl : $h+k=2n$ $h0l$: $h,l=2n$ $0kl$: $k=2n$ $hk0$: $h+k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$

$A1n1$



UNIQUE AXIS b, CELL CHOICE 2

Origin on glide plane n

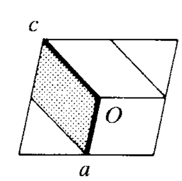
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+$		General:
4	a	1	(1) x,y,z	(2) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	hkl : $k+l=2n$ $h0l$: $h,l=2n$ $0kl$: $k+l=2n$ $hk0$: $k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$

$I1a1$



UNIQUE AXIS b, CELL CHOICE 3

Origin on glide plane a

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)

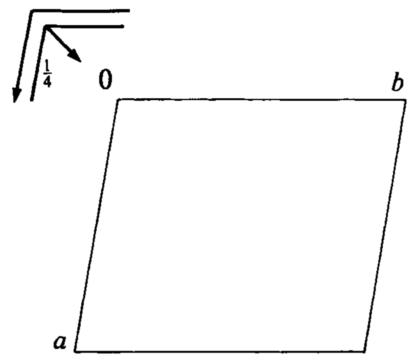
Positions

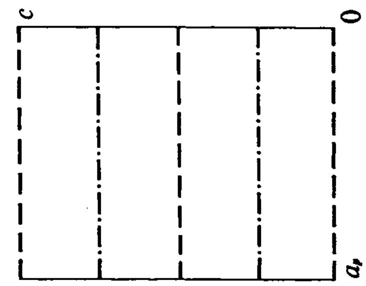
Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$		General:
4	a	1	(1) x,y,z	(2) $x+\frac{1}{2},\bar{y},z$	hkl : $h+k+l=2n$ $h0l$: $h,l=2n$ $0kl$: $k+l=2n$ $hk0$: $h+k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$

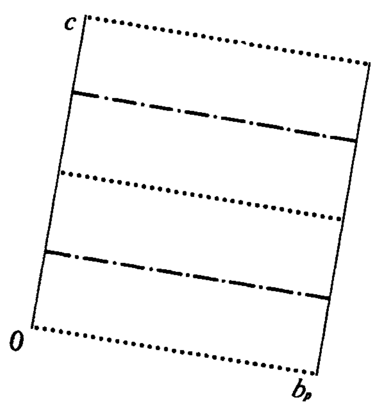
Cc $\quad C_s^4$ $\quad m$ $\quad$ Monoclinic

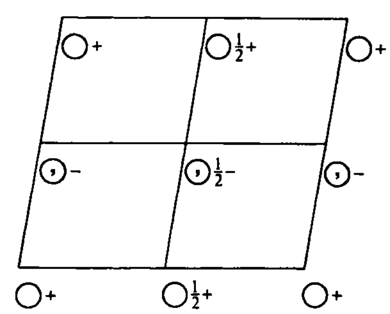
No. 9 $\quad A11a$ $\quad$ Patterson symmetry $A112/m$

UNIQUE AXIS c, CELL CHOICE 1









Origin on glide plane a

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 $\qquad$ (2) $a \quad x,y,0$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ $\qquad$ (2) $n(\frac{1}{2},\frac{1}{2},0) \quad x,y,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	General:
4	a	1	(1) x,y,z	(2) $x+\frac{1}{2},y,\bar{z}$	$hkl: k+l=2n$ $hk0: h,k=2n$ $0kl: k+l=2n$ $h0l: l=2n$ $00l: l=2n$ $h00: h=2n$ $0k0: k=2n$

Symmetry of special projections

Along [001] $p1$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $c11m$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p1g1$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $A1$ ($P1$, 1) 1+

IIa [2] $P11a$ (Pc, 7) 1; 2
[2] $P11n$ (Pc, 7) 1; $2+(0,\frac{1}{2},\frac{1}{2})$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $A11a$ ($\mathbf{c}'=3\mathbf{c}$) (Cc, 9); [3] $A11a$ ($\mathbf{a}'=3\mathbf{a}$) (Cc, 9); [3] $A11a$ ($\mathbf{b}'=3\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=3\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}+\mathbf{b},\mathbf{b}'=3\mathbf{b}$) ($Cc$, 9)

Minimal non-isomorphic supergroups

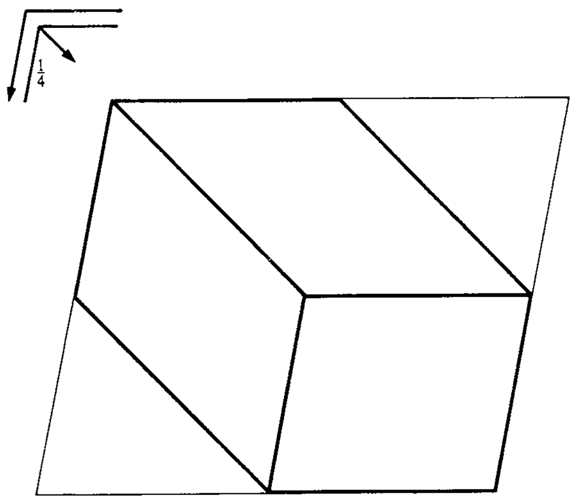
I [2] $C2/c$ (15); [2] $Cmc2_1$ (36); [2] $Ccc2$ (37); [2] $Ama2$ (40); [2] $Aea2$ (41); [2] $Fdd2$ (43); [2] $Iba2$ (45); [2] $Ima2$ (46); [3] $P3c1$ (158); [3] $P31c$ (159); [3] $R3c$ (161)

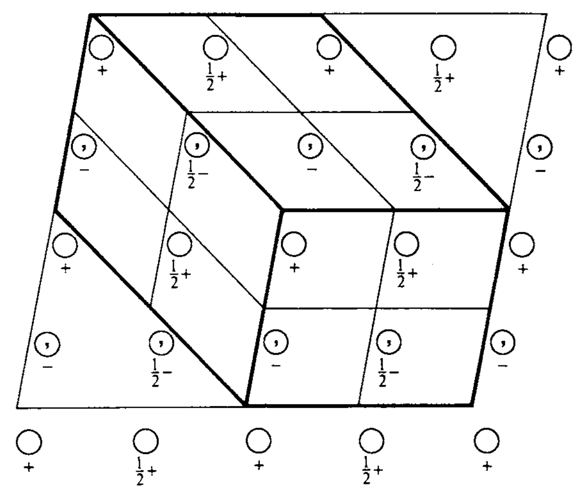
II [2] $F11m$ (Cm, 8); [2] $A11m$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Cm$, 8); [2] $P11a$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($Pc$, 7)

Cc $\quad C_s^4 \quad m \quad$ Monoclinic

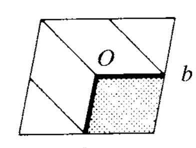
No. 9

UNIQUE AXIS c, DIFFERENT CELL CHOICES





$A\,1\,1\,a$



UNIQUE AXIS c, CELL CHOICE 1

Origin on glide plane a

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

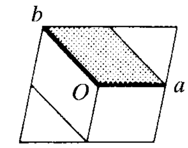
Generators selected $\quad (1);\ t(1,0,0);\ t(0,1,0);\ t(0,0,1);\ t(0,\frac{1}{2},\frac{1}{2});\ (2)$

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+$		General:
4	a	1	(1) x,y,z	(2) $x+\frac{1}{2},y,\bar{z}$	$hkl: k+l=2n$ $hk0: h,k=2n$ $0kl: k+l=2n$ $h0l: l=2n$ $00l: l=2n$ $h00: h=2n$ $0k0: k=2n$

$B\,1\,1\,n$

UNIQUE AXIS c, CELL CHOICE 2



Origin on glide plane n

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

$(0,0,0)+\quad(\frac{1}{2},0,\frac{1}{2})+$

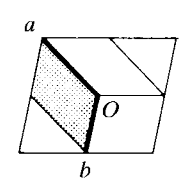
General:

4 a 1 (1) x,y,z (2) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$

hkl : $h+l=2n$
$hk0$: $h,k=2n$
$0kl$: $l=2n$
$h0l$: $h+l=2n$
$00l$: $l=2n$
$h00$: $h=2n$
$0k0$: $k=2n$

$I\,1\,1\,b$

UNIQUE AXIS c, CELL CHOICE 3



Origin on glide plane b

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

$(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

General:

4 a 1 (1) x,y,z (2) $x,y+\frac{1}{2},\bar{z}$

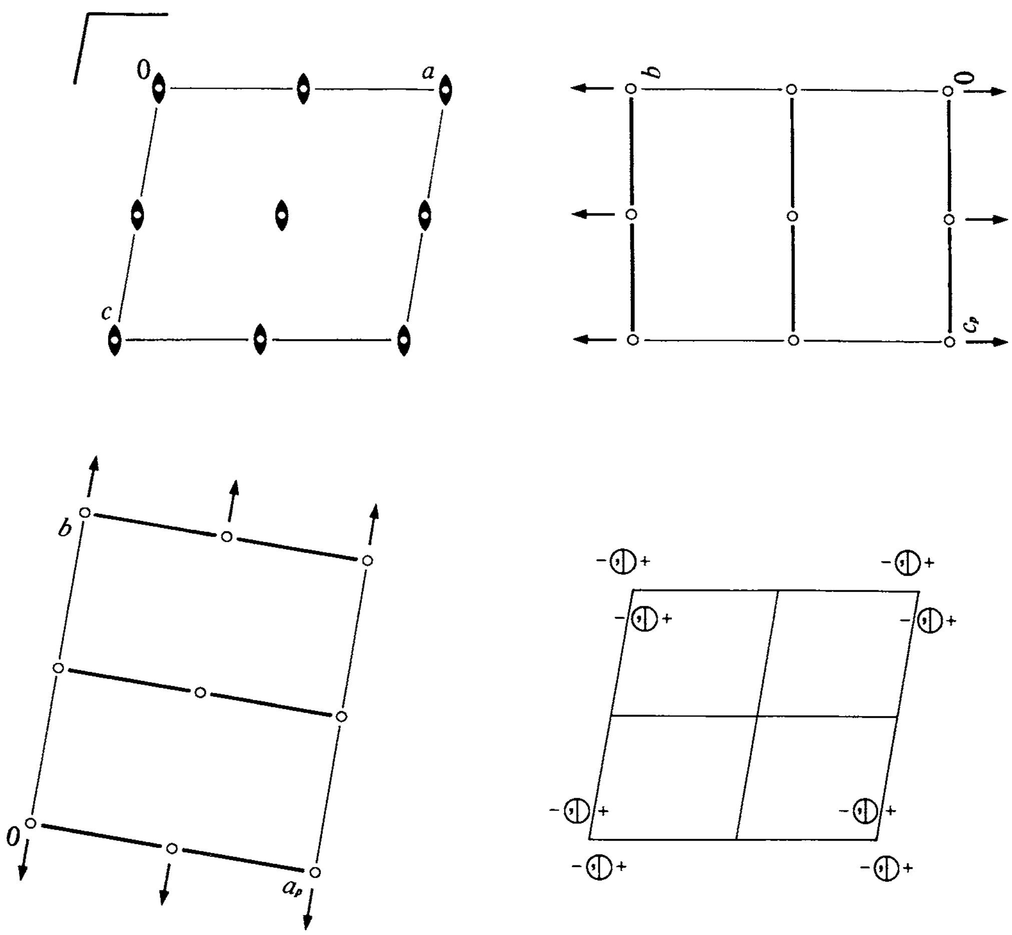
hkl : $h+k+l=2n$
$hk0$: $h,k=2n$
$0kl$: $k+l=2n$
$h0l$: $h+l=2n$
$00l$: $l=2n$
$h00$: $h=2n$
$0k0$: $k=2n$

International Tables for Crystallography (2006). Vol. A, Space group 10, pp. 160–163.

$P2/m$ $\quad C_{2h}^1$ $\quad 2/m$ $\quad$ Monoclinic

No. 10 $\quad P\,1\,2/m\,1$ $\quad$ Patterson symmetry $P\,1\,2/m\,1$

UNIQUE AXIS b



Origin at centre $(2/m)$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $\quad$ (2) $2\;\; 0,y,0$ $\quad$ (3) $\bar{1}\;\; 0,0,0$ $\quad$ (4) $m\;\; x,0,z$

Maximal isomorphic subgroups of lowest index

IIc $\quad$ [2] $P\,1\,2/m\,1$ ($\mathbf{b}' = 2\mathbf{b}$) ($P2/m$, 10); [2] $P\,1\,2/m\,1$ ($\mathbf{c}' = 2\mathbf{c}$ or $\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{a}' = \mathbf{a}+\mathbf{c}, \mathbf{c}' = -\mathbf{a}+\mathbf{c}$) ($P2/m$, 10)

Minimal non-isomorphic supergroups

I $\quad$ [2] $Pmmm$ (47); [2] $Pccm$ (49); [2] $Pmma$ (51); [2] $Pmna$ (53); [2] $Pbam$ (55); [2] $Pnnm$ (58); [2] $Cmmm$ (65); [2] $Cccm$ (66); [2] $P4/m$ (83); [2] $P4_2/m$ (84); [3] $P6/m$ (175)

II $\quad$ [2] $C\,1\,2/m\,1$ ($C2/m$, 12); [2] $A\,1\,2/m\,1$ ($C2/m$, 12); [2] $I\,1\,2/m\,1$ ($C2/m$, 12)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	o	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z$	no conditions
							Special: no extra conditions
2	n	m	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},\bar{z}$			
2	m	m	$x,0,z$	$\bar{x},0,\bar{z}$			
2	l	2	$\frac{1}{2},y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\frac{1}{2}$			
2	k	2	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			
2	j	2	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},0$			
2	i	2	$0,y,0$	$0,\bar{y},0$			
1	h	$2/m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
1	g	$2/m$	$\frac{1}{2},0,\frac{1}{2}$				
1	f	$2/m$	$0,\frac{1}{2},\frac{1}{2}$				
1	e	$2/m$	$\frac{1}{2},\frac{1}{2},0$				
1	d	$2/m$	$\frac{1}{2},0,0$				
1	c	$2/m$	$0,0,\frac{1}{2}$				
1	b	$2/m$	$0,\frac{1}{2},0$				
1	a	$2/m$	$0,0,0$				

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1m1$ (Pm, 6) 1; 4
[2] $P121$ ($P2$, 3) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

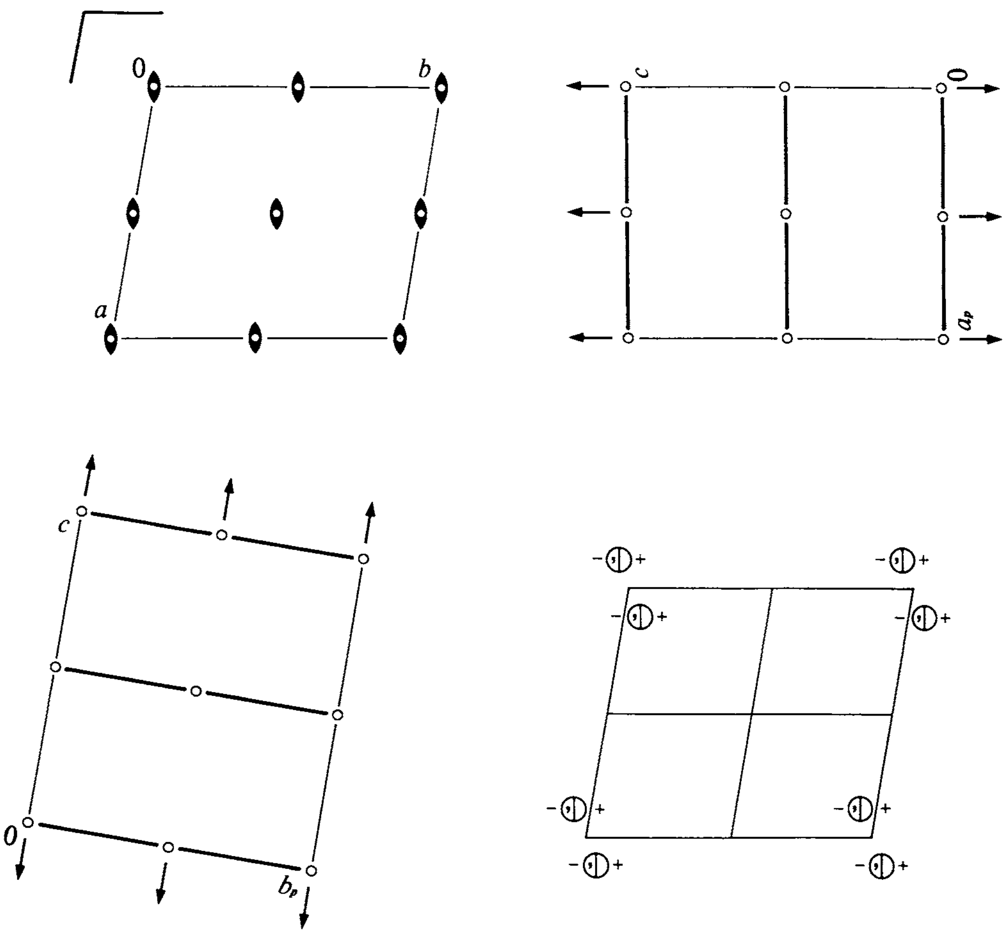
IIb [2] $P12_1/m1$ ($\mathbf{b}' = 2\mathbf{b}$) ($P2_1/m$, 11); [2] $P12/c1$ ($\mathbf{c}' = 2\mathbf{c}$) ($P2/c$, 13); [2] $P12/a1$ ($\mathbf{a}' = 2\mathbf{a}$) ($P2/c$, 13); [2] $B12/e1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($P2/c$, 13); [2] $C12/m1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($C2/m$, 12); [2] $A12/m1$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12); [2] $F12/m1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12)

(*Continued on preceding page*)

$P2/m$ $\quad C_{2h}^1$ $\quad 2/m$ $\quad$ Monoclinic

No. 10 $\quad P\,1\,1\,2/m$ $\quad$ Patterson symmetry $P\,1\,1\,2/m$

UNIQUE AXIS c



Origin at centre ($2/m$)

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 $\qquad$ (2) $2 \quad 0,0,z$ $\qquad$ (3) $\bar{1} \quad 0,0,0$ $\qquad$ (4) $m \quad x,y,0$

Maximal isomorphic subgroups of lowest index

IIc $\quad$ [2] $P\,1\,1\,2/m$ ($\mathbf{c}' = 2\mathbf{c}$) ($P2/m$, 10); [2] $P\,1\,1\,2/m$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b}$) ($P2/m$, 10)

Minimal non-isomorphic supergroups

I $\quad$ [2] $Pmmm$ (47); [2] $Pccm$ (49); [2] $Pmma$ (51); [2] $Pmna$ (53); [2] $Pbam$ (55); [2] $Pnnm$ (58); [2] $Cmmm$ (65); [2] $Cccm$ (66); [2] $P4/m$ (83); [2] $P4_2/m$ (84); [3] $P6/m$ (175)

II $\quad$ [2] $A\,1\,1\,2/m$ ($C2/m$, 12); [2] $B\,1\,1\,2/m$ ($C2/m$, 12); [2] $I\,1\,1\,2/m$ ($C2/m$, 12)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	o	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}$	no conditions
							Special: no extra conditions
2	n	m	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$			
2	m	m	$x,y,0$	$\bar{x},\bar{y},0$			
2	l	2	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			
2	k	2	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$			
2	j	2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			
2	i	2	$0,0,z$	$0,0,\bar{z}$			
1	h	$2/m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
1	g	$2/m$	$\frac{1}{2},\frac{1}{2},0$				
1	f	$2/m$	$\frac{1}{2},0,\frac{1}{2}$				
1	e	$2/m$	$0,\frac{1}{2},\frac{1}{2}$				
1	d	$2/m$	$0,\frac{1}{2},0$				
1	c	$2/m$	$\frac{1}{2},0,0$				
1	b	$2/m$	$0,0,\frac{1}{2}$				
1	a	$2/m$	$0,0,0$				

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P11m$ (Pm, 6) 1; 4
[2] $P112$ ($P2$, 3) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb [2] $P112_1/m$ ($\mathbf{c}' = 2\mathbf{c}$) ($P2_1/m$, 11); [2] $P112/a$ ($\mathbf{a}' = 2\mathbf{a}$) ($P2/c$, 13); [2] $P112/b$ ($\mathbf{b}' = 2\mathbf{b}$) ($P2/c$, 13); [2] $C112/e$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P2/c$, 13); [2] $A112/m$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12); [2] $B112/m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12); [2] $F112/m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12)

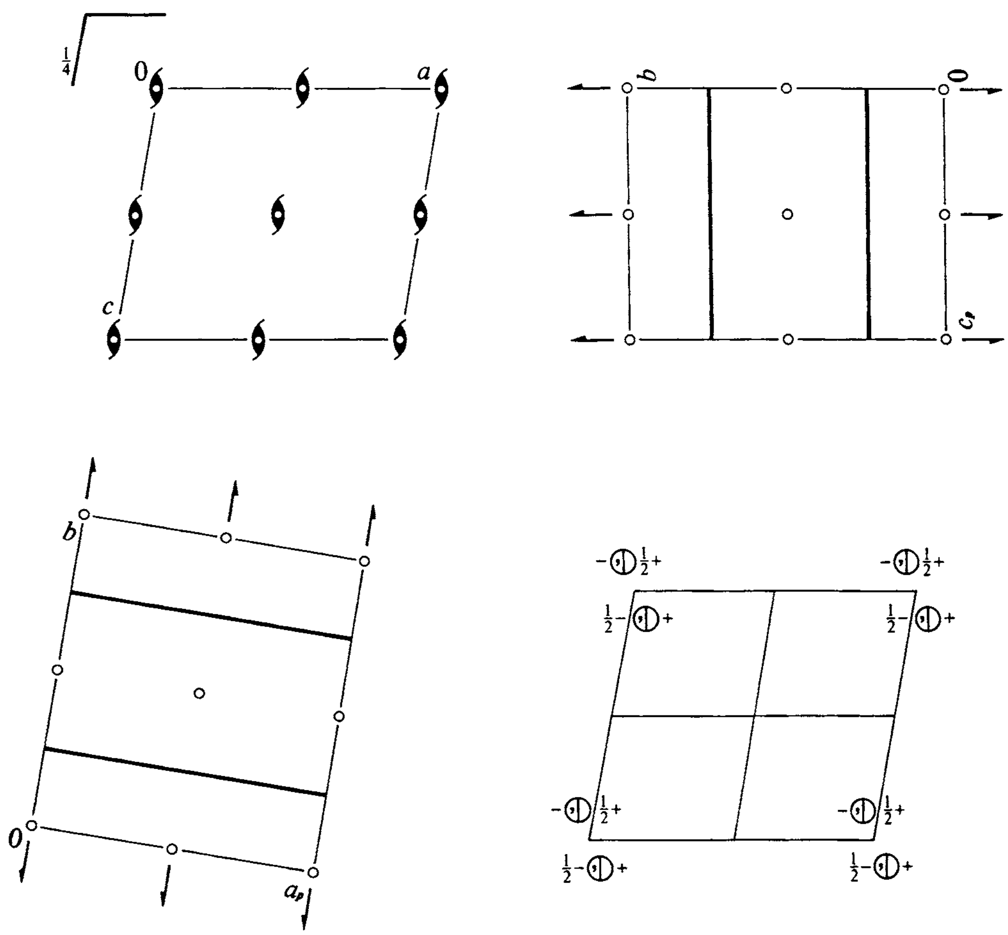
(*Continued on preceding page*)

International Tables for Crystallography (2006). Vol. A, Space group 11, pp. 164–167.

$P2_1/m$ $\quad C_{2h}^2$ $\quad 2/m$ $\quad$ Monoclinic

No. 11 $\quad P1\,2_1/m\,1$ $\quad$ Patterson symmetry $P1\,2/m\,1$

UNIQUE AXIS b



Origin at $\bar{1}$ on 2_1

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $\qquad$ (2) $2(0,\frac{1}{2},0)\quad 0,y,0$ $\qquad$ (3) $\bar{1}\quad 0,0,0$ $\qquad$ (4) $m\quad x,\frac{1}{4},z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	f	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z$	$0k0$: $k=2n$
							Special: as above, plus
2	e	m	$x,\frac{1}{4},z$	$\bar{x},\frac{3}{4},\bar{z}$			no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $k=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $k=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $k=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},0$			hkl : $k=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1m1$ (Pm, 6) 1; 4
[2] $P12_11$ ($P2_1$, 4) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb [2] $P12_1/c1$ ($\mathbf{c}'=2\mathbf{c}$) ($P2_1/c$, 14); [2] $P12_1/a1$ ($\mathbf{a}'=2\mathbf{a}$) ($P2_1/c$, 14); [2] $B12_1/e1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{c}'=2\mathbf{c}$) ($P2_1/c$, 14)

Maximal isomorphic subgroups of lowest index

IIc [2] $P12_1/m1$ ($\mathbf{c}'=2\mathbf{c}$ or $\mathbf{a}'=2\mathbf{a}$ or $\mathbf{a}'=\mathbf{a}+\mathbf{c},\mathbf{c}'=-\mathbf{a}+\mathbf{c}$) ($P2_1/m$, 11); [3] $P12_1/m1$ ($\mathbf{b}'=3\mathbf{b}$) ($P2_1/m$, 11)

Minimal non-isomorphic supergroups

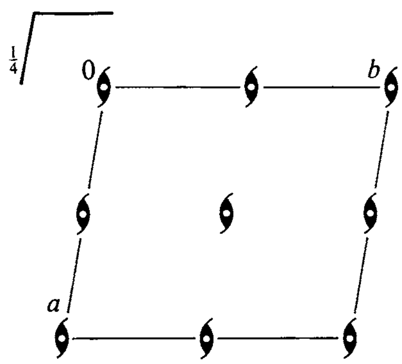
I [2] $Pmma$ (51); [2] $Pbcm$ (57); [2] $Pmmn$ (59); [2] $Pnma$ (62); [2] $Cmcm$ (63); [3] $P6_3/m$ (176)

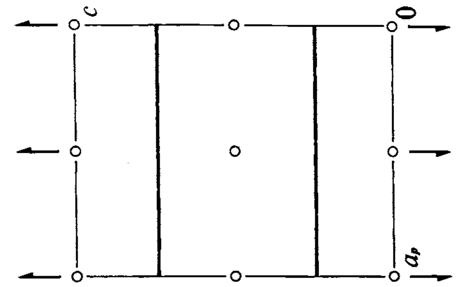
II [2] $C12/m1$ ($C2/m$, 12); [2] $A12/m1$ ($C2/m$, 12); [2] $I12/m1$ ($C2/m$, 12); [2] $P12/m1$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($P2/m$, 10)

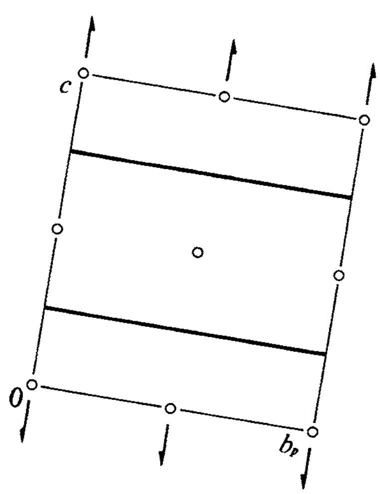
$P2_1/m$ $\quad C_{2h}^2$ $\quad 2/m$ $\quad$ Monoclinic

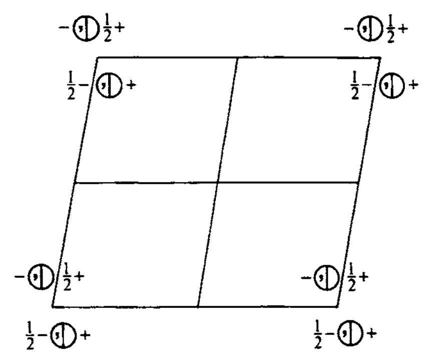
No. 11 $\quad P112_1/m$ $\quad$ Patterson symmetry $P112/m$

UNIQUE AXIS c









Origin at $\bar{1}$ on 2_1

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1 $\qquad$ (2) $2(0,0,\frac{1}{2})\quad 0,0,z$ $\qquad$ (3) $\bar{1}\quad 0,0,0$ $\qquad$ (4) $m\quad x,y,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}+\frac{1}{2}$	$00l$: $l=2n$
							Special: as above, plus
2	e	m	$x,y,\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$			no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
2	c	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $l=2n$
2	b	$\bar{1}$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mg$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P11m$ (Pm, 6) 1; 4
[2] $P112_1$ ($P2_1$, 4) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb [2] $P112_1/a$ ($\mathbf{a}'=2\mathbf{a}$) ($P2_1/c$, 14); [2] $P112_1/b$ ($\mathbf{b}'=2\mathbf{b}$) ($P2_1/c$, 14); [2] $C112_1/e$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P2_1/c$, 14)

Maximal isomorphic subgroups of lowest index

IIc [2] $P112_1/m$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{b}'=2\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{a}+\mathbf{b}$) ($P2_1/m$, 11); [3] $P112_1/m$ ($\mathbf{c}'=3\mathbf{c}$) ($P2_1/m$, 11)

Minimal non-isomorphic supergroups

I [2] $Pmma$ (51); [2] $Pbcm$ (57); [2] $Pmmn$ (59); [2] $Pnma$ (62); [2] $Cmcm$ (63); [3] $P6_3/m$ (176)

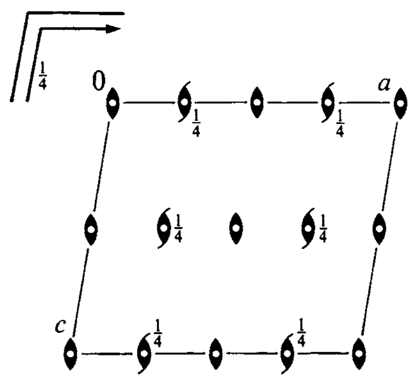
II [2] $A112/m$ ($C2/m$, 12); [2] $B112/m$ ($C2/m$, 12); [2] $I112/m$ ($C2/m$, 12); [2] $P112/m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P2/m$, 10)

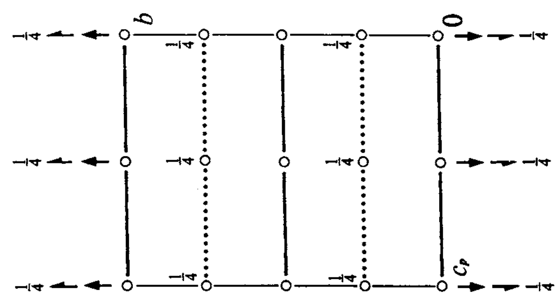
International Tables for Crystallography (2006). Vol. A, Space group 12, pp. 168–175.

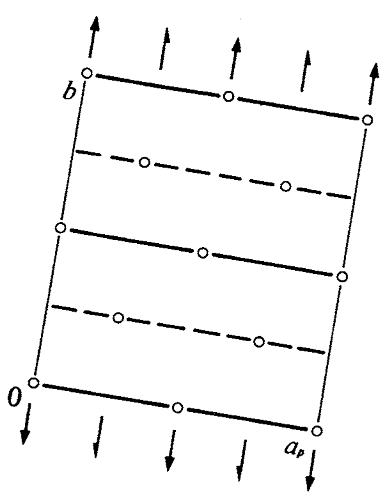
$C2/m$ C_{2h}^3 $2/m$ Monoclinic

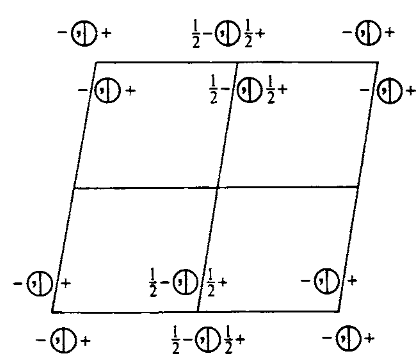
No. 12 $C12/m1$ Patterson symmetry $C12/m1$

UNIQUE AXIS b, CELL CHOICE 1









Origin at centre ($2/m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,y,0$	(3) $\bar{1}$ $0,0,0$	(4) m $x,0,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(3) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(4) a $x,\frac{1}{4},z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
8	j	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z$	$hkl: h+k=2n$ $h0l: h=2n$ $0kl: k=2n$ $hk0: h+k=2n$ $0k0: k=2n$ $h00: h=2n$
							Special: as above, plus
4	i	m	$x,0,z$	$\bar{x},0,\bar{z}$			no extra conditions
4	h	2	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			no extra conditions
4	g	2	$0,y,0$	$0,\bar{y},0$			no extra conditions
4	f	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			$hkl: h=2n$
4	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$			$hkl: h=2n$
2	d	$2/m$	$0,\frac{1}{2},\frac{1}{2}$				no extra conditions
2	c	$2/m$	$0,0,\frac{1}{2}$				no extra conditions
2	b	$2/m$	$0,\frac{1}{2},0$				no extra conditions
2	a	$2/m$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $C1m1$ (Cm, 8) (1; 4)+
[2] $C121$ ($C2$, 5) (1; 2)+
[2] $C\bar{1}$ ($P\bar{1}$, 2) (1; 3)+

IIa [2] $P12_1/a1$ ($P2_1/c$, 14) 1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $P12/a1$ ($P2/c$, 13) 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $P12_1/m1$ ($P2_1/m$, 11) 1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $P12/m1$ ($P2/m$, 10) 1; 2; 3; 4

IIb [2] $C12/c1$ ($\mathbf{c}'=2\mathbf{c}$) ($C2/c$, 15); [2] $I12/c1$ ($\mathbf{c}'=2\mathbf{c}$) ($C2/c$, 15)

Maximal isomorphic subgroups of lowest index

IIc [2] $C12/m1$ ($\mathbf{c}'=2\mathbf{c}$ or $\mathbf{a}'=\mathbf{a}+2\mathbf{c},\mathbf{c}'=2\mathbf{c}$) ($C2/m$, 12); [3] $C12/m1$ ($\mathbf{b}'=3\mathbf{b}$) ($C2/m$, 12)

Minimal non-isomorphic supergroups

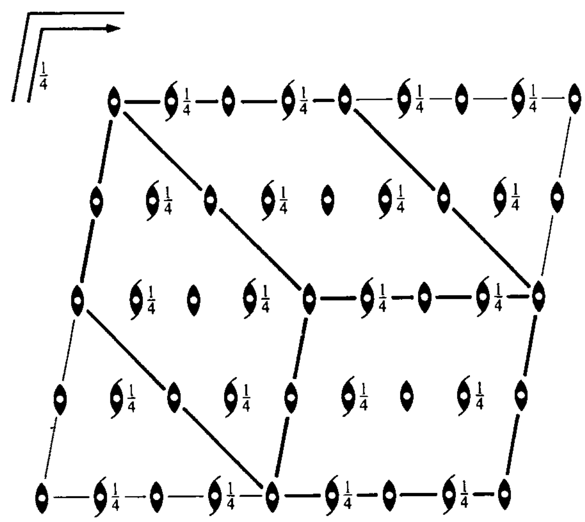
I [2] $Cmcm$ (63); [2] $Cmce$ (64); [2] $Cmmm$ (65); [2] $Cmme$ (67); [2] $Fmmm$ (69); [2] $Immm$ (71); [2] $Ibam$ (72); [2] $Imma$ (74); [2] $I4/m$ (87); [3] $P\bar{3}1m$ (162); [3] $P\bar{3}m1$ (164); [3] $R\bar{3}m$ (166)

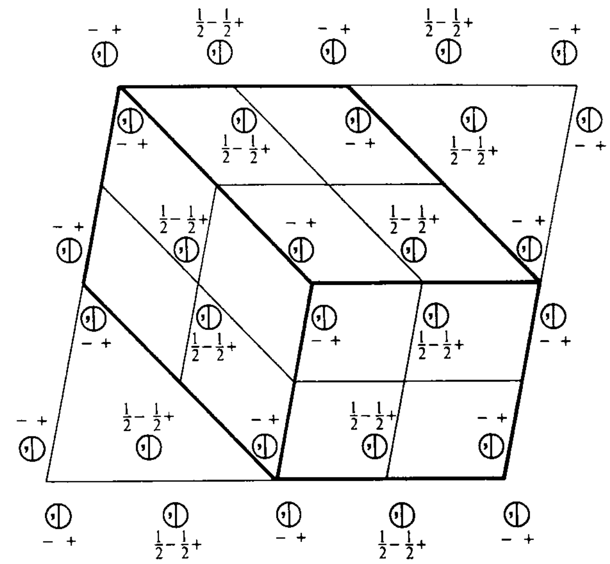
II [2] $P12/m1$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($P2/m$, 10)

$C2/m$ $\quad C_{2h}^3$ $\quad 2/m$ $\quad$ Monoclinic

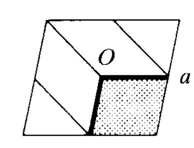
No. 12

UNIQUE AXIS b, DIFFERENT CELL CHOICES





$C12/m1$



UNIQUE AXIS b, CELL CHOICE 1

Origin at centre ($2/m$)

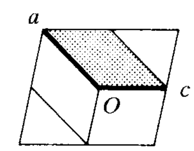
Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Generators selected $\quad$ (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates					Reflection conditions	
			$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},0)+$					General:	
8	j	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z$		hkl : $h+k=2n$ $h0l$: $h=2n$ $0kl$: $k=2n$	$hk0$: $h+k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$
								Special: as above, plus	
4	i	m	$x,0,z$	$\bar{x},0,\bar{z}$				no extra conditions	
4	h	2	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$	4 g 2	$0,y,0$	$0,\bar{y},0$	no extra conditions	
4	f	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	4 e $\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl : $h=2n$	
2	d	$2/m$	$0,\frac{1}{2},\frac{1}{2}$		2 c $2/m$	$0,0,\frac{1}{2}$		no extra conditions	
2	b	$2/m$	$0,\frac{1}{2},0$		2 a $2/m$	$0,0,0$		no extra conditions	

$A\,1\,2/m\,1$



UNIQUE AXIS b, CELL CHOICE 2

Origin at centre ($2/m$)

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates: $(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ — Reflection conditions

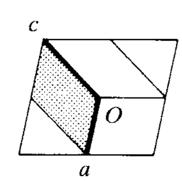
General:

8	j	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z$	hkl : $k+l=2n$ $h0l$: $l=2n$ $0kl$: $k+l=2n$	$hk0$: $k=2n$ $0k0$: $k=2n$ $00l$: $l=2n$

Special: as above, plus

4	i	m	$x,0,z$	$\bar{x},0,\bar{z}$						no extra conditions
4	h	2	$\frac{1}{2},y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\frac{1}{2}$	4	g	2	$0,y,0$	$0,\bar{y},0$	no extra conditions
4	f	$\bar{1}$	$\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	4	e	$\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{1}{4},\frac{3}{4}$	hkl : $k=2n$
2	d	$2/m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		2	c	$2/m$	$\frac{1}{2},0,\frac{1}{2}$		no extra conditions
2	b	$2/m$	$0,\frac{1}{2},0$		2	a	$2/m$	$0,0,0$		no extra conditions

$I\,1\,2/m\,1$



UNIQUE AXIS b, CELL CHOICE 3

Origin at centre ($2/m$)

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates: $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ — Reflection conditions

General:

8	j	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z$	hkl : $h+k+l=2n$ $h0l$: $h+l=2n$ $0kl$: $k+l=2n$ $hk0$: $h+k=2n$	$0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$

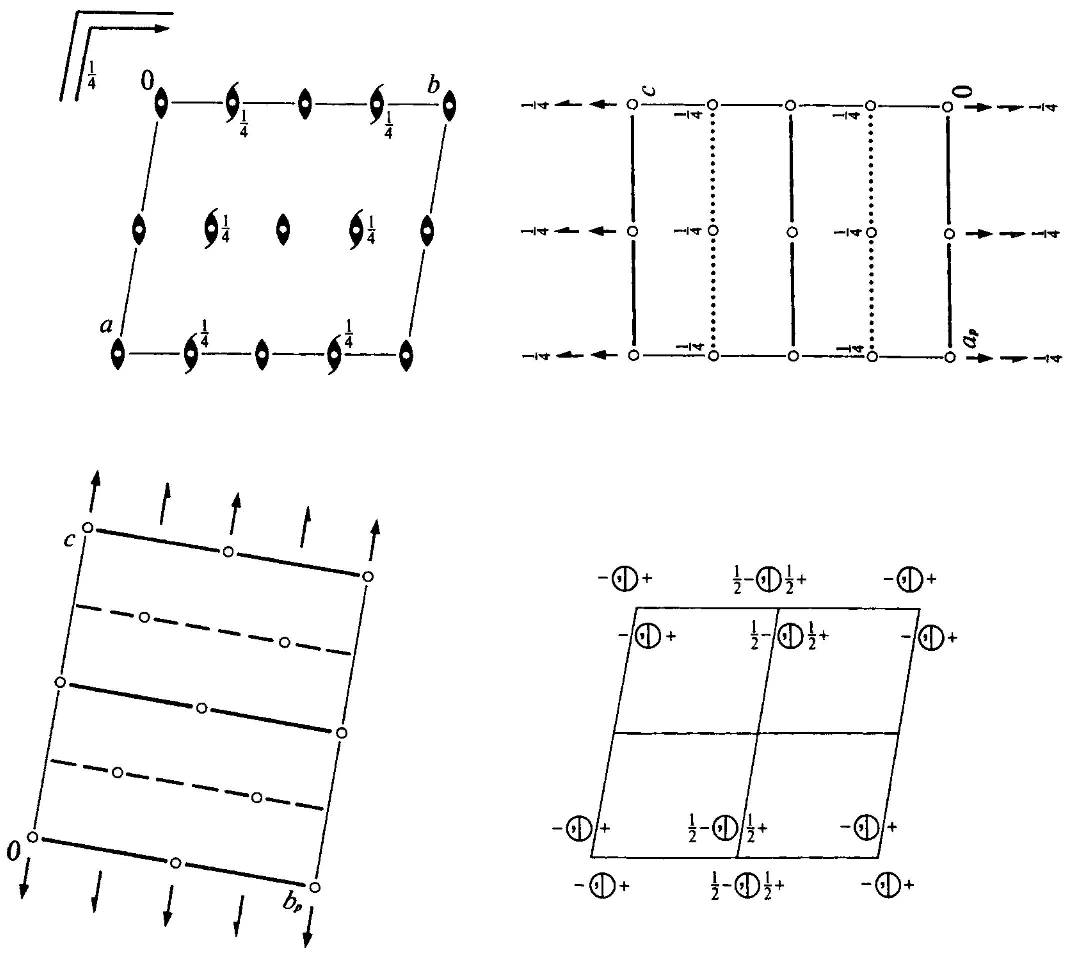
Special: as above, plus

4	i	m	$x,0,z$	$\bar{x},0,\bar{z}$						no extra conditions
4	h	2	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},0$	4	g	2	$0,y,0$	$0,\bar{y},0$	no extra conditions
4	f	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	4	e	$\bar{1}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	hkl : $k=2n$
2	d	$2/m$	$\frac{1}{2},\frac{1}{2},0$		2	c	$2/m$	$\frac{1}{2},0,0$		no extra conditions
2	b	$2/m$	$0,\frac{1}{2},0$		2	a	$2/m$	$0,0,0$		no extra conditions

$C2/m$ $\quad$ C_{2h}^3 $\quad$ $2/m$ $\quad$ Monoclinic

No. 12 $\quad$ $A\,1\,1\,2/m$ $\quad$ Patterson symmetry $A\,1\,1\,2/m$

UNIQUE AXIS c, CELL CHOICE 1



Origin at centre $(2/m)$

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2 \quad 0,0,z$	(3) $\bar{1} \quad 0,0,0$	(4) $m \quad x,y,0$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2}) \quad 0,\frac{1}{4},z$	(3) $\bar{1} \quad 0,\frac{1}{4},\frac{1}{4}$	(4) $b \quad x,y,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(0,\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
8	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}$	hkl : $k+l=2n$ $hk0$: $k=2n$ $0kl$: $k+l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	i	m	$x,y,0$	$\bar{x},\bar{y},0$			no extra conditions
4	h	2	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$			no extra conditions
4	g	2	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	f	$\bar{1}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$			hkl : $k=2n$
4	e	$\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$			hkl : $k=2n$
2	d	$2/m$	$\frac{1}{2},0,\frac{1}{2}$				no extra conditions
2	c	$2/m$	$\frac{1}{2},0,0$				no extra conditions
2	b	$2/m$	$0,0,\frac{1}{2}$				no extra conditions
2	a	$2/m$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}'=\mathbf{a}\quad \mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}_p\quad \mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}\quad \mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $A11m$ (Cm, 8)	(1; 4)+
	[2] $A112$ ($C2$, 5)	(1; 2)+
	[2] $A\bar{1}$ ($P\bar{1}$, 2)	(1; 3)+
IIa	[2] $P112_1/b$ ($P2_1/c$, 14)	1; 3; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$
	[2] $P112/b$ ($P2/c$, 13)	1; 2; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$
	[2] $P112_1/m$ ($P2_1/m$, 11)	1; 4; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$
	[2] $P112/m$ ($P2/m$, 10)	1; 2; 3; 4

IIb [2] $A112/a$ ($\mathbf{a}'=2\mathbf{a}$) ($C2/c$, 15); [2] $I112/a$ ($\mathbf{a}'=2\mathbf{a}$) ($C2/c$, 15)

Maximal isomorphic subgroups of lowest index

IIc [2] $A112/m$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) ($C2/m$, 12); [3] $A112/m$ ($\mathbf{c}'=3\mathbf{c}$) ($C2/m$, 12)

Minimal non-isomorphic supergroups

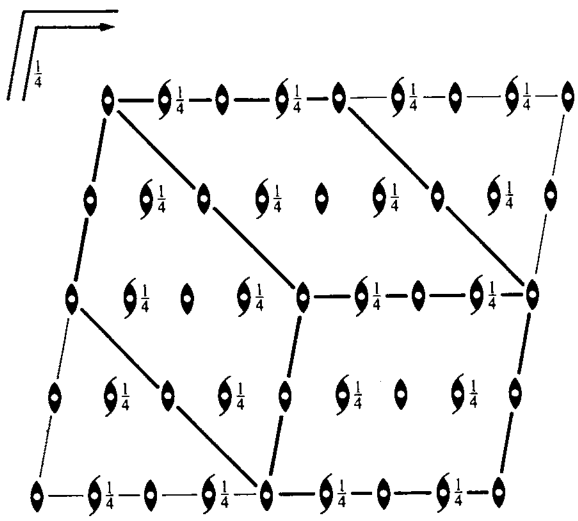
I [2] $Cmcm$ (63); [2] $Cmce$ (64); [2] $Cmmm$ (65); [2] $Cmme$ (67); [2] $Fmmm$ (69); [2] $Immm$ (71); [2] $Ibam$ (72); [2] $Imma$ (74); [2] $I4/m$ (87); [3] $P\bar{3}1m$ (162); [3] $P\bar{3}m1$ (164); [3] $R\bar{3}m$ (166)

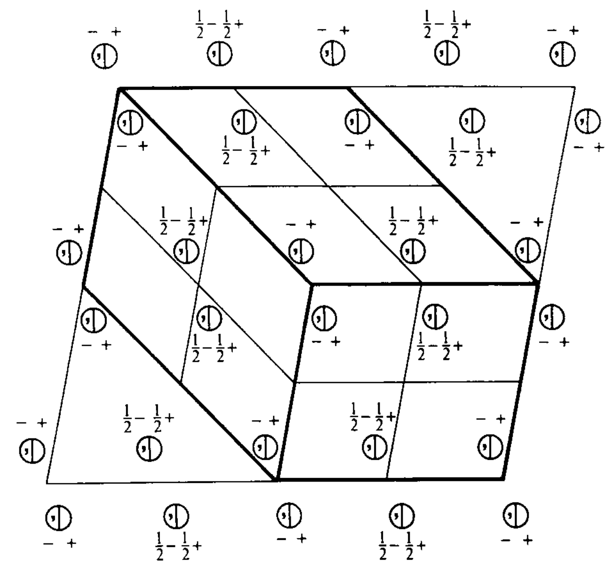
II [2] $P112/m$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P2/m$, 10)

$C2/m$ $\quad C^3_{2h}$ $\quad 2/m$ $\quad$ Monoclinic

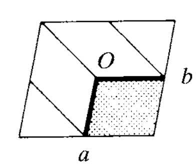
No. 12

UNIQUE AXIS c, DIFFERENT CELL CHOICES





$A112/m$



UNIQUE AXIS c, CELL CHOICE 1

Origin at centre $(2/m)$

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Generators selected $\quad (1);\ t(1,0,0);\ t(0,1,0);\ t(0,0,1);\ t(0,\frac{1}{2},\frac{1}{2});\ (2);\ (3)$

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+$

Reflection conditions

General:

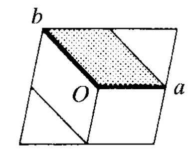
							Reflection conditions
8	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}$	$hkl: k+l=2n$; $h0l: l=2n$; $hk0: k=2n$; $00l: l=2n$; $0kl: k+l=2n$; $0k0: k=2n$

Special: as above, plus

4	i	m	$x,y,0$	$\bar{x},\bar{y},0$						no extra conditions
4	h	2	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$	4	g	2	$0,0,z$	$0,0,\bar{z}$	no extra conditions
4	f	$\bar{1}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$	4	e	$\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$hkl: k=2n$
2	d	$2/m$	$\frac{1}{2},0,\frac{1}{2}$		2	c	$2/m$	$\frac{1}{2},0,0$		no extra conditions
2	b	$2/m$	$0,0,\frac{1}{2}$		2	a	$2/m$	$0,0,0$		no extra conditions

$B112/m$

UNIQUE AXIS c, CELL CHOICE 2



Origin at centre ($2/m$)

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3)

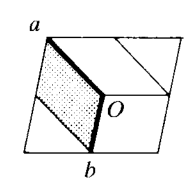
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+\quad(\frac{1}{2},0,\frac{1}{2})+$				General:
8	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}$	hkl : $h+l=2n$ $hk0$: $h=2n$ $0kl$: $l=2n$ $h0l$: $h+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$

										Special: as above, plus
4	i	m	$x,y,0$	$\bar{x},\bar{y},0$						no extra conditions
4	h	2	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	4	g	2	$0,0,z$	$0,0,\bar{z}$	no extra conditions
4	f	$\bar{1}$	$\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\frac{1}{2},\frac{1}{4}$	4	e	$\bar{1}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{3}{4},0,\frac{1}{4}$	hkl : $h=2n$
2	d	$2/m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		2	c	$2/m$	$\frac{1}{2},\frac{1}{2},0$		no extra conditions
2	b	$2/m$	$0,0,\frac{1}{2}$		2	a	$2/m$	$0,0,0$		no extra conditions

$I112/m$

UNIQUE AXIS c, CELL CHOICE 3



Origin at centre ($2/m$)

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
8	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}$	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$ $0k0$: $k=2n$

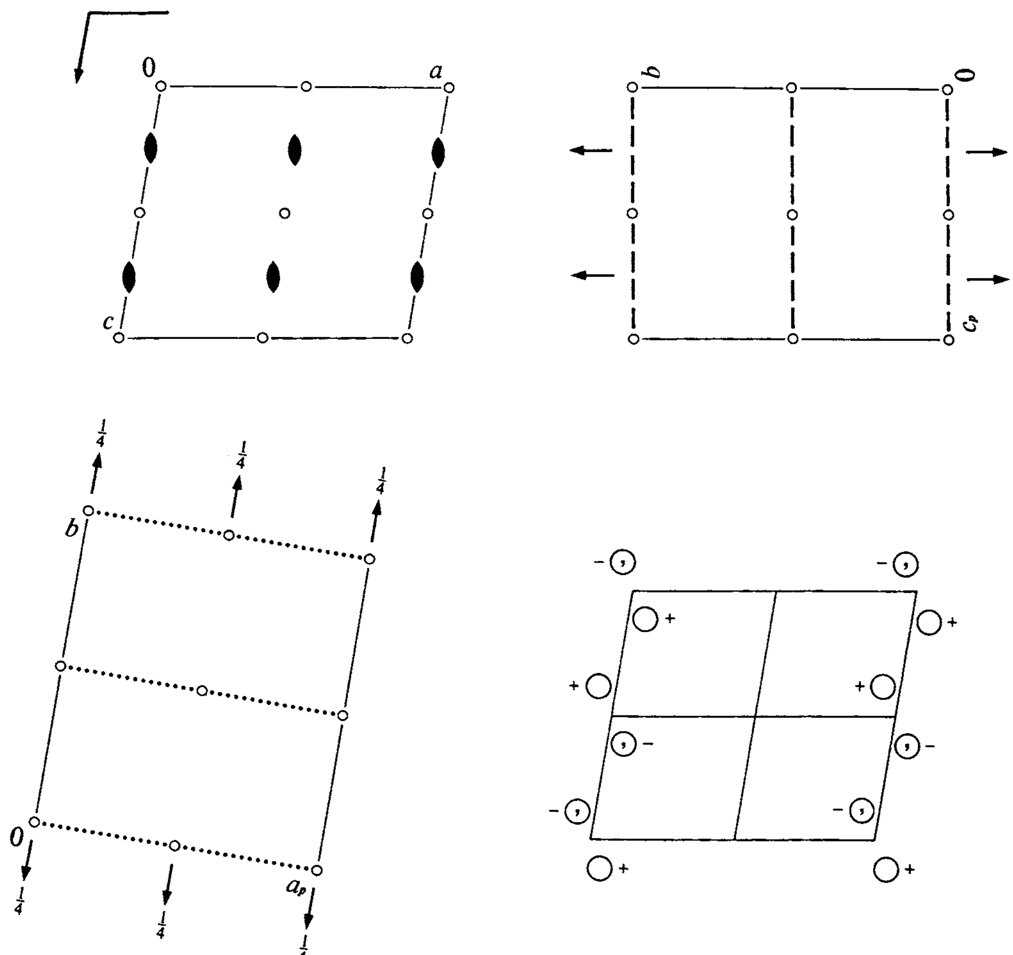
										Special: as above, plus
4	i	m	$x,y,0$	$\bar{x},\bar{y},0$						no extra conditions
4	h	2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	4	g	2	$0,0,z$	$0,0,\bar{z}$	no extra conditions
4	f	$\bar{1}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	4	e	$\bar{1}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	hkl : $l=2n$
2	d	$2/m$	$0,\frac{1}{2},\frac{1}{2}$		2	c	$2/m$	$0,\frac{1}{2},0$		no extra conditions
2	b	$2/m$	$0,0,\frac{1}{2}$		2	a	$2/m$	$0,0,0$		no extra conditions

International Tables for Crystallography (2006). Vol. A, Space group 13, pp. 176–183.

$P2/c$ $\quad C_{2h}^4$ $\quad 2/m$ $\quad$ Monoclinic

No. 13 $\quad P\,1\,2/c\,1$ $\quad$ Patterson symmetry $P\,1\,2/m\,1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$ on glide plane c

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 $\qquad$ (2) $2 \quad 0,y,\frac{1}{4}$ $\qquad$ (3) $\bar{1} \quad 0,0,0$ $\qquad$ (4) $c \quad x,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	g	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z+\frac{1}{2}$	$h0l$: $l=2n$ $00l$: $l=2n$
							Special: as above, plus
2	f	2	$\frac{1}{2},y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{3}{4}$			no extra conditions
2	e	2	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $l=2n$
2	c	$\bar{1}$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
2	b	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc, 7) 1; 4
[2] $P121$ ($P2$, 3) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb [2] $P12_1/c1$ ($\mathbf{b}'=2\mathbf{b}$) ($P2_1/c$, 14); [2] $C12/c1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($C2/c$, 15)

Maximal isomorphic subgroups of lowest index

IIc [2] $P12/c1$ ($\mathbf{b}'=2\mathbf{b}$) ($P2/c$, 13); [2] $P12/c1$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{a}'=2\mathbf{a},\mathbf{c}'=2\mathbf{a}+\mathbf{c}$) ($P2/c$, 13)

Minimal non-isomorphic supergroups

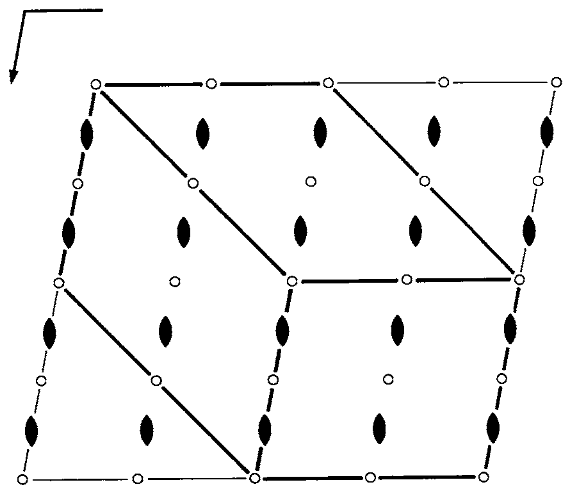
I [2] $Pnnn$ (48); [2] $Pccm$ (49); [2] $Pban$ (50); [2] $Pmma$ (51); [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pmmn$ (59); [2] $Pbcn$ (60); [2] $Cmme$ (67); [2] $Ccce$ (68); [2] $P4/n$ (85); [2] $P4_2/n$ (86)

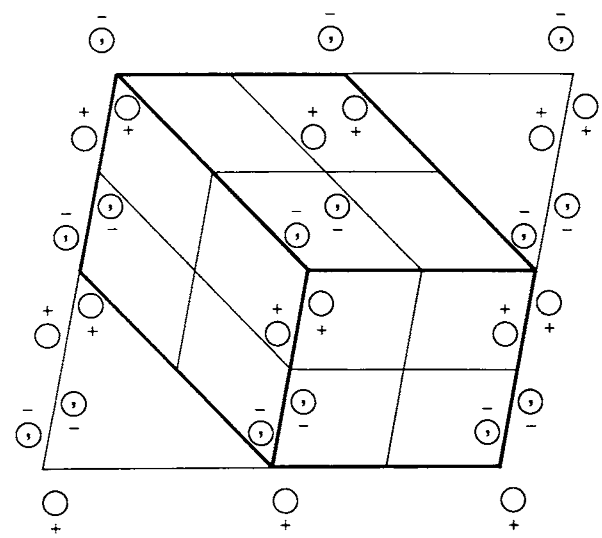
II [2] $A12/m1$ ($C2/m$, 12); [2] $C12/c1$ ($C2/c$, 15); [2] $I12/c1$ ($C2/c$, 15); [2] $P12/m1$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P2/m$, 10)

$P2/c$ C_{2h}^4 $2/m$ Monoclinic

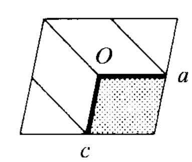
No. 13

UNIQUE AXIS b, DIFFERENT CELL CHOICES





$P12/c1$



UNIQUE AXIS b, CELL CHOICE 1

Origin at $\bar{1}$ on glide plane c

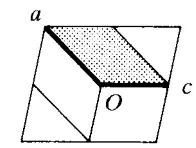
Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates							Reflection conditions
										General:
4	g	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z+\frac{1}{2}$				$h0l$: $l=2n$ $00l$: $l=2n$
										Special: as above, plus
2	f	2	$\frac{1}{2},y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{3}{4}$						no extra conditions
2	e	2	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$						no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$	2	c	$\bar{1}$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	hkl : $l=2n$
2	b	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	2	a	$\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$	hkl : $l=2n$

$P\,1\,2/n\,1$



UNIQUE AXIS b, CELL CHOICE 2

Origin at $\bar{1}$ on glide plane n

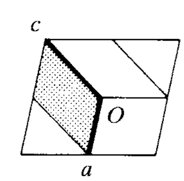
Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	$h0l:\ h+l=2n$ $h00:\ h=2n$ $00l:\ l=2n$
							Special: as above, plus
2	f	2	$\frac{3}{4},y,\frac{1}{4}$	$\frac{1}{4},\bar{y},\frac{3}{4}$			no extra conditions
2	e	2	$\frac{3}{4},y,\frac{3}{4}$	$\frac{1}{4},\bar{y},\frac{1}{4}$			no extra conditions
2	d	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	2 c $\bar{1}$	$0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkl:\ h+l=2n$
2	b	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	2 a $\bar{1}$	$0,0,0$ $\frac{1}{2},0,\frac{1}{2}$	$hkl:\ h+l=2n$

$P\,1\,2/a\,1$



UNIQUE AXIS b, CELL CHOICE 3

Origin at $\bar{1}$ on glide plane a

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{2}$

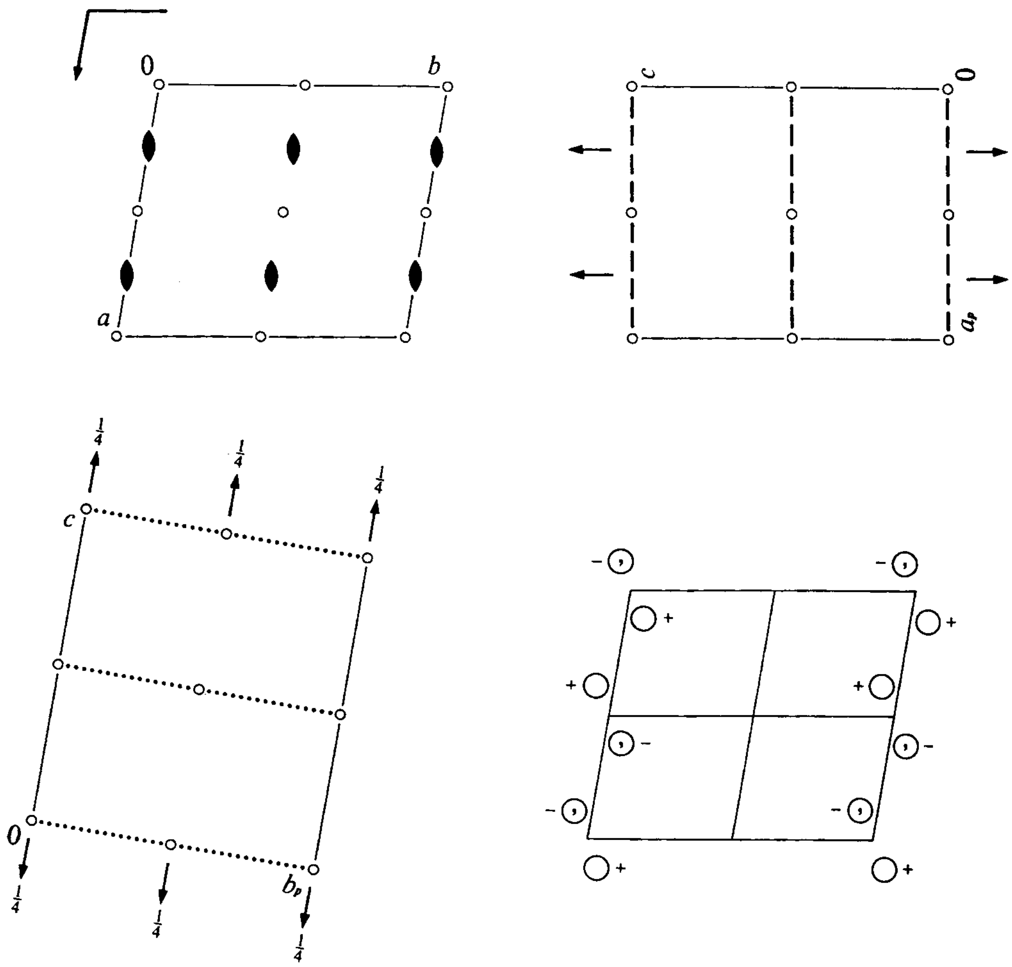
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},y,\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},z$	$h0l:\ h=2n$ $h00:\ h=2n$
							Special: as above, plus
2	f	2	$\frac{3}{4},y,\frac{1}{2}$	$\frac{1}{4},\bar{y},\frac{1}{2}$			no extra conditions
2	e	2	$\frac{1}{4},y,0$	$\frac{3}{4},\bar{y},0$			no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$0,0,\frac{1}{2}$	2 c $\bar{1}$	$0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},0$	$hkl:\ h=2n$
2	b	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	2 a $\bar{1}$	$0,0,0$ $\frac{1}{2},0,0$	$hkl:\ h=2n$

$P2/c$	C_{2h}^4	$2/m$	Monoclinic
No. 13	$P112/a$		Patterson symmetry $P112/m$

UNIQUE AXIS c, CELL CHOICE 1



Origin at $\bar{1}$ on glide plane a

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $\qquad$ (2) $2 \quad \frac{1}{4},0,z$ $\qquad$ (3) $\bar{1} \quad 0,0,0$ $\qquad$ (4) $a \quad x,y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}$	$hk0$: $h=2n$ $h00$: $h=2n$
							Special: as above, plus
2	f	2	$\frac{1}{4},\frac{1}{2},z$	$\frac{3}{4},\frac{1}{2},\bar{z}$			no extra conditions
2	e	2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}$			no extra conditions
2	d	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h=2n$
2	b	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$			hkl : $h=2n$

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P11a$ (Pc, 7) 1; 4
[2] $P112$ ($P2$, 3) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb [2] $P112_1/a$ ($\mathbf{c}'=2\mathbf{c}$) ($P2_1/c$, 14); [2] $A112/a$ ($\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($C2/c$, 15)

Maximal isomorphic subgroups of lowest index

IIc [2] $P112/a$ ($\mathbf{c}'=2\mathbf{c}$) ($P2/c$, 13); [2] $P112/a$ ($\mathbf{b}'=2\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=2\mathbf{b}$) ($P2/c$, 13)

Minimal non-isomorphic supergroups

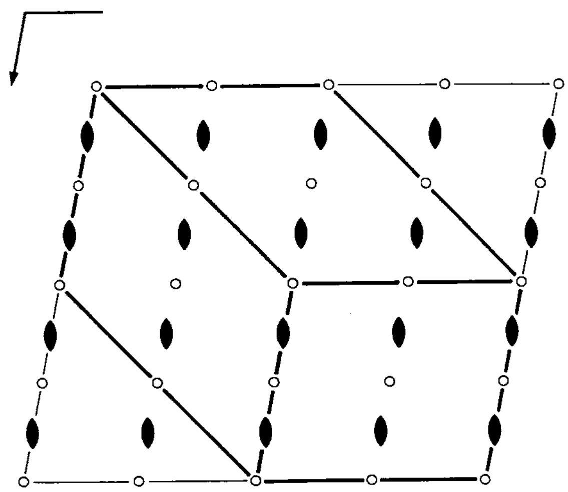
I [2] $Pnnn$ (48); [2] $Pccm$ (49); [2] $Pban$ (50); [2] $Pmma$ (51); [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pmmn$ (59); [2] $Pbcn$ (60); [2] $Cmme$ (67); [2] $Ccce$ (68); [2] $P4/n$ (85); [2] $P4_2/n$ (86)

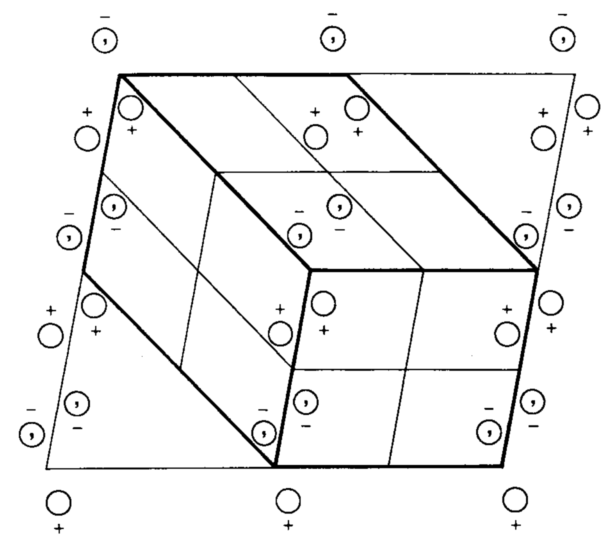
II [2] $A112/a$ ($C2/c$, 15); [2] $B112/m$ ($C2/m$, 12); [2] $I112/a$ ($C2/c$, 15); [2] $P112/m$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($P2/m$, 10)

$P2/c$ $\quad C_{2h}^4$ $\quad 2/m$ $\quad$ Monoclinic

No. 13

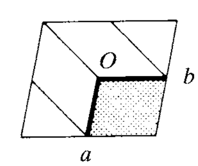
UNIQUE AXIS c, DIFFERENT CELL CHOICES





$P112/a$

UNIQUE AXIS c, CELL CHOICE 1



Origin at $\bar{1}$ on glide plane a

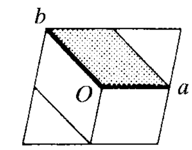
Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Generators selected $\quad (1);\ t(1,0,0);\ t(0,1,0);\ t(0,0,1);\ (2);\ (3)$

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}$	$hk0: h=2n$ $h00: h=2n$
							Special: as above, plus
2	f	2	$\frac{1}{4},\frac{1}{2},z$	$\frac{3}{4},\frac{1}{2},\bar{z}$			no extra conditions
2	e	2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}$			no extra conditions
2	d	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	2 $\quad c \quad \bar{1}$	$0,0,\frac{1}{2}$ $\quad \frac{1}{2},0,\frac{1}{2}$	$hkl: h=2n$
2	b	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	2 $\quad a \quad \bar{1}$	$0,0,0$ $\quad \frac{1}{2},0,0$	$hkl: h=2n$

$P112/n$



UNIQUE AXIS c, CELL CHOICE 2

Origin at $\bar{1}$ on glide plane n

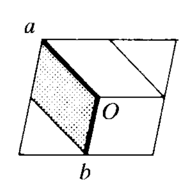
Asymmetric unit $0 \le x \le \frac{1}{4};\quad 0 \le y \le 1;\quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	$hk0:\ h+k=2n$ $h00:\ h=2n$ $0k0:\ k=2n$
							Special: as above, plus
2	f	2	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$			no extra conditions
2	e	2	$\frac{3}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}$			no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	2 c $\bar{1}$ $0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkl:\ h+k=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	2 a $\bar{1}$ $0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$hkl:\ h+k=2n$

$P112/b$



UNIQUE AXIS c, CELL CHOICE 3

Origin at $\bar{1}$ on glide plane b

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

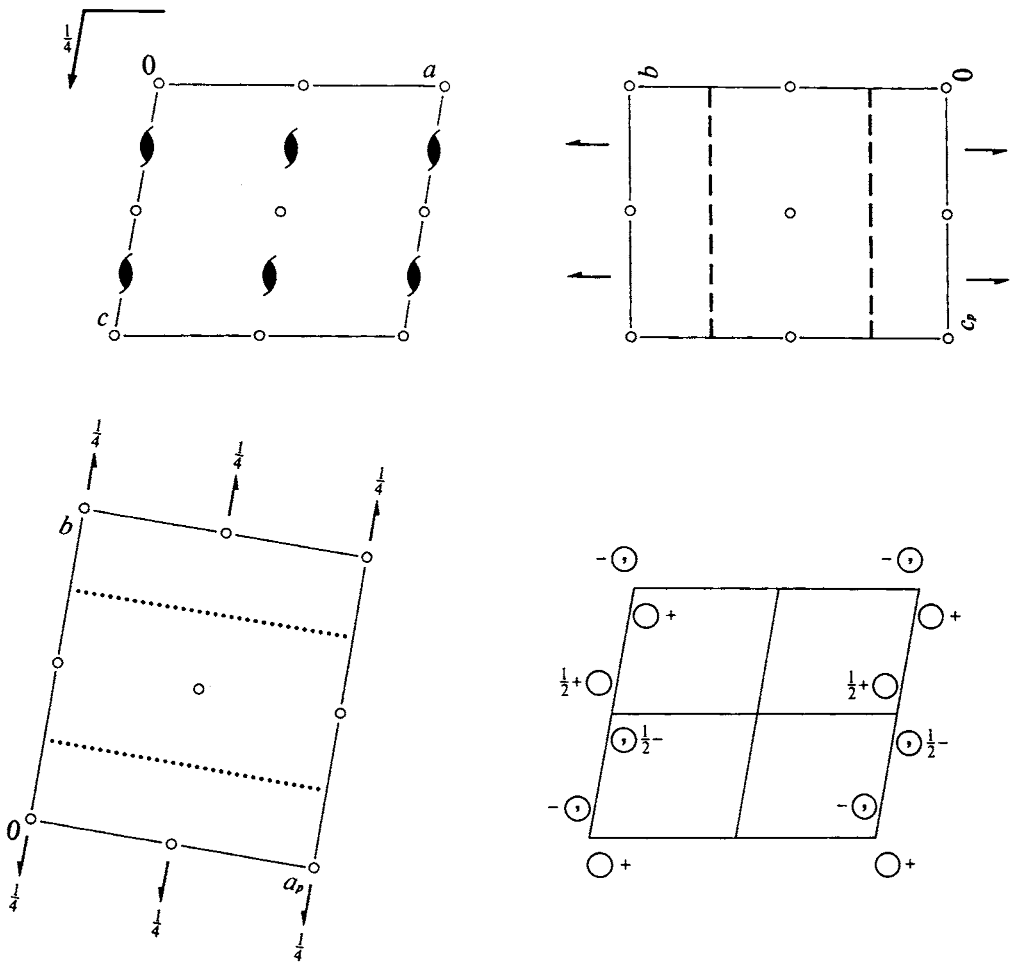
Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	g	1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y+\frac{1}{2},\bar{z}$	$hk0:\ k=2n$ $0k0:\ k=2n$
							Special: as above, plus
2	f	2	$\frac{1}{2},\frac{3}{4},z$	$\frac{1}{2},\frac{1}{4},\bar{z}$			no extra conditions
2	e	2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}$			no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	2 c $\bar{1}$ $0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$hkl:\ k=2n$
2	b	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	2 a $\bar{1}$ $0,0,0$	$0,\frac{1}{2},0$	$hkl:\ k=2n$

International Tables for Crystallography (2006). Vol. A, Space group 14, pp. 184–191.

$P2_1/c$ $\quad$ C_{2h}^5 $\quad$ $2/m$ $\quad$ Monoclinic

No. 14 $\quad$ $P1\,2_1/c\,1$ $\quad$ Patterson symmetry $P1\,2/m\,1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $\qquad$ (2) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$ $\qquad$ (3) $\bar{1}\quad 0,0,0$ $\qquad$ (4) $c\quad x,\frac{1}{4},z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $k+l=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl : $k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc, 7) 1; 4
[2] $P12_11$ ($P2_1$, 4) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $P12_1/c1$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{a}'=2\mathbf{a},\mathbf{c}'=2\mathbf{a}+\mathbf{c}$) ($P2_1/c$, 14); [3] $P12_1/c1$ ($\mathbf{b}'=3\mathbf{b}$) ($P2_1/c$, 14)

Minimal non-isomorphic supergroups

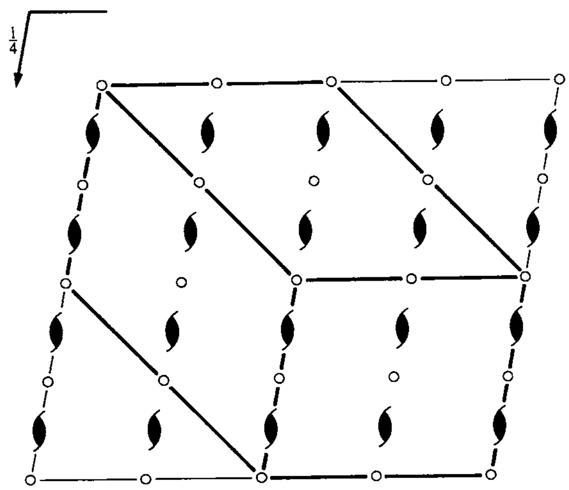
I [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pbam$ (55); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pnnm$ (58); [2] $Pbcn$ (60); [2] $Pbca$ (61); [2] $Pnma$ (62); [2] $Cmce$ (64)

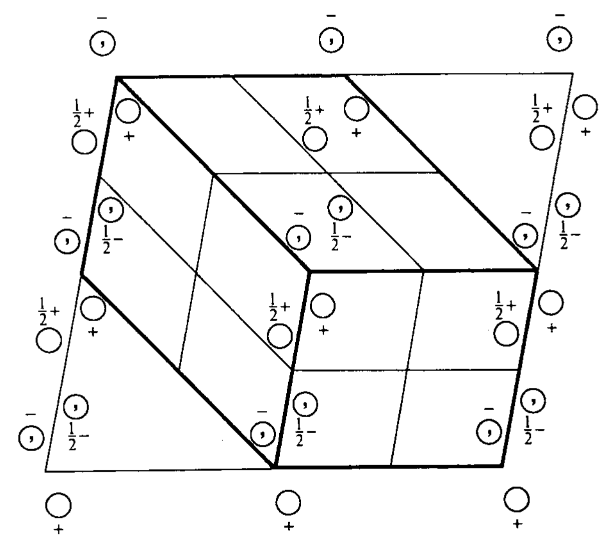
II [2] $A12/m1$ ($C2/m$, 12); [2] $C12/c1$ ($C2/c$, 15); [2] $I12/c1$ ($C2/c$, 15); [2] $P12_1/m1$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P2_1/m$, 11); [2] $P12/c1$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($P2/c$, 13)

$P2_1/c$ $\quad C_{2h}^5$ $\quad 2/m$ $\quad$ Monoclinic

No. 14

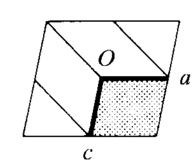
UNIQUE AXIS b, DIFFERENT CELL CHOICES





$P12_1/c1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$

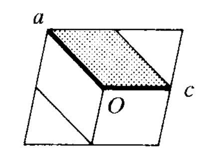
Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Generators selected $\quad$ (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	*e*	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l: l=2n$ $0k0: k=2n$ $00l: l=2n$
							Special: as above, plus
2	*d*	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			$hkl: k+l=2n$
2	*c*	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			$hkl: k+l=2n$
2	*b*	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$hkl: k+l=2n$
2	*a*	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			$hkl: k+l=2n$

$P\,1\,2_1/n\,1$



UNIQUE AXIS b, CELL CHOICE 2

Origin at $\bar{1}$

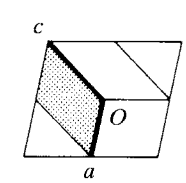
Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $h+l=2n$ $0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $h+k+l=2n$
2	c	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl : $h+k+l=2n$
2	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k+l=2n$

$P\,1\,2_1/a\,1$



UNIQUE AXIS b, CELL CHOICE 3

Origin at $\bar{1}$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

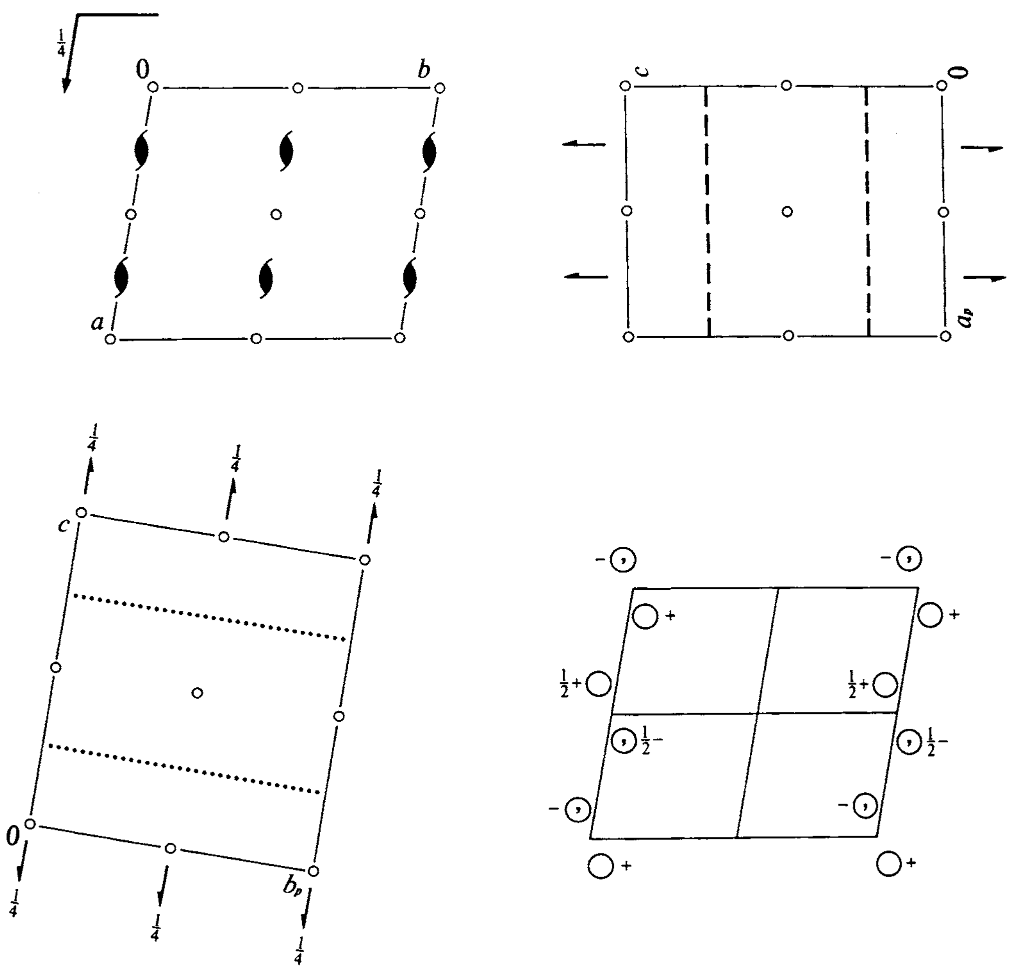
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	$h0l$: $h=2n$ $0k0$: $k=2n$ $h00$: $h=2n$
							Special: as above, plus
2	d	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	c	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			hkl : $h+k=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k=2n$

$P2_1/c$	C_{2h}^5	$2/m$	Monoclinic
No. 14	$P112_1/a$		Patterson symmetry $P112/m$

UNIQUE AXIS c, CELL CHOICE 1



Origin at $\bar{1}$

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) $\bar{1}$ $0,0,0$ (4) a $x,y,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	*e*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	$hk0: h=2n$ $00l: l=2n$ $h00: h=2n$
							Special: as above, plus
2	*d*	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			$hkl: h+l=2n$
2	*c*	$\bar{1}$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$			$hkl: h+l=2n$
2	*b*	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$hkl: h+l=2n$
2	*a*	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$			$hkl: h+l=2n$

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gg$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P11a$ (Pc, 7) 1; 4
[2] $P112_1$ ($P2_1$, 4) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $P112_1/a$ ($\mathbf{b}'=2\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=2\mathbf{b}$) ($P2_1/c$, 14); [3] $P112_1/a$ ($\mathbf{c}'=3\mathbf{c}$) ($P2_1/c$, 14)

Minimal non-isomorphic supergroups

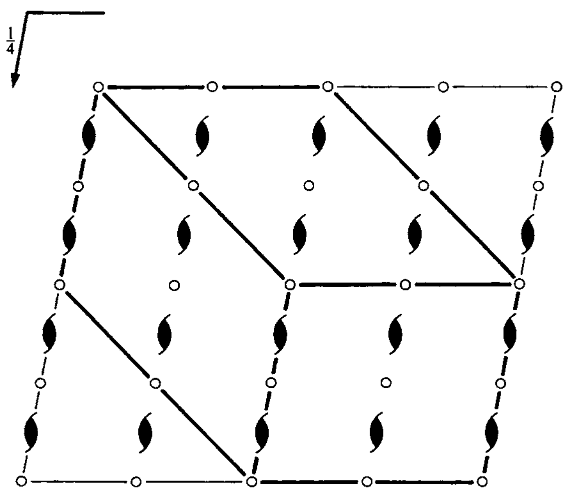
I [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pbam$ (55); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pnnm$ (58); [2] $Pbcn$ (60); [2] $Pbca$ (61); [2] $Pnma$ (62); [2] $Cmce$ (64)

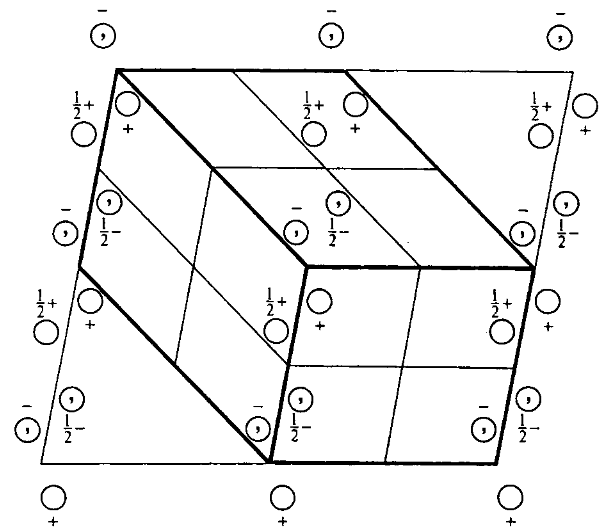
II [2] $A112/a$ ($C2/c$, 15); [2] $B112/m$ ($C2/m$, 12); [2] $I112/a$ ($C2/c$, 15); [2] $P112_1/m$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($P2_1/m$, 11); [2] $P112/a$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P2/c$, 13)

$P2_1/c$ C_{2h}^5 $2/m$ Monoclinic

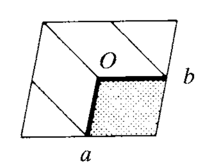
No. 14

UNIQUE AXIS c, DIFFERENT CELL CHOICES





$P112_1/a$



UNIQUE AXIS c, CELL CHOICE 1

Origin at $\bar{1}$

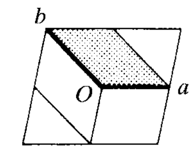
Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	$hk0:\ h=2n$ $00l:\ l=2n$ $h00:\ h=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			$hkl:\ h+l=2n$
2	c	$\bar{1}$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$			$hkl:\ h+l=2n$
2	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$hkl:\ h+l=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$			$hkl:\ h+l=2n$

$P112_1/n$



UNIQUE AXIS c, CELL CHOICE 2

Origin at $\bar{1}$

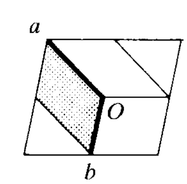
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	$hk0:\ h+k=2n$ $00l:\ l=2n$ $h00:\ h=2n$ $0k0:\ k=2n$
							Special: as above, plus
2	d	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			$hkl:\ h+k+l=2n$
2	c	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$0,0,\frac{1}{2}$			$hkl:\ h+k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$			$hkl:\ h+k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$hkl:\ h+k+l=2n$

$P112_1/b$



UNIQUE AXIS c, CELL CHOICE 3

Origin at $\bar{1}$

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

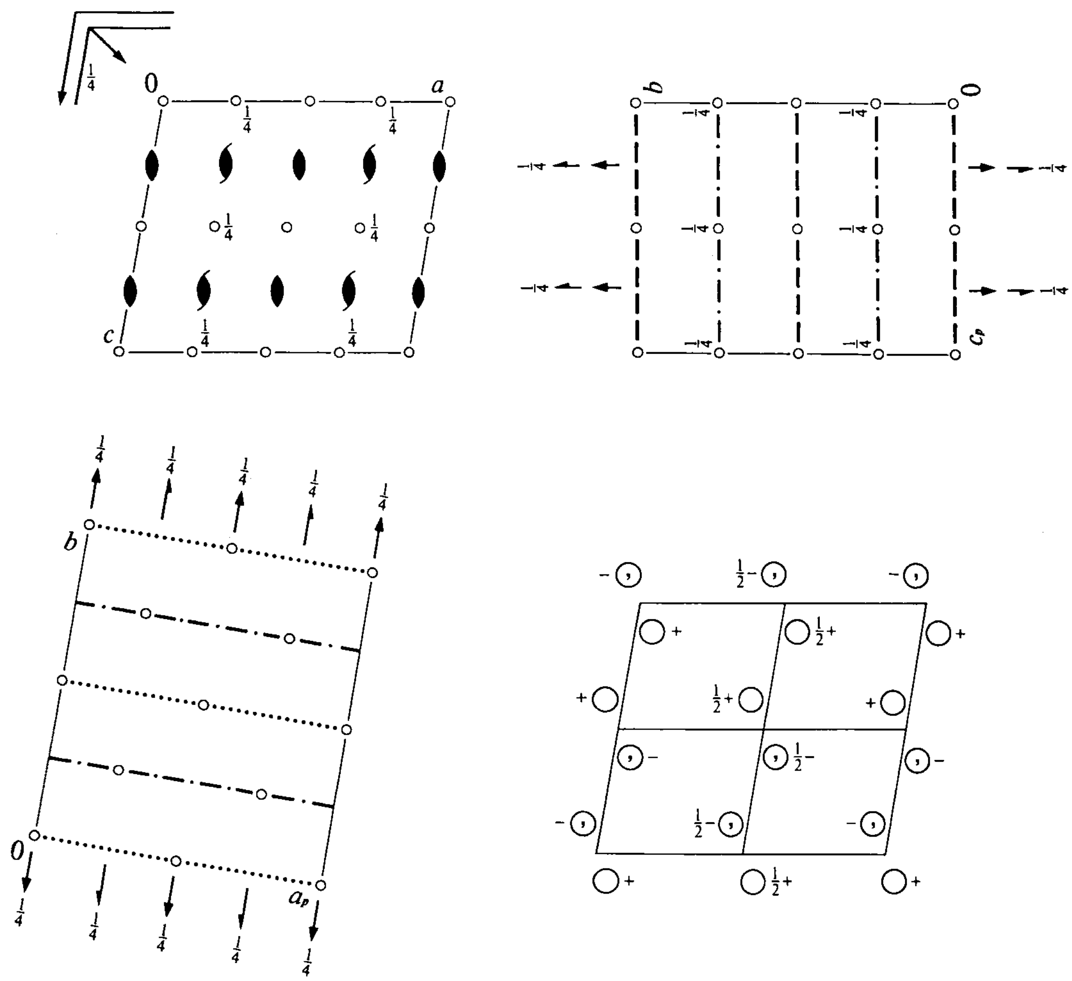
Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	$hk0:\ k=2n$ $00l:\ l=2n$ $0k0:\ k=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$hkl:\ k+l=2n$
2	c	$\bar{1}$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$			$hkl:\ k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			$hkl:\ k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			$hkl:\ k+l=2n$

International Tables for Crystallography (2006). Vol. A, Space group 15, pp. 192–199.

$C2/c$ $\quad$ C_{2h}^{6} $\quad$ $2/m$ $\quad$ Monoclinic

No. 15 $\quad$ $C12/c1$ $\quad$ Patterson symmetry $C12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$ on glide plane c

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 $\qquad$ (2) $2 \quad 0,y,\frac{1}{4}$ $\qquad$ (3) $\bar{1} \quad 0,0,0$ $\qquad$ (4) $c \quad x,0,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ $\qquad$ (2) $2(0,\frac{1}{2},0) \quad \frac{1}{4},y,\frac{1}{4}$ $\qquad$ (3) $\bar{1} \quad \frac{1}{4},\frac{1}{4},0$ $\qquad$ (4) $n(\frac{1}{2},0,\frac{1}{2}) \quad x,\frac{1}{4},z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				General:
8	f	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z+\frac{1}{2}$	hkl : $h+k=2n$ $h0l$: $h,l=2n$ $0kl$: $k=2n$ $hk0$: $h+k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus
4	e	2	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			no extra conditions
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},0$			hkl : $k+l=2n$
4	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl : $k+l=2n$
4	b	$\bar{1}$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
4	a	$\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $C1c1$ (Cc, 9)	(1; 4)+
	[2] $C121$ ($C2$, 5)	(1; 2)+
	[2] $C\bar{1}$ ($P\bar{1}$, 2)	(1; 3)+
IIa	[2] $P12_1/n1$ ($P2_1/c$, 14)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P12_1/c1$ ($P2_1/c$, 14)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P12/c1$ ($P2/c$, 13)	1; 2; 3; 4
	[2] $P12/n1$ ($P2/c$, 13)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $C12/c1$ ($\mathbf{b}'=3\mathbf{b}$) ($C2/c$, 15); [3] $C12/c1$ ($\mathbf{c}'=3\mathbf{c}$) ($C2/c$, 15); [3] $C12/c1$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{a}'=3\mathbf{a},\mathbf{c}'=-\mathbf{a}+\mathbf{c}$ or $\mathbf{a}'=3\mathbf{a},\mathbf{c}'=\mathbf{a}+\mathbf{c}$) ($C2/c$, 15)

Minimal non-isomorphic supergroups

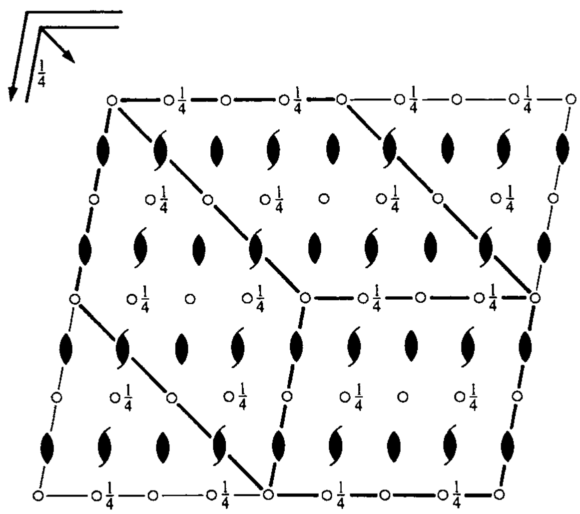
I [2] $Cmcm$ (63); [2] $Cmce$ (64); [2] $Cccm$ (66); [2] $Ccce$ (68); [2] $Fddd$ (70); [2] $Ibam$ (72); [2] $Ibca$ (73); [2] $Imma$ (74); [2] $I4_1/a$ (88); [3] $P\bar{3}1c$ (163); [3] $P\bar{3}c1$ (165); [3] $R\bar{3}c$ (167)

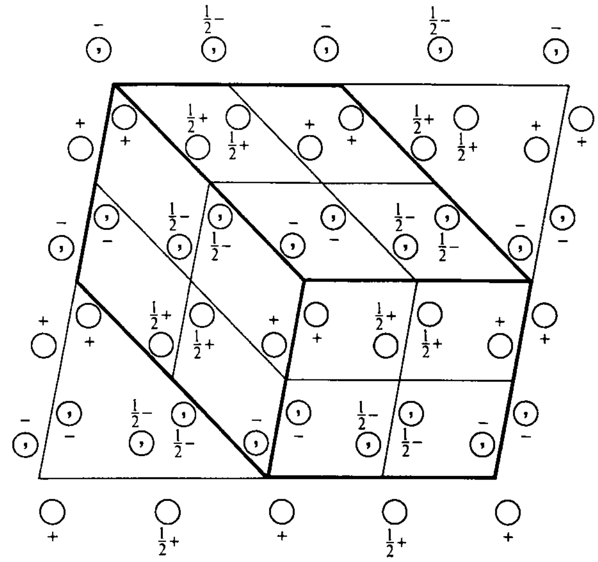
II [2] $F12/m1$ ($C2/m$, 12); [2] $C12/m1$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($C2/m$, 12); [2] $P12/c1$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($P2/c$, 13)

$C2/c$ $\quad C_{2h}^{6}$ $\quad 2/m$ $\quad$ Monoclinic

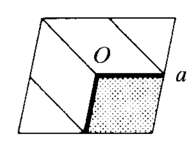
No. 15

UNIQUE AXIS b, DIFFERENT CELL CHOICES





$C\,1\,2/c\,1$



UNIQUE AXIS b, CELL CHOICE 1

Origin at $\bar{1}$ on glide plane c

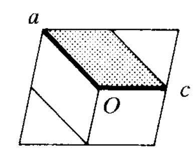
Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Generators selected $\quad (1);\ t(1,0,0);\ t(0,1,0);\ t(0,0,1);\ t(\frac{1}{2},\frac{1}{2},0);\ (2);\ (3)$

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},0)+$				General:
8	f	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z+\frac{1}{2}$	$hkl:\ h+k=2n$; $h0l:\ h,l=2n$; $0kl:\ k=2n$; $hk0:\ h+k=2n$; $0k0:\ k=2n$; $h00:\ h=2n$; $00l:\ l=2n$
							Special: as above, plus
4	e	2	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			no extra conditions
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},0$			
4	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			$hkl:\ k+l=2n$
4	b	$\bar{1}$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			
4	a	$\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$			$hkl:\ l=2n$

$A\,1\,2/n\,1$



UNIQUE AXIS b, CELL CHOICE 2

Origin at $\bar{1}$ on glide plane n

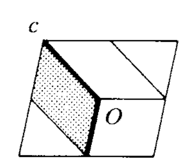
Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(0,\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
8	f	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	hkl : $k+l=2n$ $h0l$: $h,l=2n$ $0kl$: $k+l=2n$ $hk0$: $k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus
4	e	2	$\frac{3}{4},y,\frac{3}{4}$	$\frac{1}{4},\bar{y},\frac{1}{4}$			no extra conditions
4	d	$\bar{1}$	$\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$0,\frac{1}{4},\frac{3}{4}$			
4	c	$\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$			hkl : $h=2n$
4	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k=2n$

$I\,1\,2/a\,1$



UNIQUE AXIS b, CELL CHOICE 3

Origin at $\bar{1}$ on glide plane a

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

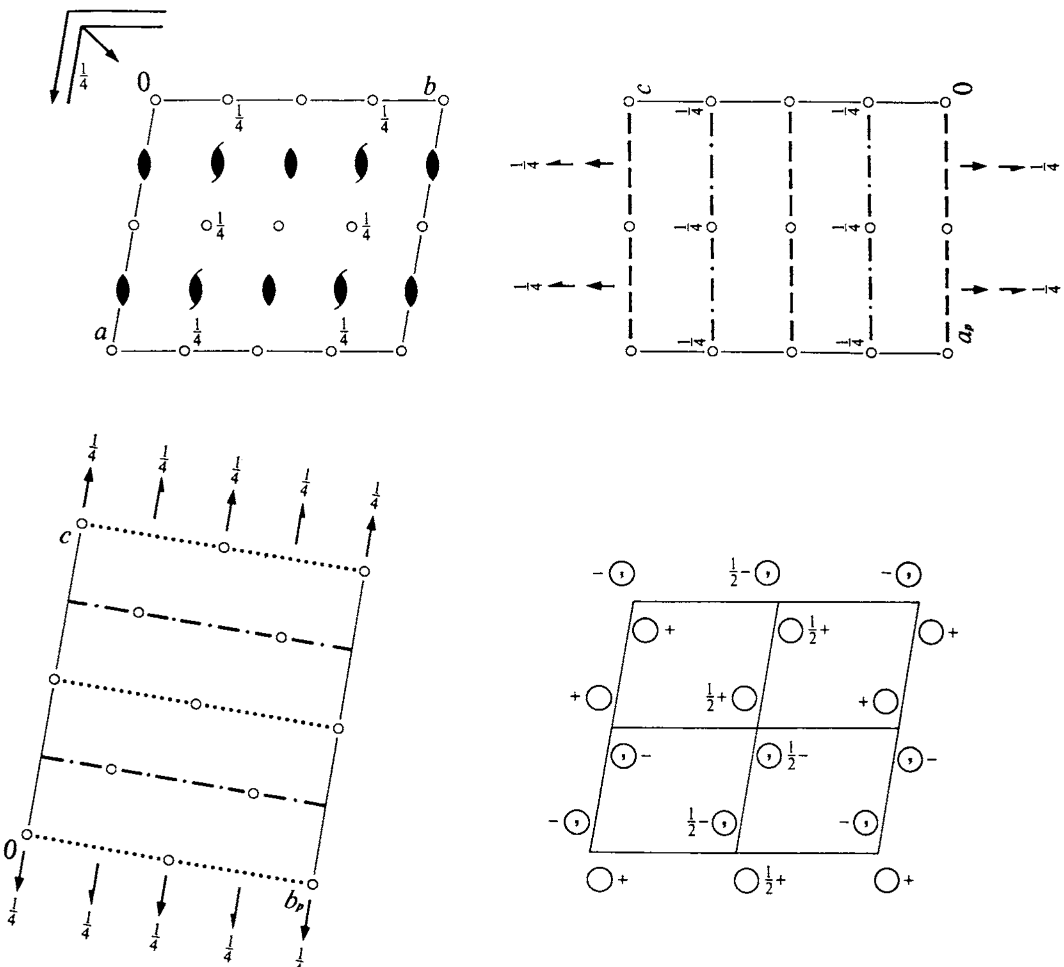
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
8	f	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},y,\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},z$	hkl : $h+k+l=2n$ $h0l$: $h,l=2n$ $0kl$: $k+l=2n$ $hk0$: $h+k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus
4	e	2	$\frac{1}{4},y,0$	$\frac{3}{4},\bar{y},0$			no extra conditions
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$			
4	c	$\bar{1}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$			hkl : $l=2n$
4	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$			hkl : $h=2n$

$C2/c$ $\quad C_{2h}^6 \quad 2/m$ Monoclinic

No. 15 $\quad A\,1\,1\,2/a$ Patterson symmetry $A\,1\,1\,2/m$

UNIQUE AXIS c, CELL CHOICE 1



Origin at $\bar{1}$ on glide plane a

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad \frac{1}{4},0,z$	(3) $\bar{1}\quad 0,0,0$	(4) $a\quad x,y,0$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},\frac{1}{4},z$	(3) $\bar{1}\quad 0,\frac{1}{4},\frac{1}{4}$	(4) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+$				General:
8	f	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}$	$hkl: k+l=2n$ $hk0: h,k=2n$ $0kl: k+l=2n$ $h0l: l=2n$ $00l: l=2n$ $h00: h=2n$ $0k0: k=2n$
							Special: as above, plus
4	e	2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}$			no extra conditions
4	d	$\bar{1}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$			$hkl: h+k=2n$
4	c	$\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$			$hkl: h+k=2n$
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			$hkl: h=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$			$hkl: h=2n$

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{a} \quad \mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}_p \quad \mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c} \quad \mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $A11a$ (Cc, 9)	(1; 4)+
	[2] $A112$ ($C2$, 5)	(1; 2)+
	[2] $A\bar{1}$ ($P\bar{1}$, 2)	(1; 3)+
IIa	[2] $P112_1/n$ ($P2_1/c$, 14)	1; 3; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$
	[2] $P112_1/a$ ($P2_1/c$, 14)	1; 4; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$
	[2] $P112/a$ ($P2/c$, 13)	1; 2; 3; 4
	[2] $P112/n$ ($P2/c$, 13)	1; 2; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $A112/a$ ($\mathbf{c}'=3\mathbf{c}$) ($C2/c$, 15); [3] $A112/a$ ($\mathbf{a}'=3\mathbf{a}$) ($C2/c$, 15); [3] $A112/a$ ($\mathbf{b}'=3\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=3\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}+\mathbf{b},\mathbf{b}'=3\mathbf{b}$) ($C2/c$, 15)

Minimal non-isomorphic supergroups

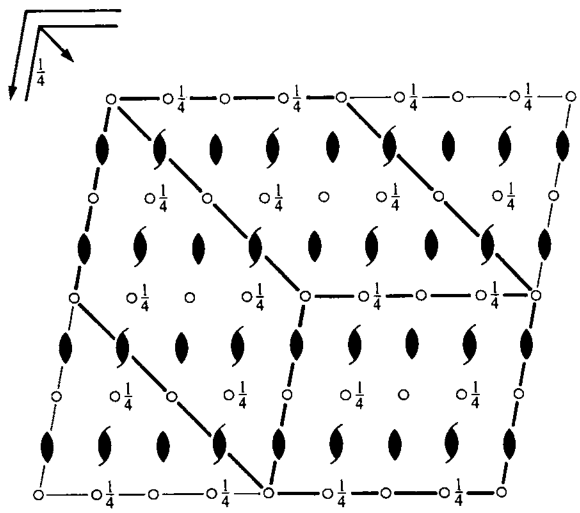
I [2] $Cmcm$ (63); [2] $Cmce$ (64); [2] $Cccm$ (66); [2] $Ccce$ (68); [2] $Fddd$ (70); [2] $Ibam$ (72); [2] $Ibca$ (73); [2] $Imma$ (74); [2] $I4_1/a$ (88); [3] $P\bar{3}1c$ (163); [3] $P\bar{3}c1$ (165); [3] $R\bar{3}c$ (167)

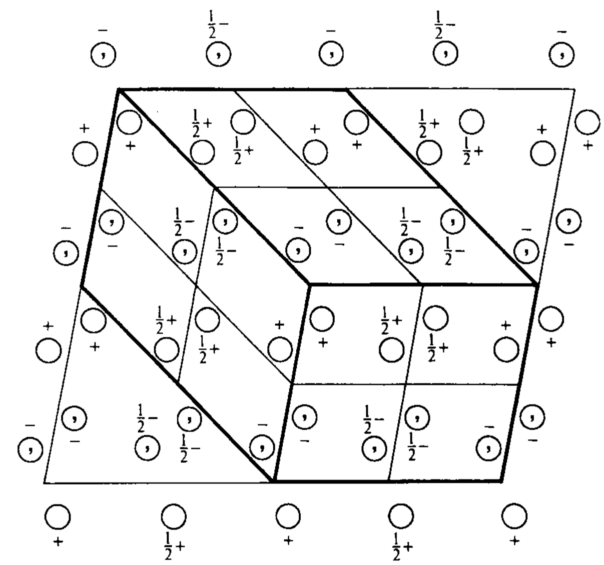
II [2] $F112/m$ ($C2/m$, 12); [2] $A112/m$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($C2/m$, 12); [2] $P112/a$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P2/c$, 13)

$C2/c$ $\quad C_{2h}^{6}$ $\quad 2/m$ $\quad$ Monoclinic

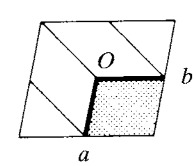
No. 15

UNIQUE AXIS c, DIFFERENT CELL CHOICES





$A112/a$



UNIQUE AXIS c, CELL CHOICE 1

Origin at $\bar{1}$ on glide plane a

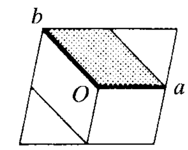
Asymptotic unit $0 \le x \le \frac{1}{2}$; $\quad 0 \le y \le \frac{1}{2}$; $\quad 0 \le z \le \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+$				General:
8	f	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}$	hkl : $k+l=2n$; $hk0$: $h,k=2n$; $0kl$: $k+l=2n$; $h0l$: $l=2n$; $00l$: $l=2n$; $h00$: $h=2n$; $0k0$: $k=2n$
							Special: as above, plus
4	e	2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}$			no extra conditions
4	d	$\bar{1}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	4 c $\bar{1}$: $0,\frac{1}{4},\frac{1}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$	hkl : $h+k=2n$
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	4 a $\bar{1}$: $0,0,0$	$\frac{1}{2},0,0$	hkl : $h=2n$

$B112/n$



UNIQUE AXIS c, CELL CHOICE 2

Origin at $\bar{1}$ on glide plane n

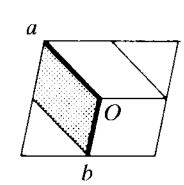
Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},0,\frac{1}{2})+$				General:
8	f	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	$hkl: h+l=2n$; $hk0: h,k=2n$; $0kl: l=2n$; $h0l: h+l=2n$; $00l: l=2n$; $h00: h=2n$; $0k0: k=2n$
							Special: as above, plus
4	e	2	$\frac{3}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}$			no extra conditions
4	d	$\bar{1}$	$\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},0,\frac{1}{4}$			
4	c	$\bar{1}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},\frac{1}{2},\frac{1}{4}$			$hkl: k=2n$
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			$hkl: h+k=2n$

$I112/b$



UNIQUE AXIS c, CELL CHOICE 3

Origin at $\bar{1}$ on glide plane b

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le 1$; $0 \le z \le \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

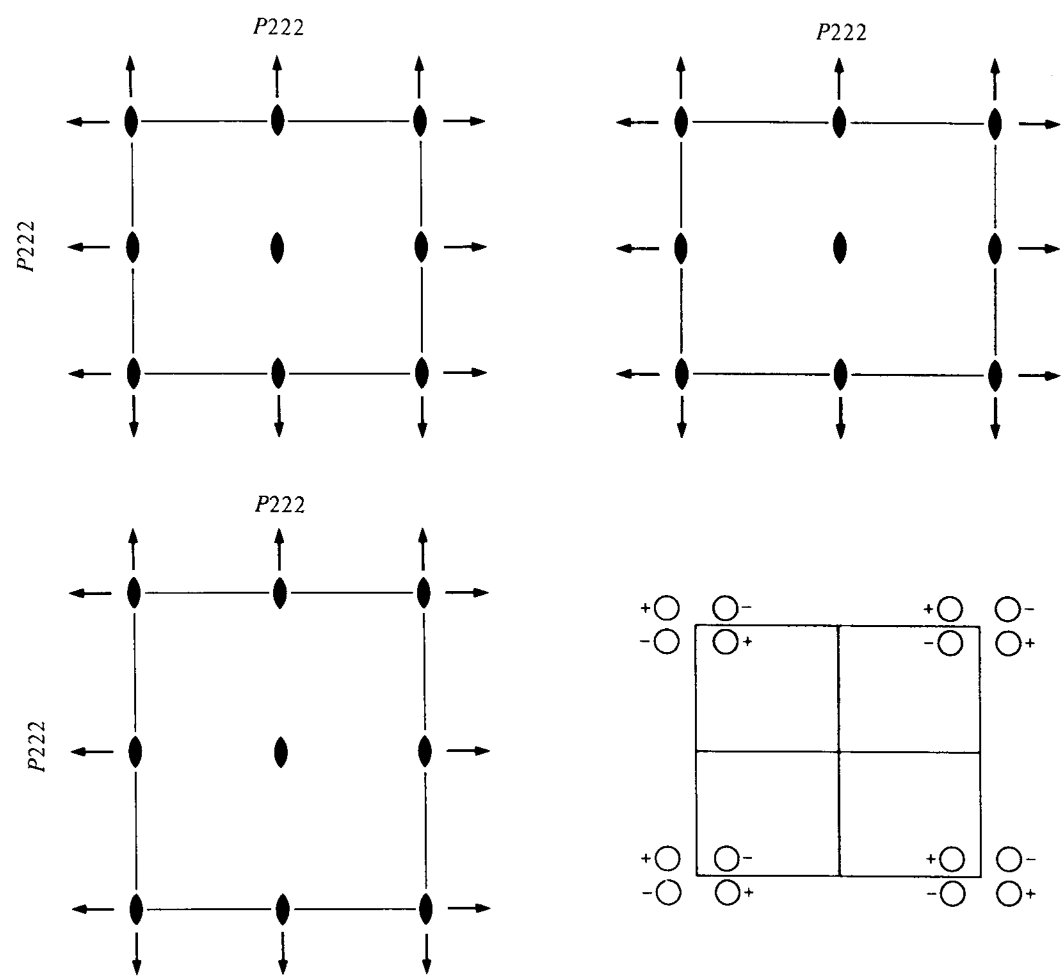
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
8	f	1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y+\frac{1}{2},\bar{z}$	$hkl: h+k+l=2n$; $hk0: h,k=2n$; $0kl: k+l=2n$; $h0l: h+l=2n$; $00l: l=2n$; $h00: h=2n$; $0k0: k=2n$
							Special: as above, plus
4	e	2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}$			no extra conditions
4	d	$\bar{1}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$			
4	c	$\bar{1}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$			$hkl: h=2n$
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			
4	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},0$			$hkl: k=2n$

International Tables for Crystallography (2006). Vol. A, Space group 16, pp. 200–201.

$P222$ $\quad D_2^1$ $\quad 222$ $\quad$ Orthorhombic

No. 16 $\quad P222$ $\quad$ Patterson symmetry $Pmmm$



Origin at 222

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $\quad$ (2) 2 $\;0,0,z$ $\quad$ (3) 2 $\;0,y,0$ $\quad$ (4) 2 $\;x,0,0$

Maximal non-isomorphic subgroups

I $\quad$ [2] $P112$ ($P2$, 3) $\quad$ 1; 2
[2] $P121$ ($P2$, 3) $\quad$ 1; 3
[2] $P211$ ($P2$, 3) $\quad$ 1; 4

IIa $\quad$ none

IIb $\quad$ [2] $P2_122$ ($\mathbf{a}' = 2\mathbf{a}$) ($P222_1$, 17); [2] $P22_12$ ($\mathbf{b}' = 2\mathbf{b}$) ($P222_1$, 17); [2] $P222_1$ ($\mathbf{c}' = 2\mathbf{c}$) (17);
[2] $A222$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C222$, 21); [2] $B222$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($C222$, 21); [2] $C222$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (21);
[2] $F222$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (22)

Maximal isomorphic subgroups of lowest index

IIc $\quad$ [2] $P222$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{c}' = 2\mathbf{c}$) (16)

Minimal non-isomorphic supergroups

I $\quad$ [2] $Pmmm$ (47); [2] $Pnnn$ (48); [2] $Pccm$ (49); [2] $Pban$ (50); [2] $P422$ (89); [2] $P4_222$ (93); [2] $P\bar{4}2c$ (112); [2] $P\bar{4}2m$ (111);
[3] $P23$ (195)

II $\quad$ [2] $A222$ ($C222$, 21); [2] $B222$ ($C222$, 21); [2] $C222$ (21); [2] $I222$ (23)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	u	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	no conditions
							Special: no extra conditions
2	t	. . 2	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			
2	s	. . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			
2	r	. . 2	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$			
2	q	. . 2	$0,0,z$	$0,0,\bar{z}$			
2	p	. 2 .	$\frac{1}{2},y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\frac{1}{2}$			
2	o	. 2 .	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},0$			
2	n	. 2 .	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			
2	m	. 2 .	$0,y,0$	$0,\bar{y},0$			
2	l	2 . .	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$			
2	k	2 . .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$			
2	j	2 . .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$			
2	i	2 . .	$x,0,0$	$\bar{x},0,0$			
1	h	2 2 2	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
1	g	2 2 2	$0,\frac{1}{2},\frac{1}{2}$				
1	f	2 2 2	$\frac{1}{2},0,\frac{1}{2}$				
1	e	2 2 2	$\frac{1}{2},\frac{1}{2},0$				
1	d	2 2 2	$0,0,\frac{1}{2}$				
1	c	2 2 2	$0,\frac{1}{2},0$				
1	b	2 2 2	$\frac{1}{2},0,0$				
1	a	2 2 2	$0,0,0$				

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

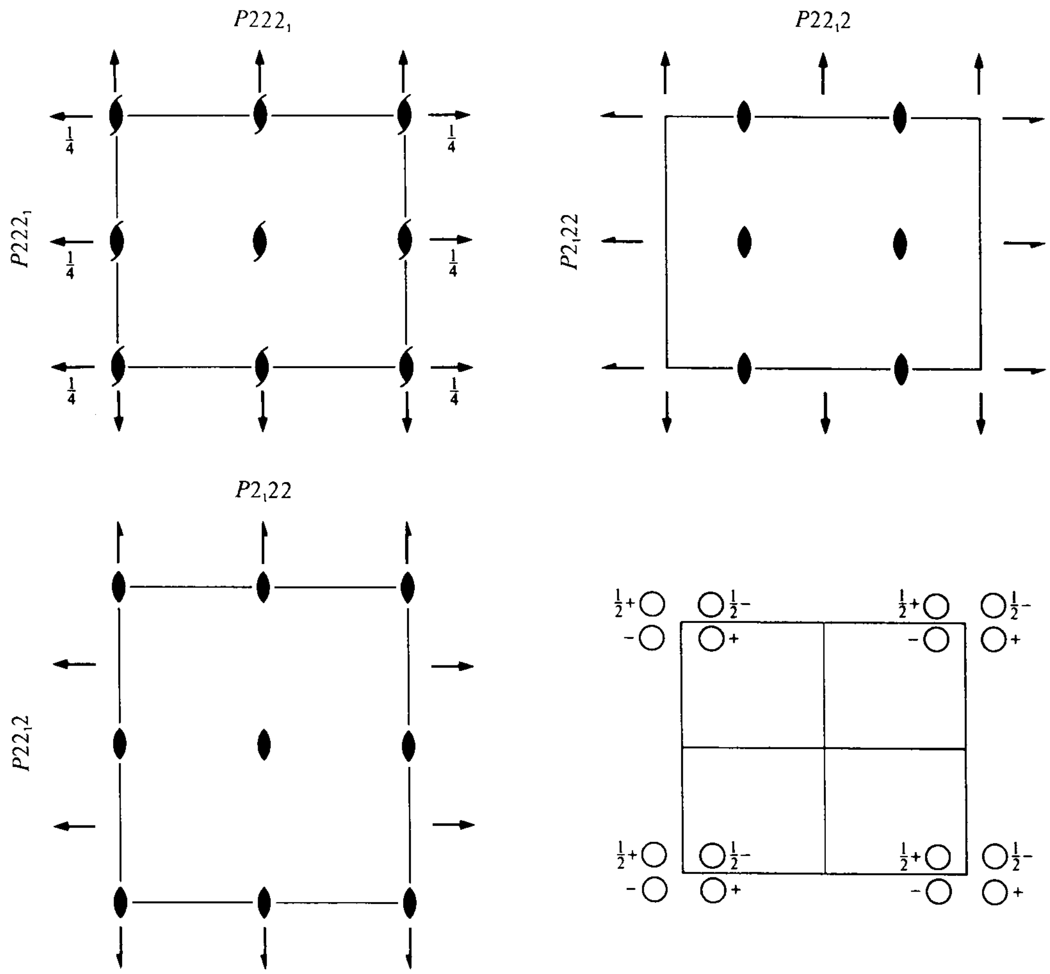
Along [010] $p2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

(*Continued on preceding page*)

International Tables for Crystallography (2006). Vol. A, Space group 17, pp. 202–203.

$P222_1$ D_2^2 222 Orthorhombic

No. 17 $P222_1$ Patterson symmetry $Pmmm$



Origin at $2\,1\,2_1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) 2 $0,y,\frac{1}{4}$ (4) 2 $x,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$	$00l$: $l=2n$
							Special: as above, plus
2	d	. 2 .	$\frac{1}{2},y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{3}{4}$			$h0l$: $l=2n$
2	c	. 2 .	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			$h0l$: $l=2n$
2	b	2 . .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},\frac{1}{2}$			$0kl$: $l=2n$
2	a	2 . .	$x,0,0$	$\bar{x},0,\frac{1}{2}$			$0kl$: $l=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mg$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,\frac{1}{4}$

Maximal non-isomorphic subgroups

I [2] $P112_1$ ($P2_1$, 4) 1; 2
[2] $P121$ ($P2$, 3) 1; 3
[2] $P211$ ($P2$, 3) 1; 4

IIa none

IIb [2] $P2_122_1$ ($\mathbf{a}'=2\mathbf{a}$) ($P2_12_12$, 18); [2] $P22_12_1$ ($\mathbf{b}'=2\mathbf{b}$) ($P2_12_12$, 18); [2] $C222_1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (20)

Maximal isomorphic subgroups of lowest index

IIc [2] $P222_1$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{b}'=2\mathbf{b}$) (17); [3] $P222_1$ ($\mathbf{c}'=3\mathbf{c}$) (17)

Minimal non-isomorphic supergroups

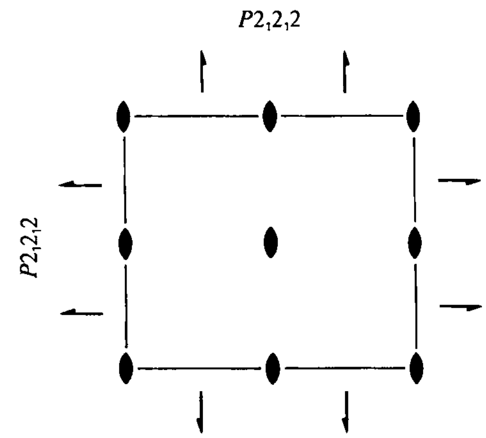
I [2] $Pmma$ (51); [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $P4_122$ (91); [2] $P4_322$ (95)

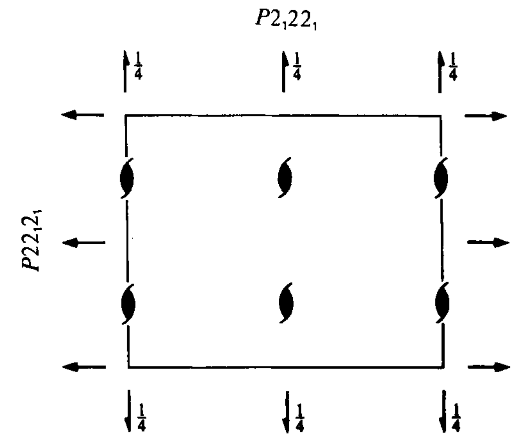
II [2] $C222_1$ (20); [2] $A222$ ($C222$, 21); [2] $B222$ ($C222$, 21); [2] $I2_12_12_1$ (24); [2] $P222$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (16)

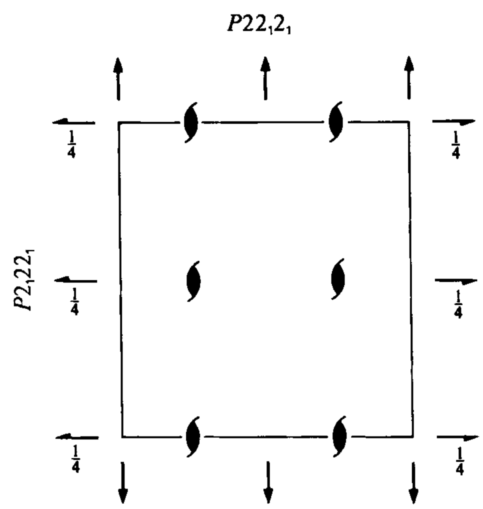
International Tables for Crystallography (2006). Vol. A, Space group 18, pp. 204–205.

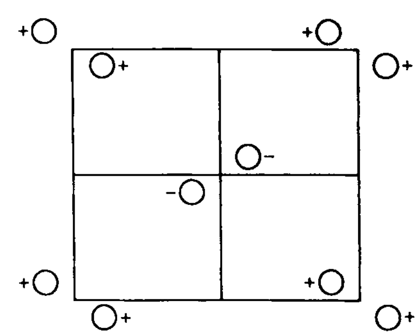
$P2_12_12$ D_2^3 222 Orthorhombic

No. 18 $P2_12_12$ Patterson symmetry $Pmmm$









Origin at intersection of 2 with perpendicular plane containing 2_1 axes

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
2	b	$..2$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			$hk0$: $h+k=2n$
2	a	$..2$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			$hk0$: $h+k=2n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [010] $p2gm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $\frac{1}{4},y,0$

Maximal non-isomorphic subgroups

I [2] $P12_11$ ($P2_1$, 4) 1; 3
[2] $P2_111$ ($P2_1$, 4) 1; 4
[2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $P2_12_12_1$ ($\mathbf{c}'=2\mathbf{c}$) (19)

Maximal isomorphic subgroups of lowest index

IIc [2] $P2_12_12$ ($\mathbf{c}'=2\mathbf{c}$) (18); [3] $P2_12_12$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (18)

Minimal non-isomorphic supergroups

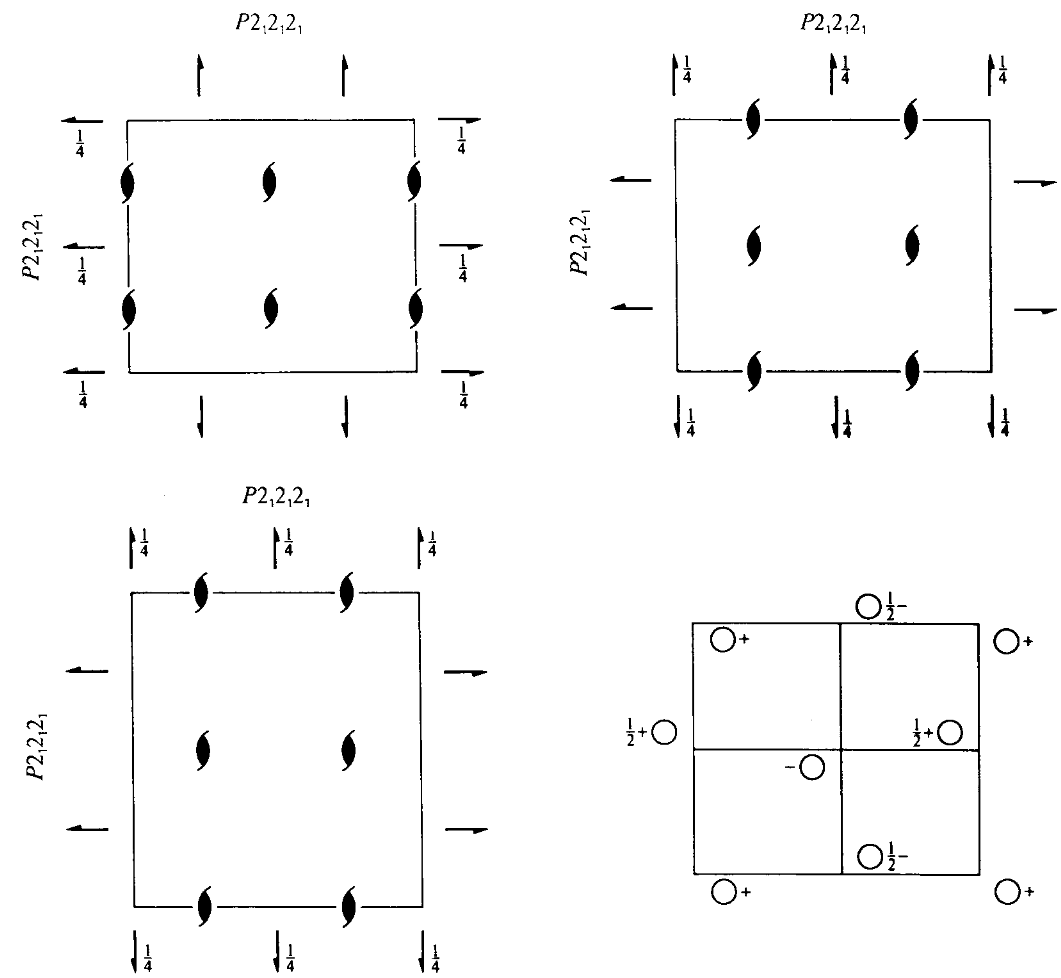
I [2] $Pbam$ (55); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pnnm$ (58); [2] $Pmmn$ (59); [2] $Pbcn$ (60); [2] $P42_12$ (90); [2] $P4_22_12$ (94); [2] $P\bar{4}2_1m$ (113); [2] $P\bar{4}2_1c$ (114)

II [2] $A2_122$ ($C222_1$, 20); [2] $B22_12$ ($C222_1$, 20); [2] $C222$ (21); [2] $I222$ (23); [2] $P22_12$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($P222_1$, 17); [2] $P2_122$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($P222_1$, 17)

International Tables for Crystallography (2006). Vol. A, Space group 19, pp. 206–207.

$P2_12_12_1$ D_2^4 222 Orthorhombic

No. 19 $P2_12_12_1$ Patterson symmetry $Pmmm$



Origin at midpoint of three non-intersecting pairs of parallel 2_1 axes

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 *a* 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},0,z$

Along [100] $p2gg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [010] $p2gg$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,\frac{1}{4}$

Maximal non-isomorphic subgroups

I [2] $P112_1$ ($P2_1$, 4) 1; 2
[2] $P12_11$ ($P2_1$, 4) 1; 3
[2] $P2_111$ ($P2_1$, 4) 1; 4

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P2_12_12_1$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$ or $\mathbf{c}'=3\mathbf{c}$) (19)

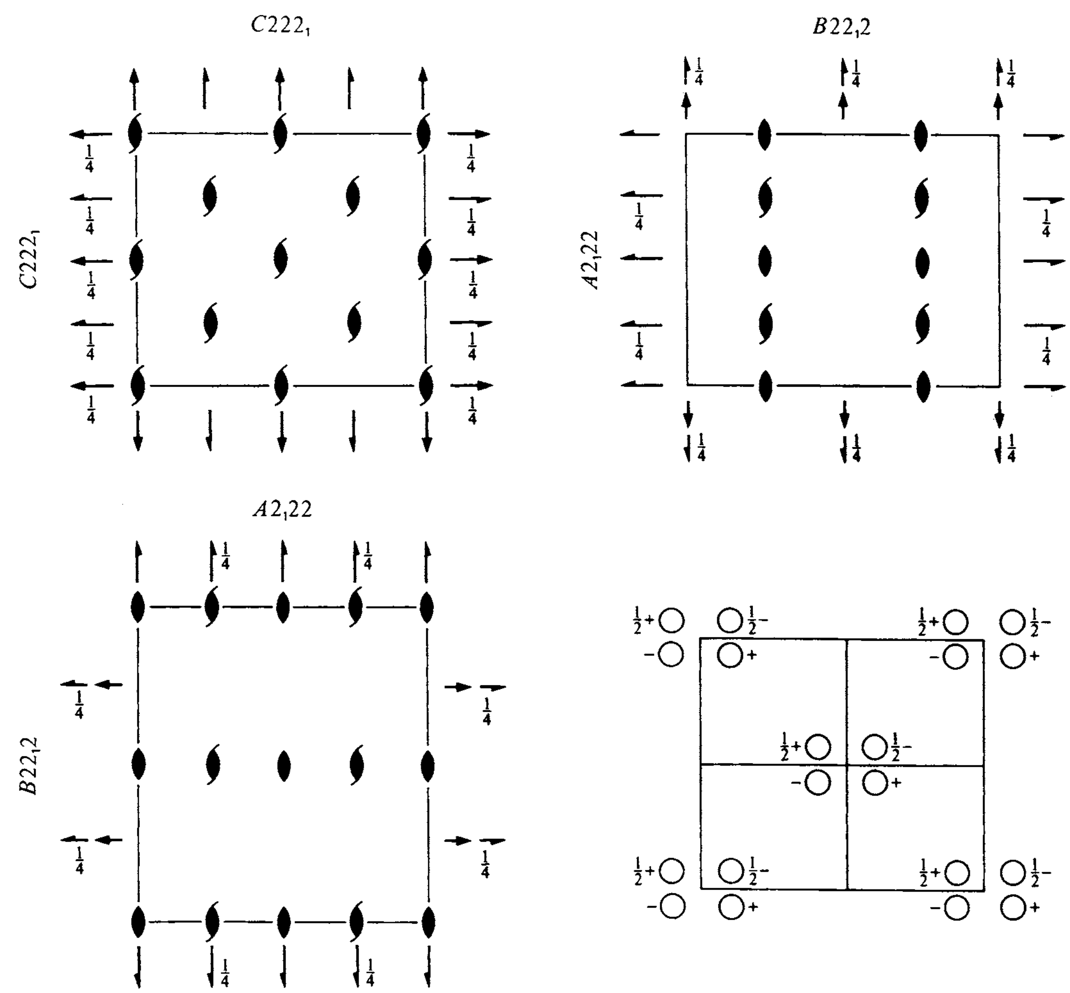
Minimal non-isomorphic supergroups

I [2] $Pbca$ (61); [2] $Pnma$ (62); [2] $P4_12_12$ (92); [2] $P4_32_12$ (96); [3] $P2_13$ (198)

II [2] $A2_122$ ($C222_1$, 20); [2] $B22_12$ ($C222_1$, 20); [2] $C222_1$ (20); [2] $I2_12_12_1$ (24); [2] $P22_12_1$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($P2_12_12$, 18); [2] $P2_122_1$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($P2_12_12$, 18); [2] $P2_12_12$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (18)

$C222_1$ D_2^5 222 Orthorhombic

No. 20 $C222_1$ Patterson symmetry $Cmmm$



Origin at 212_1

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) $2(0,0,\frac{1}{2})\ \ 0,0,z$ (3) $2\ \ 0,y,\frac{1}{4}$ (4) $2\ \ x,0,0$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$ (3) $2(0,\frac{1}{2},0)\ \ \frac{1}{4},y,\frac{1}{4}$ (4) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				General:
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$	$hkl: h+k=2n$ $0kl: k=2n$ $h0l: h=2n$ $hk0: h+k=2n$ $h00: h=2n$ $0k0: k=2n$ $00l: l=2n$
							Special: as above, plus
4	b	. 2 .	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			$h0l: l=2n$
4	a	2 . .	$x,0,0$	$\bar{x},0,\frac{1}{2}$			$0kl: l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mg$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,\frac{1}{4}$

Maximal non-isomorphic subgroups

I	[2] $C121$ ($C2$, 5)	(1; 3)+
	[2] $C211$ ($C2$, 5)	(1; 4)+
	[2] $C112_1$ ($P2_1$, 4)	(1; 2)+
IIa	[2] $P2_12_12_1$ (19)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P2_122_1$ ($P2_12_12$, 18)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P22_12_1$ ($P2_12_12$, 18)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $P222_1$ (17)	1; 2; 3; 4
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $C222_1$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (20); [3] $C222_1$ ($\mathbf{c}'=3\mathbf{c}$) (20)

Minimal non-isomorphic supergroups

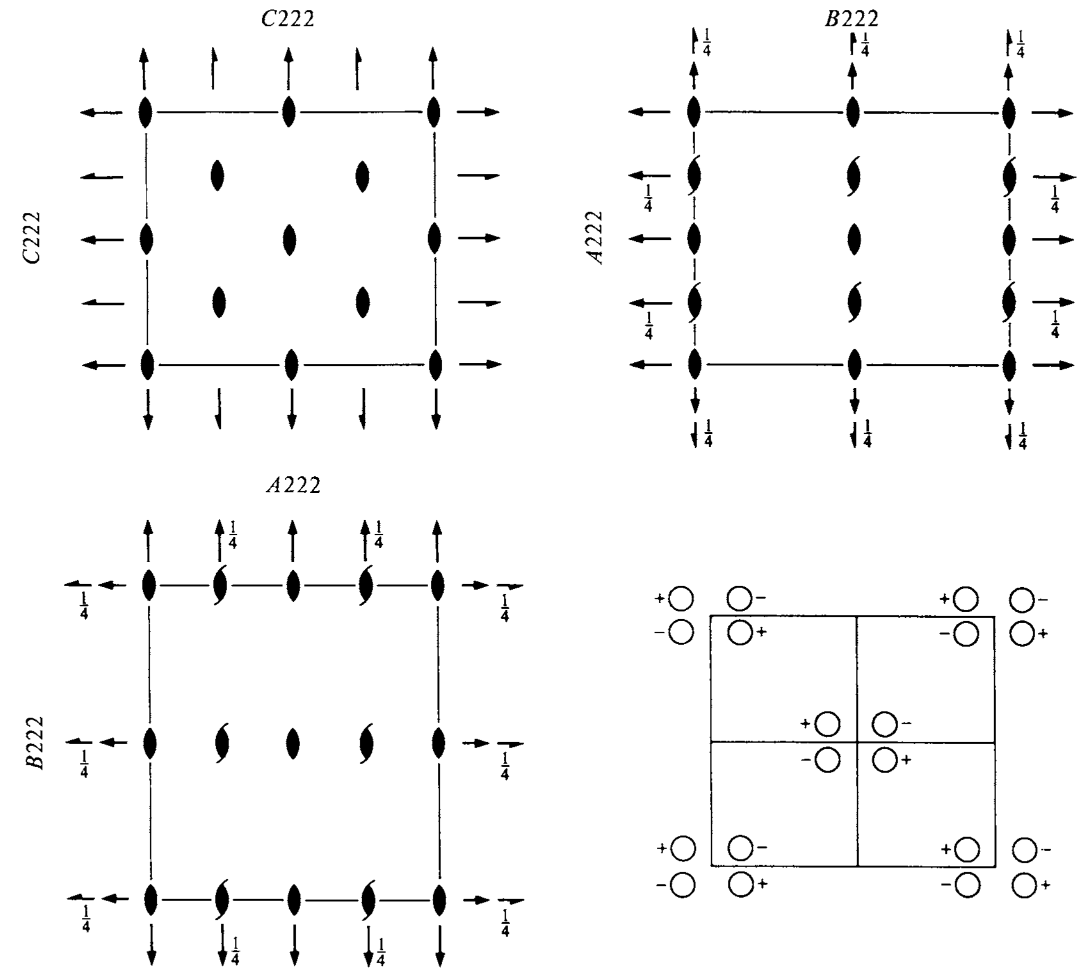
I [2] $Cmcm$ (63); [2] $Cmce$ (64); [2] $P4_122$ (91); [2] $P4_12_12$ (92); [2] $P4_322$ (95); [2] $P4_32_12$ (96); [3] $P6_122$ (178); [3] $P6_522$ (179); [3] $P6_322$ (182)

II [2] $F222$ (22); [2] $P222_1$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (17); [2] $C222$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (21)

International Tables for Crystallography (2006). Vol. A, Space group 21, pp. 210–211.

$C222$ $\quad D_2^6$ $\quad 222$ $\quad$ Orthorhombic

No. 21 $\quad C222$ $\quad$ Patterson symmetry $Cmmm$



Origin at 222

Asymmetric unit $\quad 0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2 \quad 0,0,z$	(3) $2 \quad 0,y,0$	(4) $2 \quad x,0,0$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2 \quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0) \quad \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0) \quad x,\frac{1}{4},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				General:
8	*l*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hkl : $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	*k*	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$			$hk0$: $h=2n$
4	*j*	. . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			no extra conditions
4	*i*	. . 2	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	*h*	. 2 .	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			no extra conditions
4	*g*	. 2 .	$0,y,0$	$0,\bar{y},0$			no extra conditions
4	*f*	2 . .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$			no extra conditions
4	*e*	2 . .	$x,0,0$	$\bar{x},0,0$			no extra conditions
2	*d*	2 2 2	$0,0,\frac{1}{2}$				no extra conditions
2	*c*	2 2 2	$\frac{1}{2},0,\frac{1}{2}$				no extra conditions
2	*b*	2 2 2	$0,\frac{1}{2},0$				no extra conditions
2	*a*	2 2 2	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $C121$ ($C2$, 5) (1; 3)+
[2] $C211$ ($C2$, 5) (1; 4)+
[2] $C112$ ($P2$, 3) (1; 2)+

IIa [2] $P2_12_12$ (18) 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $P2_122$ ($P222_1$, 17) 1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $P22_12$ ($P222_1$, 17) 1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $P222$ (16) 1; 2; 3; 4

IIb [2] $I2_12_12_1$ ($\mathbf{c}'=2\mathbf{c}$) (24); [2] $I222$ ($\mathbf{c}'=2\mathbf{c}$) (23); [2] $C222_1$ ($\mathbf{c}'=2\mathbf{c}$) (20)

Maximal isomorphic subgroups of lowest index

IIc [2] $C222$ ($\mathbf{c}'=2\mathbf{c}$) (21); [3] $C222$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (21)

Minimal non-isomorphic supergroups

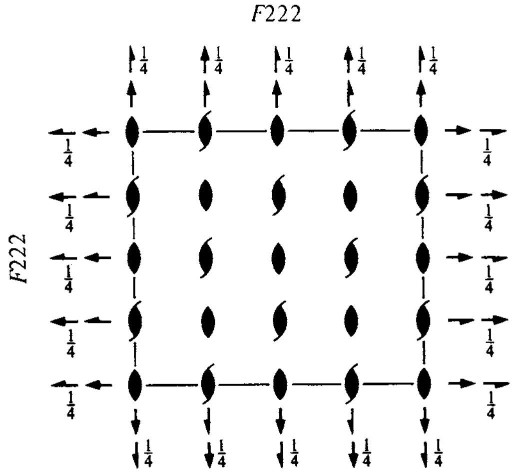
I [2] $Cmmm$ (65); [2] $Cccm$ (66); [2] $Cmme$ (67); [2] $Ccce$ (68); [2] $P422$ (89); [2] $P42_12$ (90); [2] $P4_222$ (93); [2] $P4_22_12$ (94); [2] $P\bar{4}m2$ (115); [2] $P\bar{4}c2$ (116); [2] $P\bar{4}b2$ (117); [2] $P\bar{4}n2$ (118); [3] $P622$ (177); [3] $P6_222$ (180); [3] $P6_422$ (181)

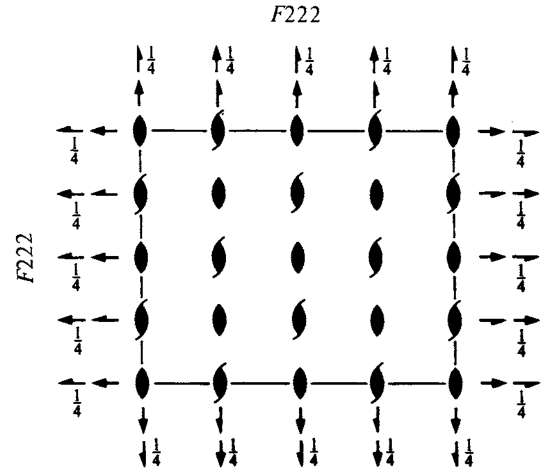
II [2] $F222$ (22); [2] $P222$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (16)

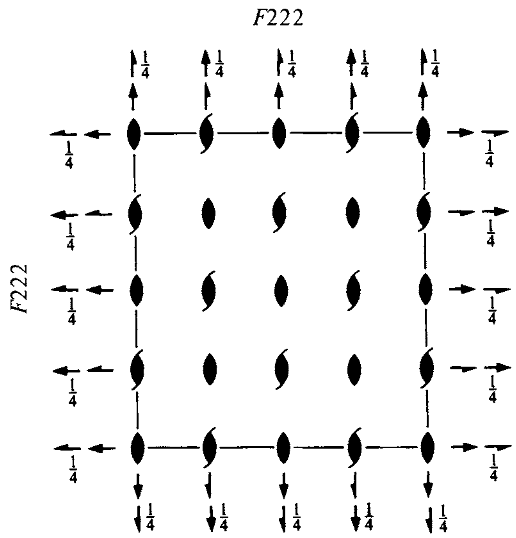
International Tables for Crystallography (2006). Vol. A, Space group 22, pp. 212–213.

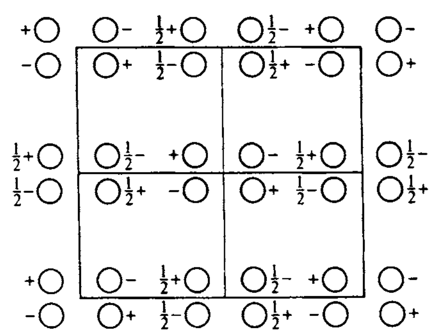
$F\,2\,2\,2$ $\quad D_2^7$ $\quad 2\,2\,2$ $\quad$ Orthorhombic

No. 22 $\quad F\,2\,2\,2$ $\quad$ Patterson symmetry $F\,m\,m\,m$









Origin at $2\,2\,2$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4};\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2\quad x,\frac{1}{4},\frac{1}{4}$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,0,\frac{1}{4}$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$

Maximal isomorphic subgroups of lowest index

IIc $\quad$ [3] $F\,2\,2\,2$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (22)

Minimal non-isomorphic supergroups

I $\quad$ [2] $F\,m\,m\,m$ (69); [2] $F\,d\,d\,d$ (70); [2] $I\,4\,2\,2$ (97); [2] $I\,4_1\,2\,2$ (98); [2] $I\,\bar{4}\,m\,2$ (119); [2] $I\,\bar{4}\,c\,2$ (120); [3] $F\,2\,3$ (196)

II $\quad$ [2] $P\,2\,2\,2$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (16)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$

Multiplicity	Wyckoff letter	Site symmetry	Coordinates				Reflection conditions
							General:
16	*k*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hkl : $h+k,h+l,k+l=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: no extra conditions
8	*j*	2 . .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$			
8	*i*	. 2 .	$\frac{1}{4},y,\frac{1}{4}$	$\frac{3}{4},\bar{y},\frac{1}{4}$			
8	*h*	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$			
8	*g*	. . 2	$0,0,z$	$0,0,\bar{z}$			
8	*f*	. 2 .	$0,y,0$	$0,\bar{y},0$			
8	*e*	2 . .	$x,0,0$	$\bar{x},0,0$			
4	*d*	2 2 2	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$				
4	*c*	2 2 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$				
4	*b*	2 2 2	$0,0,\frac{1}{2}$				
4	*a*	2 2 2	$0,0,0$				

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

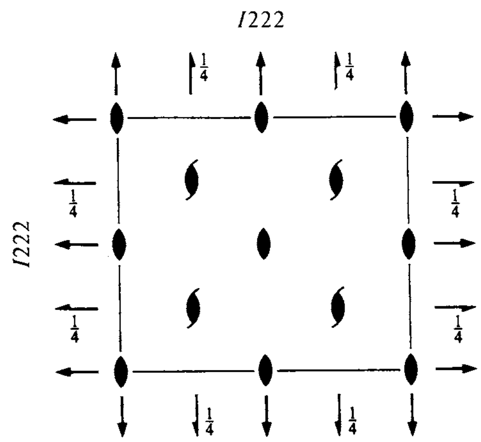
Maximal non-isomorphic subgroups

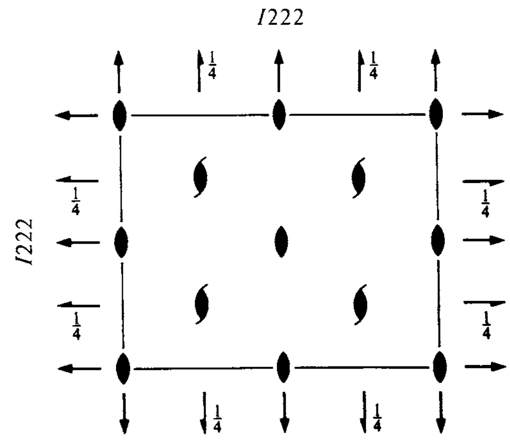
I	[2] $F112$ ($C2$, 5)	(1; 2)+
	[2] $F121$ ($C2$, 5)	(1; 3)+
	[2] $F211$ ($C2$, 5)	(1; 4)+
IIa	[2] $A222$ ($C222$, 21)	1; 2; 3; 4; (1; 2; 3; 4) + $(0,\frac{1}{2},\frac{1}{2})$
	[2] $A222$ ($C222$, 21)	1; 4; (1; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 3) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $B222$ ($C222$, 21)	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2},0,\frac{1}{2})$
	[2] $B222$ ($C222$, 21)	1; 3; (1; 3) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$
	[2] $C222$ (21)	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $C222$ (21)	1; 2; (1; 2) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 4) + $(\frac{1}{2},0,\frac{1}{2})$
	[2] $A2_122$ ($C222_1$, 20)	1; 2; (1; 2) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 4) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $A2_122$ ($C222_1$, 20)	1; 3; (1; 3) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 4) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $B22_12$ ($C222_1$, 20)	1; 2; (1; 2) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$
	[2] $B22_12$ ($C222_1$, 20)	1; 4; (1; 4) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$
	[2] $C222_1$ (20)	1; 3; (1; 3) + $(\frac{1}{2},\frac{1}{2},0)$; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 4) + $(\frac{1}{2},0,\frac{1}{2})$
	[2] $C222_1$ (20)	1; 4; (1; 4) + $(\frac{1}{2},\frac{1}{2},0)$; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 3) + $(\frac{1}{2},0,\frac{1}{2})$
IIb	none	

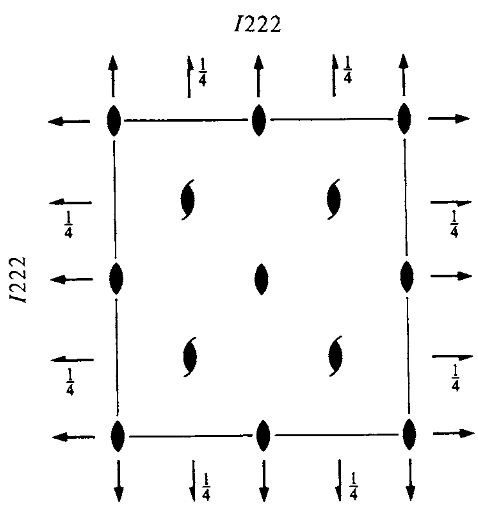
(*Continued on preceding page*)

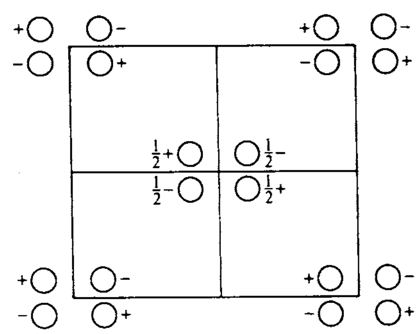
$I222$ $\quad D_2^8$ $\quad 222$ $\quad$ Orthorhombic

No. 23 $\quad I222$ $\quad$ Patterson symmetry $Immm$









Origin at 222

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2 \quad 0,0,z$	(3) $2 \quad 0,y,0$	(4) $2 \quad x,0,0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0) \quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0) \quad x,\frac{1}{4},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
8	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hkl : $h+k+l=2n$ $0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: no extra conditions
4	j	. . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			
4	i	. . 2	$0,0,z$	$0,0,\bar{z}$			
4	h	. 2 .	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},0$			
4	g	. 2 .	$0,y,0$	$0,\bar{y},0$			
4	f	2 . .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$			
4	e	2 . .	$x,0,0$	$\bar{x},0,0$			
2	d	2 2 2	$0,\frac{1}{2},0$				
2	c	2 2 2	$0,0,\frac{1}{2}$				
2	b	2 2 2	$\frac{1}{2},0,0$				
2	a	2 2 2	$0,0,0$				

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $c2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $I112$ ($C2$, 5)	(1; 2)+
	[2] $I121$ ($C2$, 5)	(1; 3)+
	[2] $I211$ ($C2$, 5)	(1; 4)+
IIa	[2] $P2_12_12$ (18)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P2_122_1$ ($P2_12_12$, 18)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P22_12_1$ ($P2_12_12$, 18)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P222$ (16)	1; 2; 3; 4
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I222$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$ or $\mathbf{c}'=3\mathbf{c}$) (23)

Minimal non-isomorphic supergroups

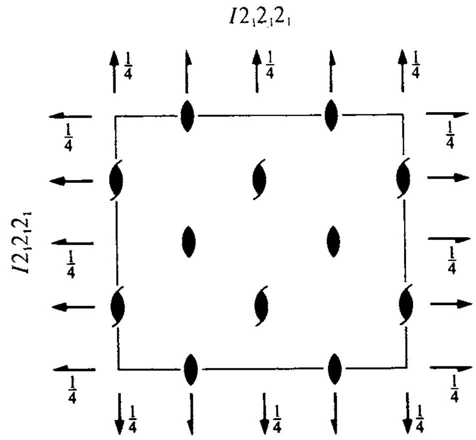
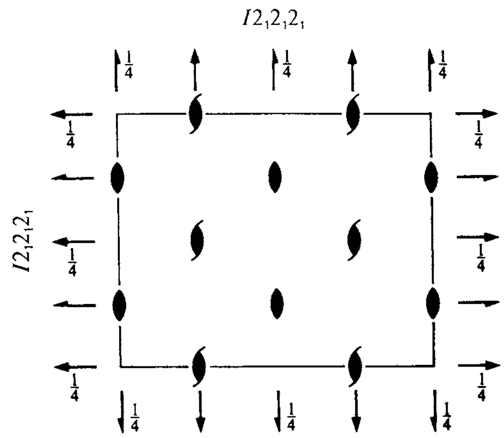
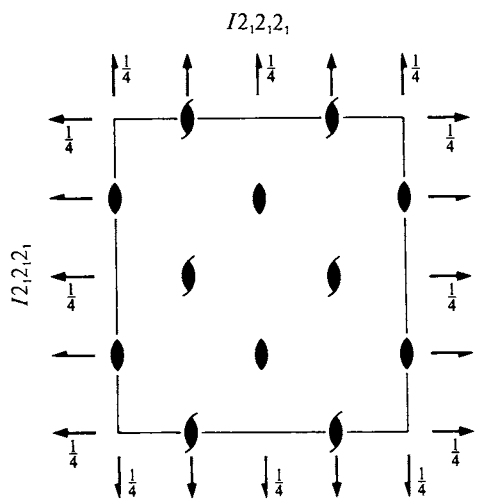
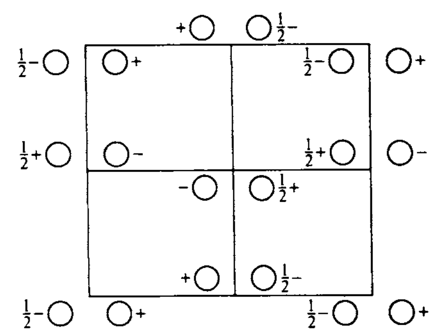
I [2] $Immm$ (71); [2] $Ibam$ (72); [2] $I422$ (97); [2] $I\bar{4}2m$ (121); [3] $I23$ (197)

II [2] $A222$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($C222$, 21); [2] $B222$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($C222$, 21); [2] $C222$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (21)

International Tables for Crystallography (2006). Vol. A, Space group 24, pp. 216–217.

$I\,2_1\,2_1\,2_1$ $\quad D_2^9$ $\quad 222$ $\quad$ Orthorhombic

No. 24 $\quad I\,2_1\,2_1\,2_1$ $\quad$ Patterson symmetry $Immm$

Origin at midpoint of three non-intersecting pairs of parallel 2 axes

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\quad 0,\frac{1}{4},z$	(3) $2\quad \frac{1}{4},y,0$	(4) $2\quad x,0,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
8	d	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	hkl : $h+k+l=2n$ $0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	c	. . 2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}+\frac{1}{2}$			$hk0$: $h=2n$
4	b	. 2 .	$\frac{1}{4},y,0$	$\frac{1}{4},\bar{y},\frac{1}{2}$			$h0l$: $h=2n$
4	a	2 . .	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$			$0kl$: $k=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [010] $c2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,\frac{1}{4}$

Maximal non-isomorphic subgroups

I [2] $I112_1$ ($C2$, 5) (1; 2)+
[2] $I12_11$ ($C2$, 5) (1; 3)+
[2] $I2_111$ ($C2$, 5) (1; 4)+

IIa [2] $P2_12_12_1$ (19) 1; 2; 3; 4
[2] $P222_1$ (17) 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P22_12$ ($P222_1$, 17) 1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P2_122$ ($P222_1$, 17) 1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I2_12_12_1$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$ or $\mathbf{c}'=3\mathbf{c}$) (24)

Minimal non-isomorphic supergroups

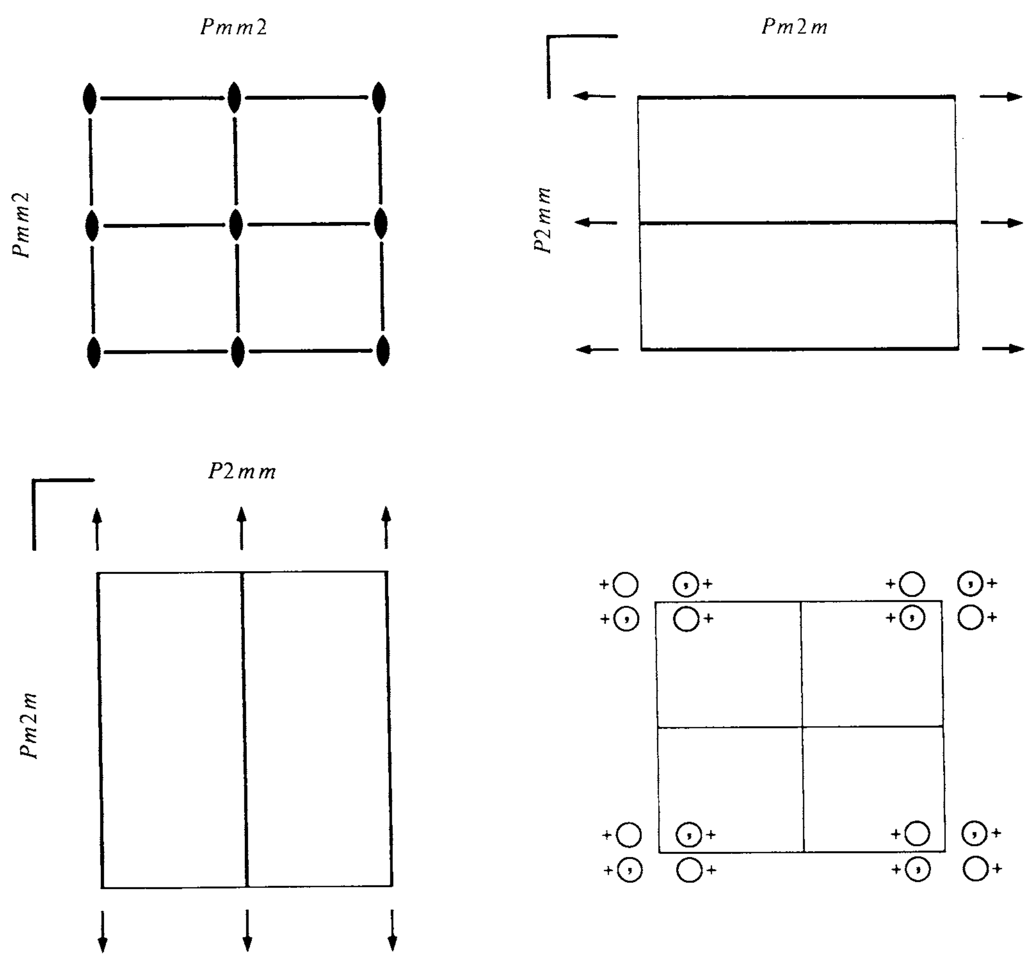
I [2] $Ibca$ (73); [2] $Imma$ (74); [2] $I4_122$ (98); [2] $I\bar{4}2d$ (122); [3] $I2_13$ (199)

II [2] $A222$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($C222$, 21); [2] $B222$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($C222$, 21); [2] $C222$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (21)

International Tables for Crystallography (2006). Vol. A, Space group 25, pp. 218–219.

$Pmm2$ $\quad C_{2v}^{1}$ $\quad mm2$ $\quad$ Orthorhombic

No. 25 $\quad Pmm2$ $\quad$ Patterson symmetry $Pmmm$



Origin on $mm2$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le 1$

Symmetry operations

(1) 1 $\qquad$ (2) $2\ \ 0,0,z$ $\qquad$ (3) $m\ \ x,0,z$ $\qquad$ (4) $m\ \ 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	no conditions
							Special: no extra conditions
2	h	$m\,.\,.$	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$			
2	g	$m\,.\,.$	$0,y,z$	$0,\bar{y},z$			
2	f	$.\,m\,.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$			
2	e	$.\,m\,.$	$x,0,z$	$\bar{x},0,z$			
1	d	$m\,m\,2$	$\frac{1}{2},\frac{1}{2},z$				
1	c	$m\,m\,2$	$\frac{1}{2},0,z$				
1	b	$m\,m\,2$	$0,\frac{1}{2},z$				
1	a	$m\,m\,2$	$0,0,z$				

Symmetry of special projections

Along [001] $p\,2\,m\,m$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,m\,1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p\,1\,1\,m$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P\,1\,m\,1$ (Pm, 6) 1; 3
[2] $P\,m\,1\,1$ (Pm, 6) 1; 4
[2] $P\,1\,1\,2$ ($P2$, 3) 1; 2

IIa none

IIb [2] $P\,m\,a\,2$ ($\mathbf{a}'=2\mathbf{a}$) (28); [2] $P\,b\,m\,2$ ($\mathbf{b}'=2\mathbf{b}$) ($P\,m\,a\,2$, 28); [2] $P\,c\,c\,2$ ($\mathbf{c}'=2\mathbf{c}$) (27); [2] $P\,m\,c\,2_1$ ($\mathbf{c}'=2\mathbf{c}$) (26); [2] $P\,c\,m\,2_1$ ($\mathbf{c}'=2\mathbf{c}$) ($P\,m\,c\,2_1$, 26); [2] $A\,e\,m\,2$ ($\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (39); [2] $A\,m\,m\,2$ ($\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (38); [2] $B\,m\,e\,2$ ($\mathbf{a}'=2\mathbf{a},\mathbf{c}'=2\mathbf{c}$) ($A\,e\,m\,2$, 39); [2] $B\,m\,m\,2$ ($\mathbf{a}'=2\mathbf{a},\mathbf{c}'=2\mathbf{c}$) ($A\,m\,m\,2$, 38); [2] $C\,m\,m\,2$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (35); [2] $F\,m\,m\,2$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (42)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\,m\,m\,2$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{b}'=2\mathbf{b}$) (25); [2] $P\,m\,m\,2$ ($\mathbf{c}'=2\mathbf{c}$) (25)

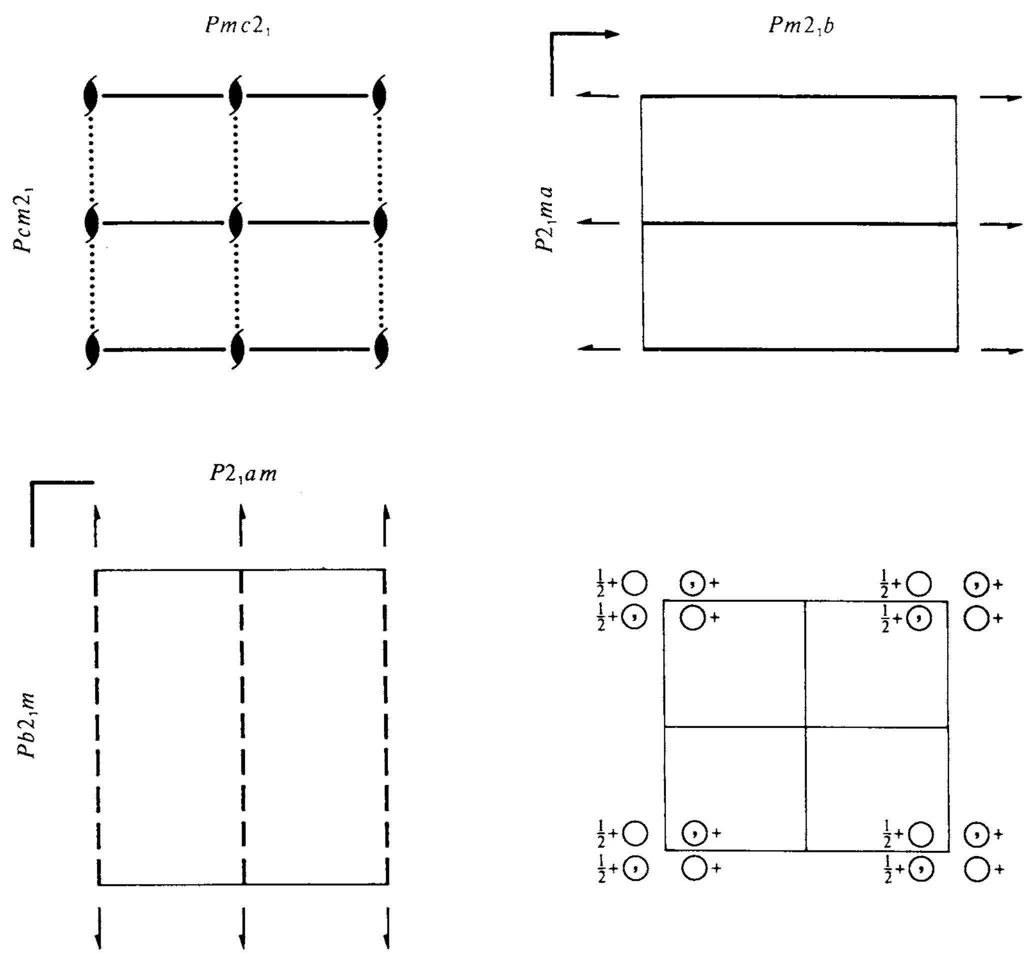
Minimal non-isomorphic supergroups

I [2] $P\,m\,m\,m$ (47); [2] $P\,m\,m\,a$ (51); [2] $P\,m\,m\,n$ (59); [2] $P\,4\,m\,m$ (99); [2] $P\,4_2\,m\,c$ (105); [2] $P\,\bar{4}\,m\,2$ (115)

II [2] $C\,m\,m\,2$ (35); [2] $A\,m\,m\,2$ (38); [2] $B\,m\,m\,2$ ($A\,m\,m\,2$, 38); [2] $I\,m\,m\,2$ (44)

$Pmc2_1$ $\quad$ C_{2v}^2 $\quad$ $mm2$ $\quad$ Orthorhombic

No. 26 $\quad$ $Pmc2_1$ $\quad$ Patterson symmetry $Pmmm$



Origin on $mc2_1$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $\quad$ (2) $2(0,0,\frac{1}{2})\ \ 0,0,z$ $\quad$ (3) $c\ \ x,0,z$ $\quad$ (4) $m\ \ 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $x,\bar{y},z+\frac{1}{2}$	(4) $\bar{x},y,z$	$h0l$: $l=2n$ $00l$: $l=2n$
							Special: no extra conditions
2	b	$m\,.\,.$	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z+\frac{1}{2}$			
2	a	$m\,.\,.$	$0,y,z$	$0,\bar{y},z+\frac{1}{2}$			

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc, 7) 1; 3
[2] $Pm11$ (Pm, 6) 1; 4
[2] $P112_1$ ($P2_1$, 4) 1; 2

IIa none

IIb [2] $Pmn2_1$ ($\mathbf{a}'=2\mathbf{a}$) (31); [2] $Pbc2_1$ ($\mathbf{b}'=2\mathbf{b}$) ($Pca2_1$, 29); [2] $Cmc2_1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (36)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmc2_1$ ($\mathbf{a}'=2\mathbf{a}$) (26); [2] $Pmc2_1$ ($\mathbf{b}'=2\mathbf{b}$) (26); [3] $Pmc2_1$ ($\mathbf{c}'=3\mathbf{c}$) (26)

Minimal non-isomorphic supergroups

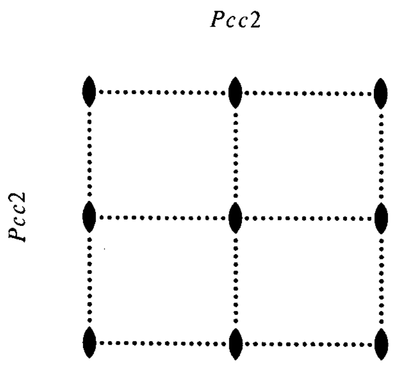
I [2] $Pmma$ (51); [2] $Pbam$ (55); [2] $Pbcm$ (57); [2] $Pnma$ (62)

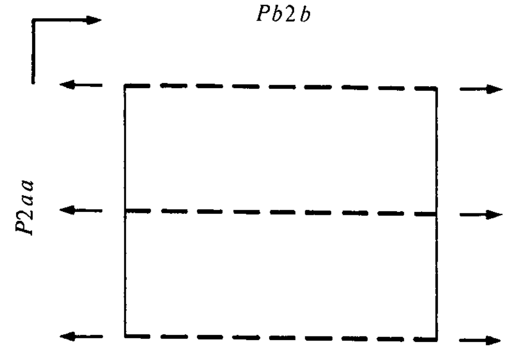
II [2] $Cmc2_1$ (36); [2] $Amm2$ (38); [2] $Bme2$ ($Aem2$, 39); [2] $Ima2$ (46); [2] $Pmm2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (25)

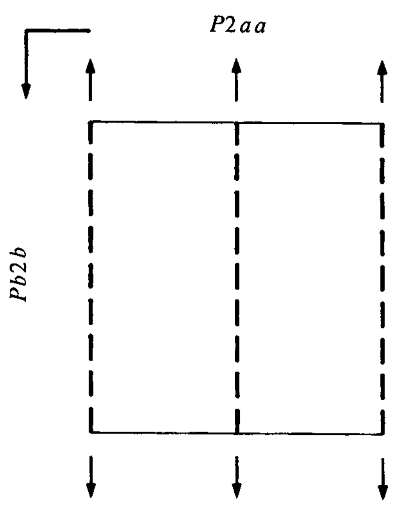
International Tables for Crystallography (2006). Vol. A, Space group 27, pp. 222–223.

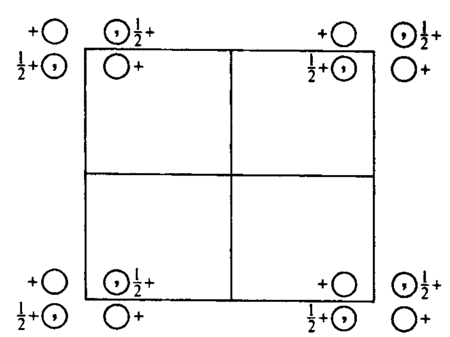
$Pcc2$ $\quad C_{2v}^{3}$ $\quad mm2$ $\quad$ Orthorhombic

No. 27 $\quad Pcc2$ $\quad$ Patterson symmetry $Pmmm$









Origin on $cc2$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $\qquad$ (2) $2 \quad 0,0,z$ $\qquad$ (3) $c \quad x,0,z$ $\qquad$ (4) $c \quad 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z+\frac{1}{2}$	(4) $\bar{x},y,z+\frac{1}{2}$	$0kl$: $l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$
							Special: as above, plus
2	d	$..2$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl : $l=2n$
2	c	$..2$	$\frac{1}{2},0,z$	$\frac{1}{2},0,z+\frac{1}{2}$			hkl : $l=2n$
2	b	$..2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$			hkl : $l=2n$
2	a	$..2$	$0,0,z$	$0,0,z+\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc, 7) 1; 3
[2] $Pc11$ (Pc, 7) 1; 4
[2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pcn2$ ($\mathbf{a}'=2\mathbf{a}$) ($Pnc2$, 30); [2] $Pnc2$ ($\mathbf{b}'=2\mathbf{b}$) (30); [2] $Ccc2$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (37)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pcc2$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{b}'=2\mathbf{b}$) (27); [3] $Pcc2$ ($\mathbf{c}'=3\mathbf{c}$) (27)

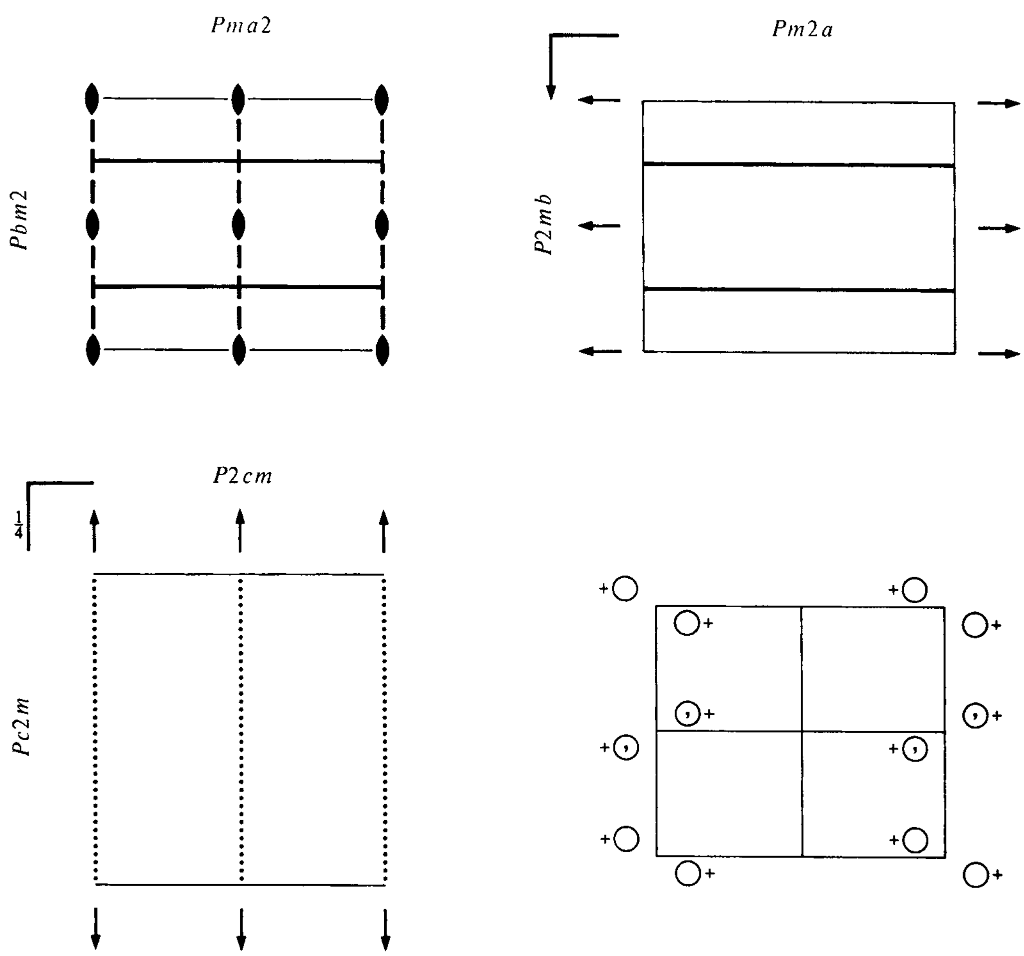
Minimal non-isomorphic supergroups

I [2] $Pccm$ (49); [2] $Pcca$ (54); [2] $Pccn$ (56); [2] $P4_2cm$ (101); [2] $P4cc$ (103); [2] $P\bar{4}c2$ (116)

II [2] $Ccc2$ (37); [2] $Aem2$ (39); [2] $Bme2$ ($Aem2$, 39); [2] $Iba2$ (45); [2] $Pmm2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (25)

$Pma2$ $\quad C_{2v}^{4}$ $\quad mm2$ $\quad$ Orthorhombic

No. 28 $\quad Pma2$ $\quad$ Patterson symmetry $Pmmm$



Origin on $1a2$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $\qquad$ (2) $2 \quad 0,0,z$ $\qquad$ (3) $a \quad x,0,z$ $\qquad$ (4) $m \quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y},z$	(4) $\bar{x}+\frac{1}{2},y,z$	$h0l$: $h=2n$ $h00$: $h=2n$
							Special: as above, plus
2	c	$m\,.\,.$	$\frac{1}{4},y,z$	$\frac{3}{4},\bar{y},z$			no extra conditions
2	b	$.\,.\,2$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$			hkl : $h=2n$
2	a	$.\,.\,2$	$0,0,z$	$\frac{1}{2},0,z$			hkl : $h=2n$

Symmetry of special projections

Along [001] $p2mg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1a1$ (Pc, 7) 1; 3
[2] $Pm11$ (Pm, 6) 1; 4
[2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pba2$ ($\mathbf{b}'=2\mathbf{b}$) (32); [2] $Pmn2_1$ ($\mathbf{c}'=2\mathbf{c}$) (31); [2] $Pcn2$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnc2$, 30); [2] $Pca2_1$ ($\mathbf{c}'=2\mathbf{c}$) (29); [2] $Aea2$ ($\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (41); [2] $Ama2$ ($\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (40)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pma2$ ($\mathbf{b}'=2\mathbf{b}$) (28); [2] $Pma2$ ($\mathbf{c}'=2\mathbf{c}$) (28); [3] $Pma2$ ($\mathbf{a}'=3\mathbf{a}$) (28)

Minimal non-isomorphic supergroups

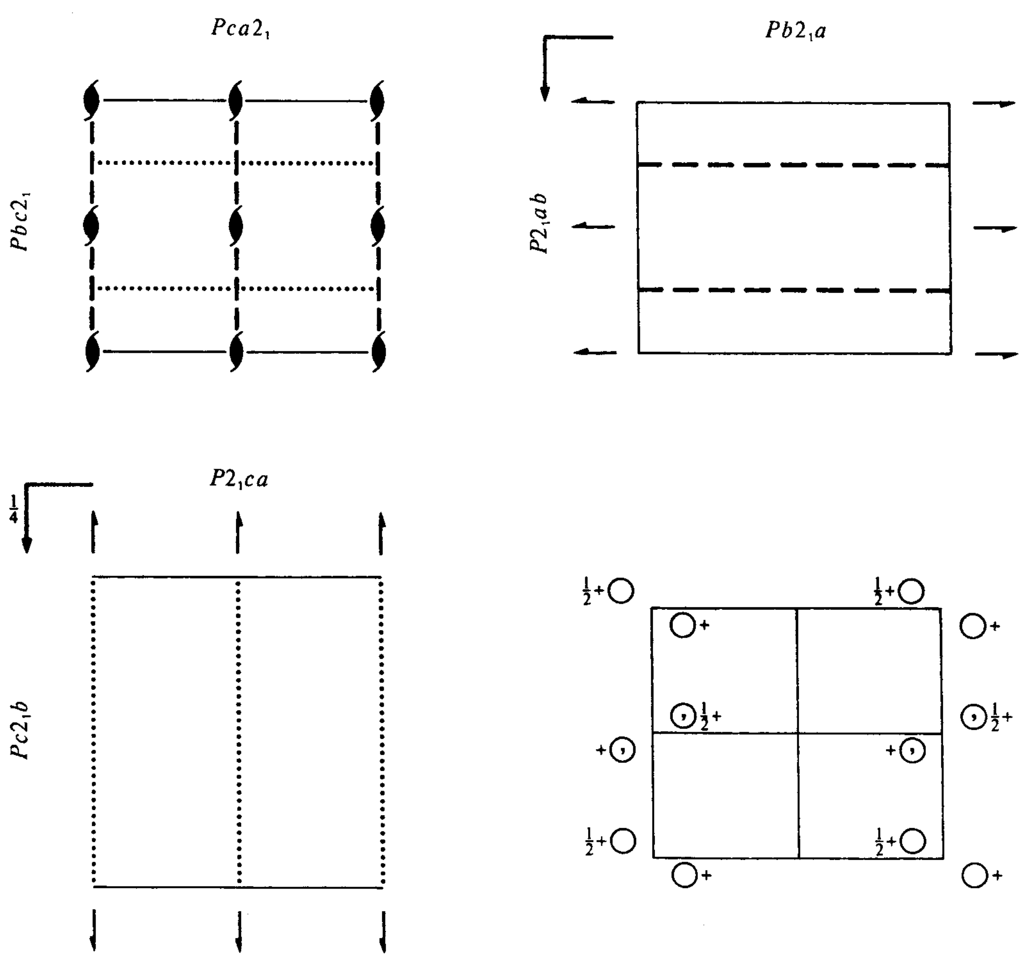
I [2] $Pccm$ (49); [2] $Pmma$ (51); [2] $Pmna$ (53); [2] $Pbcm$ (57)

II [2] $Cmm2$ (35); [2] $Bme2$ ($Aem2$, 39); [2] $Ama2$ (40); [2] $Ima2$ (46); [2] $Pmm2$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (25)

International Tables for Crystallography (2006). Vol. A, Space group 29, pp. 226–227.

$Pca2_1$ $\quad C_{2v}^5$ $\quad mm2$ $\quad$ Orthorhombic

No. 29 $\quad Pca2_1$ $\quad$ Patterson symmetry $Pmmm$



Origin on $1a2_1$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4};\quad 0 \le y \le 1;\quad 0 \le z \le 1$

Symmetry operations

(1) 1 $\qquad$ (2) $2(0,0,\frac{1}{2})\quad 0,0,z$ $\qquad$ (3) $a\quad x,0,z$ $\qquad$ (4) $c\quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 a 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $x+\frac{1}{2},\bar{y},z$	(4) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	$0kl$: $l=2n$ $h0l$: $h=2n$ $h00$: $h=2n$ $00l$: $l=2n$

Symmetry of special projections

Along [001] $p2mg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11g$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1a1$ (Pc, 7) 1; 3
[2] $Pc11$ (Pc, 7) 1; 4
[2] $P112_1$ ($P2_1$, 4) 1; 2

IIa none

IIb [2] $Pna2_1$ ($\mathbf{b}'=2\mathbf{b}$) (33)

Maximal isomorphic subgroups of lowest index

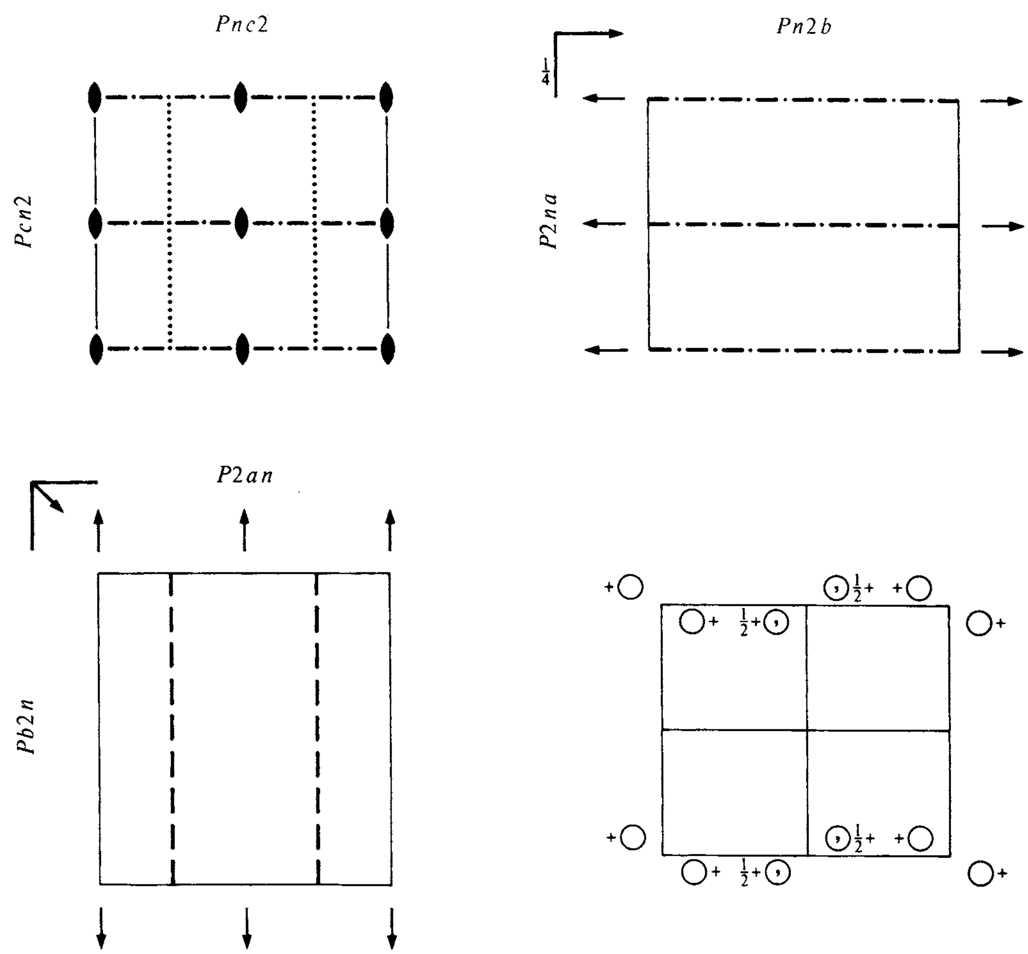
IIc [2] $Pca2_1$ ($\mathbf{b}'=2\mathbf{b}$) (29); [3] $Pca2_1$ ($\mathbf{a}'=3\mathbf{a}$) (29); [3] $Pca2_1$ ($\mathbf{c}'=3\mathbf{c}$) (29)

Minimal non-isomorphic supergroups

I [2] $Pcca$ (54); [2] $Pbcm$ (57); [2] $Pbcn$ (60); [2] $Pbca$ (61)

II [2] $Ccm2_1$ ($Cmc2_1$, 36); [2] $Bme2$ ($Aem2$, 39); [2] $Aea2$ (41); [2] $Iba2$ (45); [2] $Pcm2_1$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Pmc2_1$, 26); [2] $Pma2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (28)

$Pnc2$	C_{2v}^{6}	$mm2$	Orthorhombic
No. 30	$Pnc2$		Patterson symmetry $Pmmm$



Origin on $n\,1\,2$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 $\qquad$ (2) $2\quad 0,0,z$ $\qquad$ (3) $c\quad x,\frac{1}{4},z$ $\qquad$ (4) $n(0,\frac{1}{2},\frac{1}{2})\quad 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	b	..2	$\frac{1}{2},0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl : $k+l=2n$
2	a	..2	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{2}$			hkl : $k+l=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc, 7) 1; 3
[2] $Pn11$ (Pc, 7) 1; 4
[2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pnn2$ ($\mathbf{a}'=2\mathbf{a}$) (34)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pnc2$ ($\mathbf{a}'=2\mathbf{a}$) (30); [3] $Pnc2$ ($\mathbf{b}'=3\mathbf{b}$) (30); [3] $Pnc2$ ($\mathbf{c}'=3\mathbf{c}$) (30)

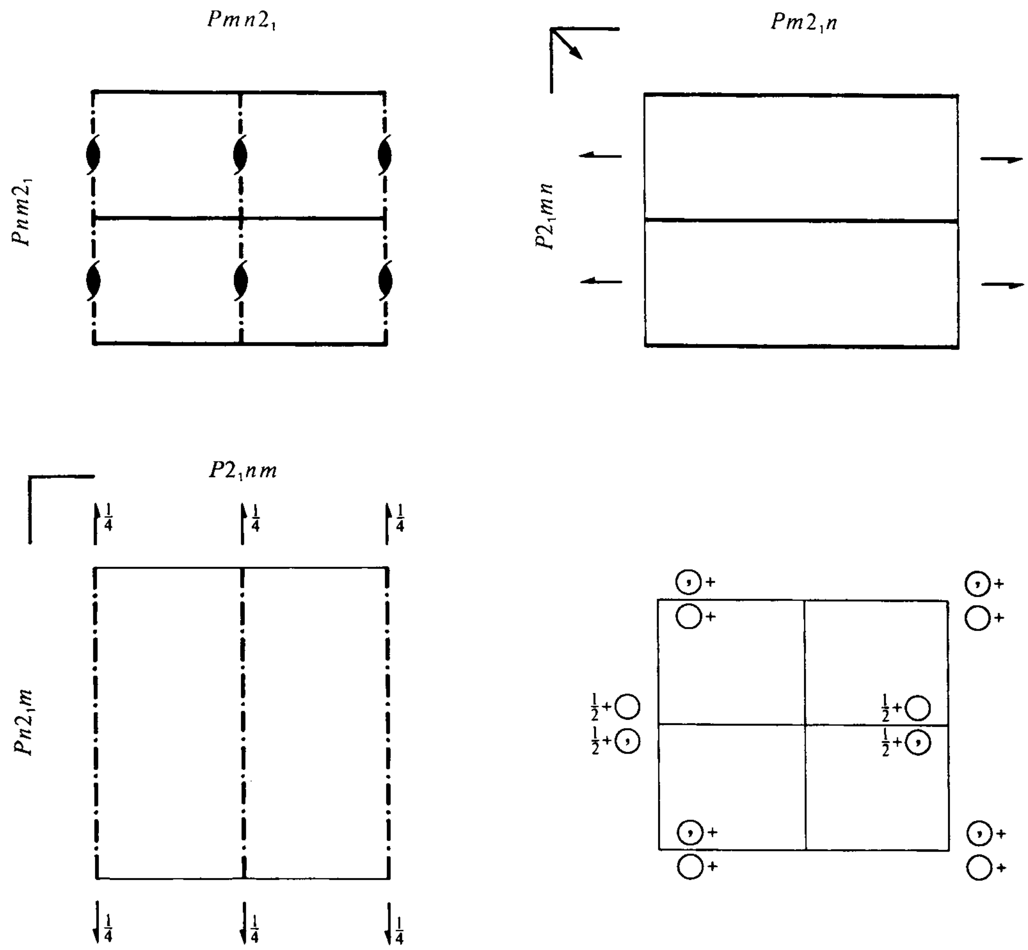
Minimal non-isomorphic supergroups

I [2] $Pban$ (50); [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pbcn$ (60)

II [2] $Ccc2$ (37); [2] $Amm2$ (38); [2] $Bbe2$ ($Aea2$, 41); [2] $Ima2$ (46); [2] $Pcc2$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (27); [2] $Pbm2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($Pma2$, 28)

$Pmn2_1$ C_{2v}^7 $mm2$ Orthorhombic

No. 31 $Pmn2_1$ Patterson symmetry $Pmmm$



Origin on $mn1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$ (4) m $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
4 b 1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (3) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (4) $\bar{x},y,z$	$h0l$: $h+l=2n$ $h00$: $h=2n$ $00l$: $l=2n$
		Special: no extra conditions
2 a $m..$	$0,y,z$ $\frac{1}{2},\bar{y},z+\frac{1}{2}$	

Symmetry of special projections

Along [001] $p2mg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},0,z$

Along [100] $p1g1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $c11m$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1n1$ (Pc, 7) 1; 3
[2] $Pm11$ (Pm, 6) 1; 4
[2] $P112_1$ ($P2_1$, 4) 1; 2

IIa none

IIb [2] $Pbn2_1$ ($\mathbf{b}'=2\mathbf{b}$) ($Pna2_1$, 33)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmn2_1$ ($\mathbf{b}'=2\mathbf{b}$) (31); [3] $Pmn2_1$ ($\mathbf{a}'=3\mathbf{a}$) (31); [3] $Pmn2_1$ ($\mathbf{c}'=3\mathbf{c}$) (31)

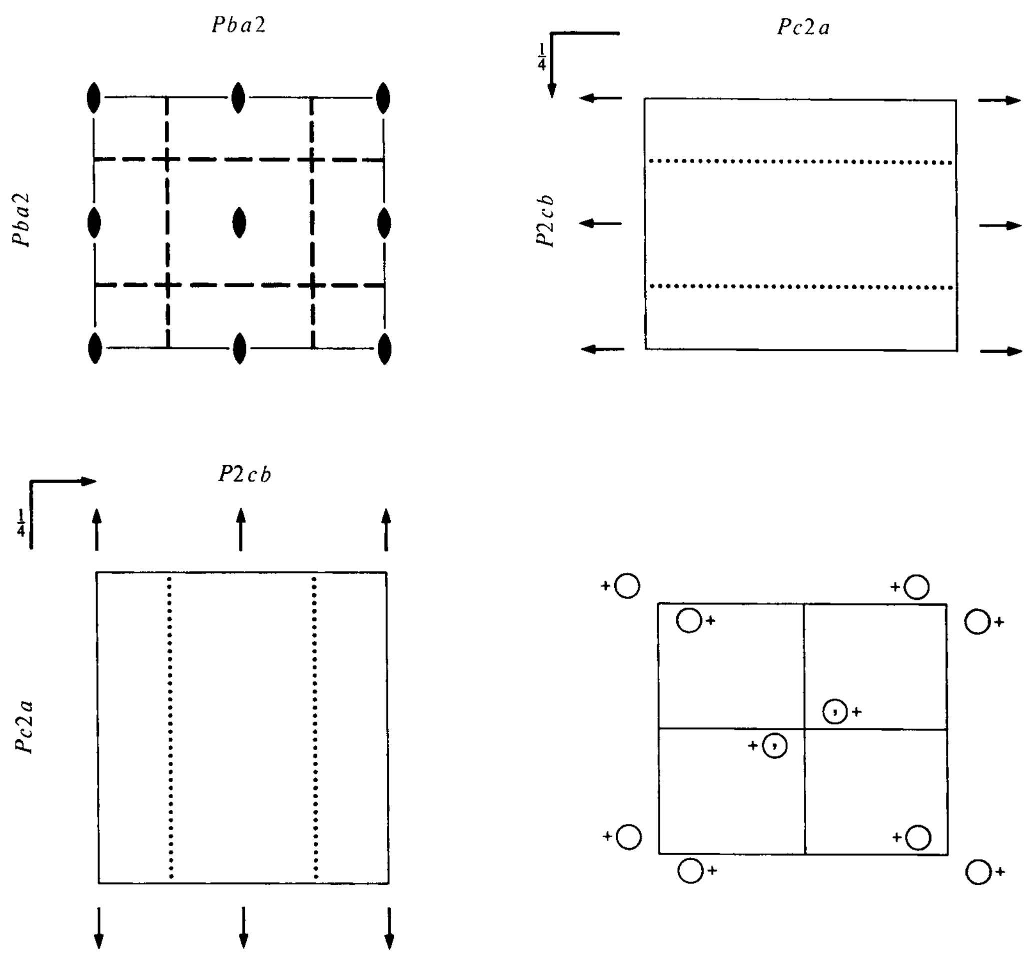
Minimal non-isomorphic supergroups

I [2] $Pmna$ (53); [2] $Pnnm$ (58); [2] $Pmmn$ (59); [2] $Pnma$ (62)

II [2] $Cmc2_1$ (36); [2] $Bmm2$ ($Amm2$, 38); [2] $Ama2$ (40); [2] $Imm2$ (44); [2] $Pmc2_1$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (26); [2] $Pma2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (28)

$Pba2$ $\quad C_{2v}^{8}$ $\quad mm2$ $\quad$ Orthorhombic

No. 32 $\quad Pba2$ $\quad$ Patterson symmetry $Pmmm$



Origin on 1 1 2

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 $\qquad$ (2) 2 $\;0,0,z$ $\qquad$ (3) $a\;\; x,\frac{1}{4},z$ $\qquad$ (4) $b\;\; \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$0kl$: $k=2n$ $h0l$: $h=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
2	b	$..2$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			hkl : $h+k=2n$
2	a	$..2$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1a1$ (Pc, 7) 1; 3
[2] $Pb11$ (Pc, 7) 1; 4
[2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pnn2$ ($\mathbf{c}'=2\mathbf{c}$) (34); [2] $Pna2_1$ ($\mathbf{c}'=2\mathbf{c}$) (33); [2] $Pbn2_1$ ($\mathbf{c}'=2\mathbf{c}$) ($Pna2_1$, 33)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pba2$ ($\mathbf{c}'=2\mathbf{c}$) (32); [3] $Pba2$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (32)

Minimal non-isomorphic supergroups

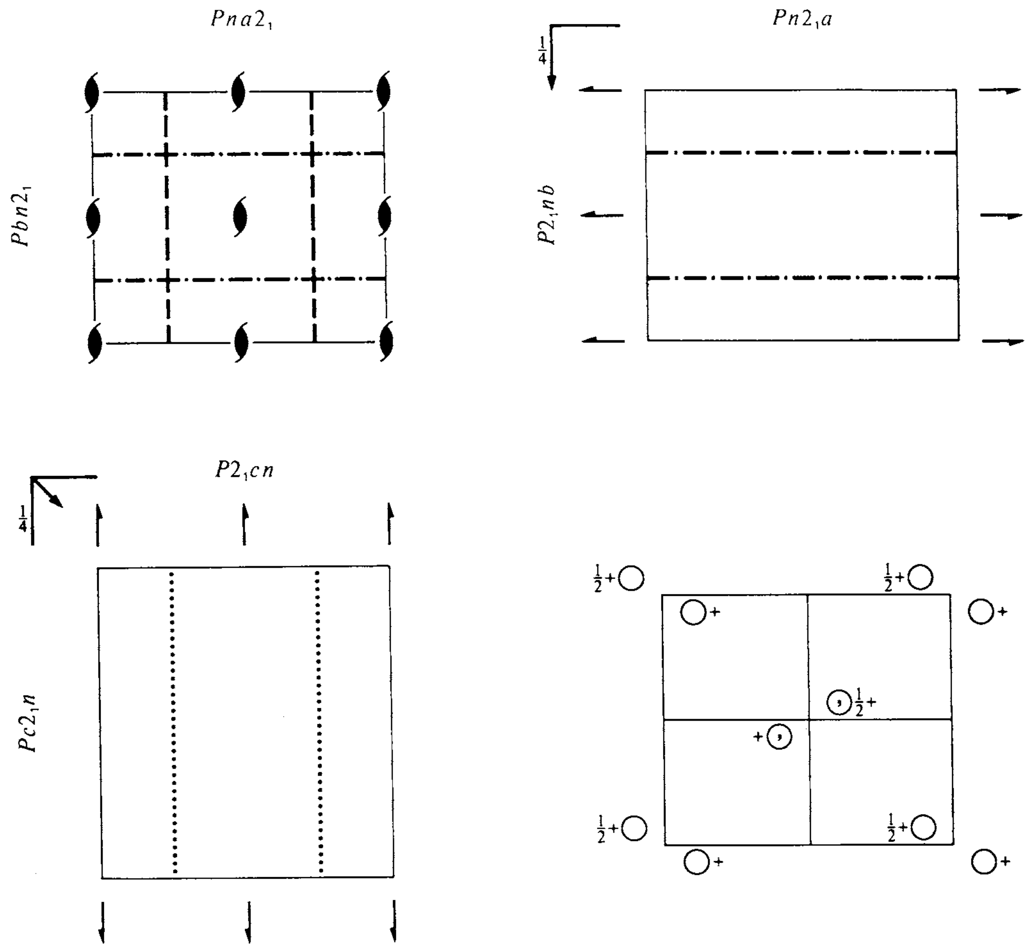
I [2] $Pban$ (50); [2] $Pcca$ (54); [2] $Pbam$ (55); [2] $P4bm$ (100); [2] $P4_2bc$ (106); [2] $P\bar{4}b2$ (117)

II [2] $Cmm2$ (35); [2] $Aea2$ (41); [2] $Bbe2$ ($Aea2$, 41); [2] $Iba2$ (45); [2] $Pbm2$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Pma2$, 28); [2] $Pma2$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (28)

International Tables for Crystallography (2006). Vol. A, Space group 33, pp. 234–235.

$Pna2_1$ C_{2v}^{9} $mm2$ Orthorhombic

No. 33 $Pna2_1$ Patterson symmetry $Pmmm$



Origin on $1\,1\,2_1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) a $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 a 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $h0l$: $h=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [010] $p11g$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1a1$ (Pc, 7) 1; 3
[2] $Pn11$ (Pc, 7) 1; 4
[2] $P112_1$ ($P2_1$, 4) 1; 2

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pna2_1$ ($\mathbf{a}'=3\mathbf{a}$) (33); [3] $Pna2_1$ ($\mathbf{b}'=3\mathbf{b}$) (33); [3] $Pna2_1$ ($\mathbf{c}'=3\mathbf{c}$) (33)

Minimal non-isomorphic supergroups

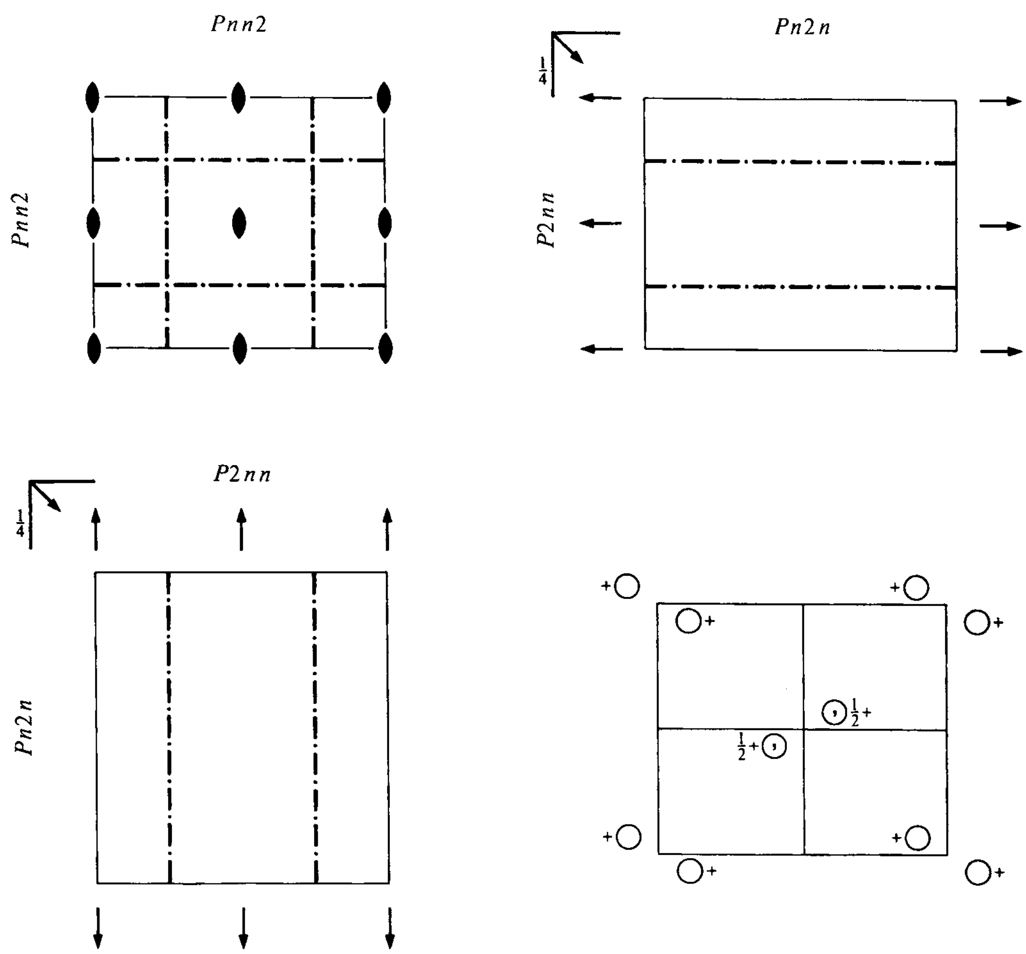
I [2] $Pnna$ (52); [2] $Pccn$ (56); [2] $Pbcn$ (60); [2] $Pnma$ (62)

II [2] $Ccm2_1$ ($Cmc2_1$, 36); [2] $Ama2$ (40); [2] $Bbe2$ ($Aea2$, 41); [2] $Ima2$ (46); [2] $Pca2_1$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (29);
[2] $Pnm2_1$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Pmn2_1$, 31); [2] $Pba2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (32)

International Tables for Crystallography (2006). Vol. A, Space group 34, pp. 236–237.

$Pnn2$ C_{2v}^{10} $mm2$ Orthorhombic

No. 34 $Pnn2$ Patterson symmetry $Pmmm$



Origin on 1 1 2

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	b	$..2$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$			hkl : $h+k+l=2n$
2	a	$..2$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $c11m$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1n1$ (Pc, 7) 1; 3
[2] $Pn11$ (Pc, 7) 1; 4
[2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Fdd2$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (43)

Maximal isomorphic subgroups of lowest index

IIc [3] $Pnn2$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (34); [3] $Pnn2$ ($\mathbf{c}'=3\mathbf{c}$) (34)

Minimal non-isomorphic supergroups

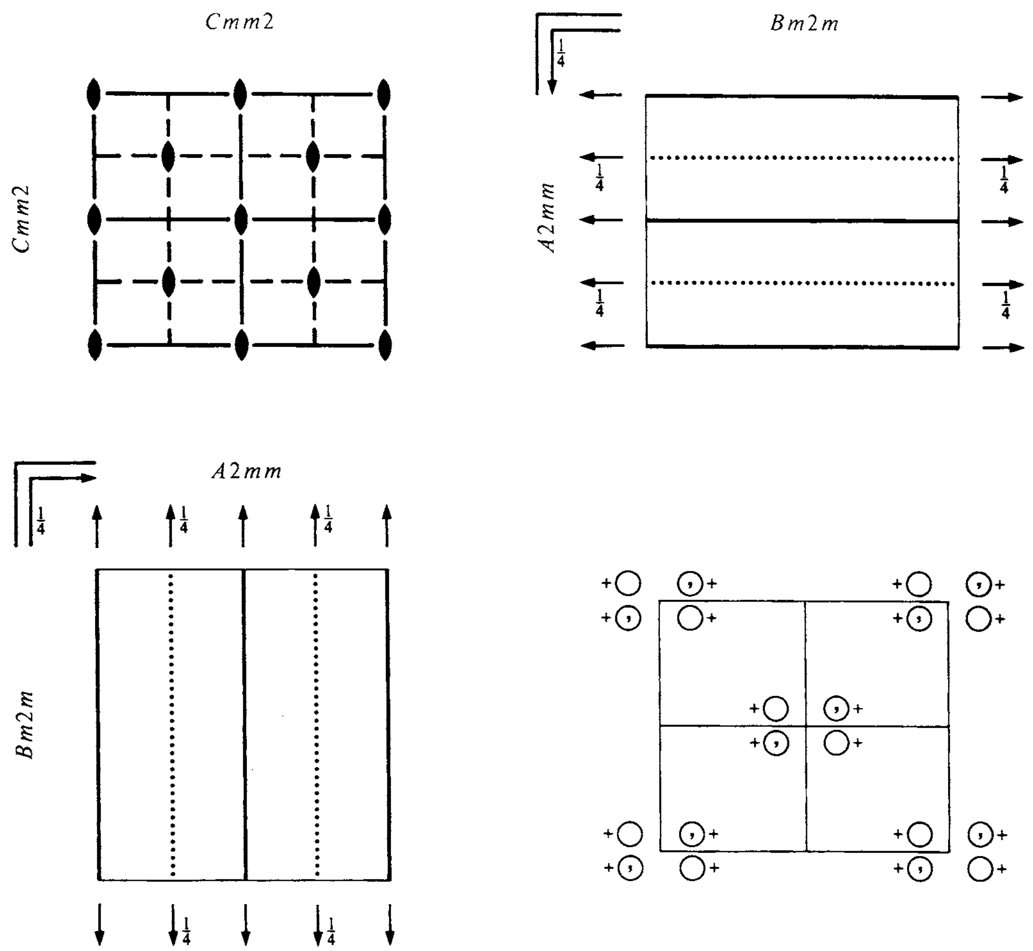
I [2] $Pnnn$ (48); [2] $Pnna$ (52); [2] $Pnnm$ (58); [2] $P4_2nm$ (102); [2] $P4nc$ (104); [2] $P\bar{4}n2$ (118)

II [2] $Ccc2$ (37); [2] $Ama2$ (40); [2] $Bbm2$ ($Ama2$, 40); [2] $Imm2$ (44); [2] $Pnc2$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (30); [2] $Pcn2$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Pnc2$, 30); [2] $Pba2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (32)

International Tables for Crystallography (2006). Vol. A, Space group 35, pp. 238–239.

$Cmm2$ $\qquad$ C_{2v}^{11} $\qquad$ $mm2$ $\qquad$ Orthorhombic

No. 35 $\qquad$ $Cmm2$ $\qquad$ Patterson symmetry $Cmmm$



Origin on $mm2$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2 \quad 0,0,z$	(3) $m \quad x,0,z$	(4) $m \quad 0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2 \quad \frac{1}{4},\frac{1}{4},z$	(3) $a \quad x,\frac{1}{4},z$	(4) $b \quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
8	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	hkl : $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	e	$m\,.\,.$	$0,y,z$	$0,\bar{y},z$			no extra conditions
4	d	$.\,m\,.$	$x,0,z$	$\bar{x},0,z$			no extra conditions
4	c	$.\,.\,2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$			hkl : $h=2n$
2	b	$m\,m\,2$	$0,\frac{1}{2},z$				no extra conditions
2	a	$m\,m\,2$	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}' = \mathbf{c} \quad \mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $C1m1$ (Cm, 8) (1; 3)+
[2] $Cm11$ (Cm, 8) (1; 4)+
[2] $C112$ ($P2$, 3) (1; 2)+

IIa [2] $Pba2$ (32) 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pbm2$ ($Pma2$, 28) 1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pma2$ (28) 1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pmm2$ (25) 1; 2; 3; 4

IIb [2] $Ima2$ ($\mathbf{c}' = 2\mathbf{c}$) (46); [2] $Ibm2$ ($\mathbf{c}' = 2\mathbf{c}$) ($Ima2$, 46); [2] $Iba2$ ($\mathbf{c}' = 2\mathbf{c}$) (45); [2] $Imm2$ ($\mathbf{c}' = 2\mathbf{c}$) (44); [2] $Ccc2$ ($\mathbf{c}' = 2\mathbf{c}$) (37); [2] $Cmc2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (36); [2] $Ccm2_1$ ($\mathbf{c}' = 2\mathbf{c}$) ($Cmc2_1$, 36)

Maximal isomorphic subgroups of lowest index

IIc [2] $Cmm2$ ($\mathbf{c}' = 2\mathbf{c}$) (35); [3] $Cmm2$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (35)

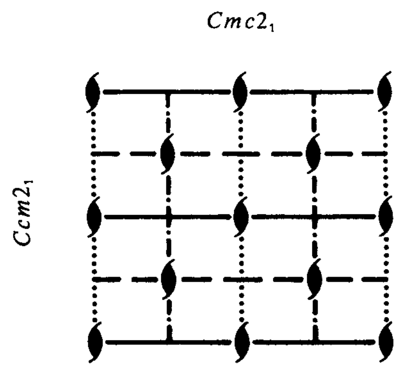
Minimal non-isomorphic supergroups

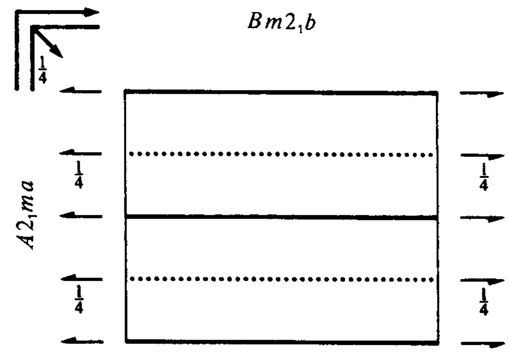
I [2] $Cmmm$ (65); [2] $Cmme$ (67); [2] $P4mm$ (99); [2] $P4bm$ (100); [2] $P4_2cm$ (101); [2] $P4_2nm$ (102); [2] $P\bar{4}2m$ (111); [2] $P\bar{4}2_1m$ (113); [3] $P6mm$ (183)

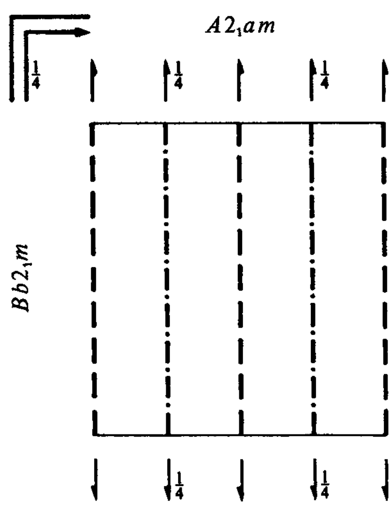
II [2] $Fmm2$ (42); [2] $Pmm2$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) (25)

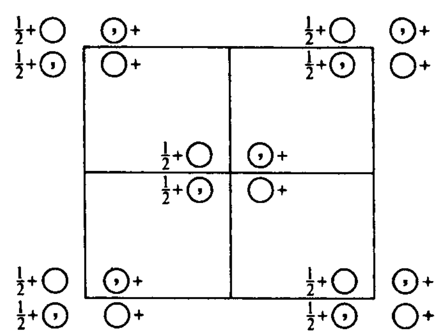
$Cmc2_1$ $\quad$ C_{2v}^{12} $\quad$ $mm2$ $\quad$ Orthorhombic

No. 36 $\quad$ $Cmc2_1$ $\quad$ Patterson symmetry $Cmmm$









Origin on $mc2_1$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 $\quad$ (2) $2(0,0,\frac{1}{2})\ \ 0,0,z$ $\quad$ (3) $c\ \ x,0,z$ $\quad$ (4) $m\ \ 0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ $\quad$ (2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$ $\quad$ (3) $n(\frac{1}{2},0,\frac{1}{2})\ \ x,\frac{1}{4},z$ $\quad$ (4) $b\ \ \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				General:
8	b	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $x,\bar{y},z+\frac{1}{2}$	(4) $\bar{x},y,z$	hkl : $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: no extra conditions
4	a	$m\,.\,.$	$0,y,z$	$0,\bar{y},z+\frac{1}{2}$			

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $C1c1$ (Cc, 9)	(1; 3)+
	[2] $Cm11$ (Cm, 8)	(1; 4)+
	[2] $C112_1$ ($P2_1$, 4)	(1; 2)+
IIa	[2] $Pbn2_1$ ($Pna2_1$, 33)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmn2_1$ (31)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbc2_1$ ($Pca2_1$, 29)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmc2_1$ (26)	1; 2; 3; 4
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Cmc2_1$ ($\mathbf{a}'=3\mathbf{a}$) (36); [3] $Cmc2_1$ ($\mathbf{b}'=3\mathbf{b}$) (36); [3] $Cmc2_1$ ($\mathbf{c}'=3\mathbf{c}$) (36)

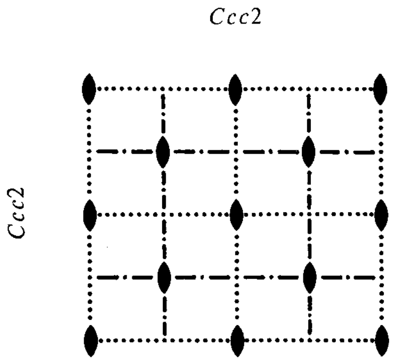
Minimal non-isomorphic supergroups

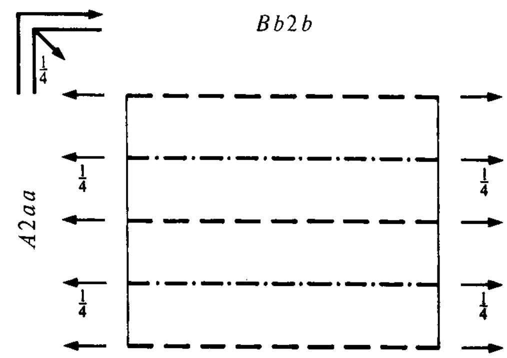
I [2] $Cmcm$ (63); [2] $Cmce$ (64); [3] $P6_3cm$ (185); [3] $P6_3mc$ (186)

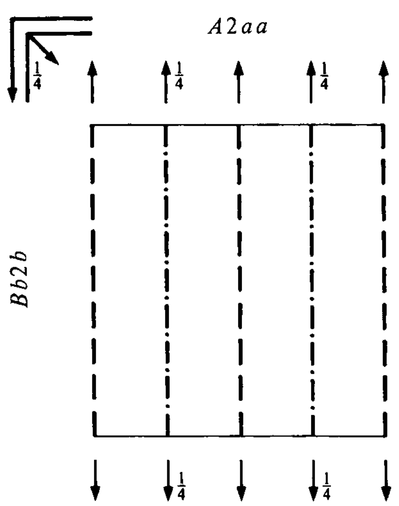
II [2] $Fmm2$ (42); [2] $Pmc2_1$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (26); [2] $Cmm2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (35)

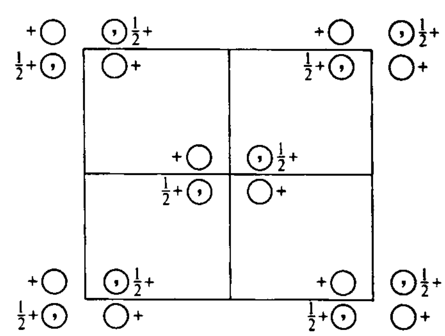
$Ccc2$ $\quad C_{2v}^{13}$ $\quad mm2$ $\quad$ Orthorhombic

No. 37 $\quad Ccc2$ $\quad$ Patterson symmetry $Cmmm$









Origin on $cc2$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $c\quad x,0,z$	(4) $c\quad 0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(4) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				General:
8	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z+\frac{1}{2}$	(4) $\bar{x},y,z+\frac{1}{2}$	hkl : $h+k=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	c	$..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$			hkl : $k+l=2n$
4	b	$..2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$			hkl : $l=2n$
4	a	$..2$	$0,0,z$	$0,0,z+\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $C1c1$ (Cc, 9)	(1; 3)+
	[2] $Cc11$ (Cc, 9)	(1; 4)+
	[2] $C112$ ($P2$, 3)	(1; 2)+
IIa	[2] $Pnn2$ (34)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pnc2$ (30)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pcn2$ ($Pnc2$, 30)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pcc2$ (27)	1; 2; 3; 4
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Ccc2$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (37); [3] $Ccc2$ ($\mathbf{c}'=3\mathbf{c}$) (37)

Minimal non-isomorphic supergroups

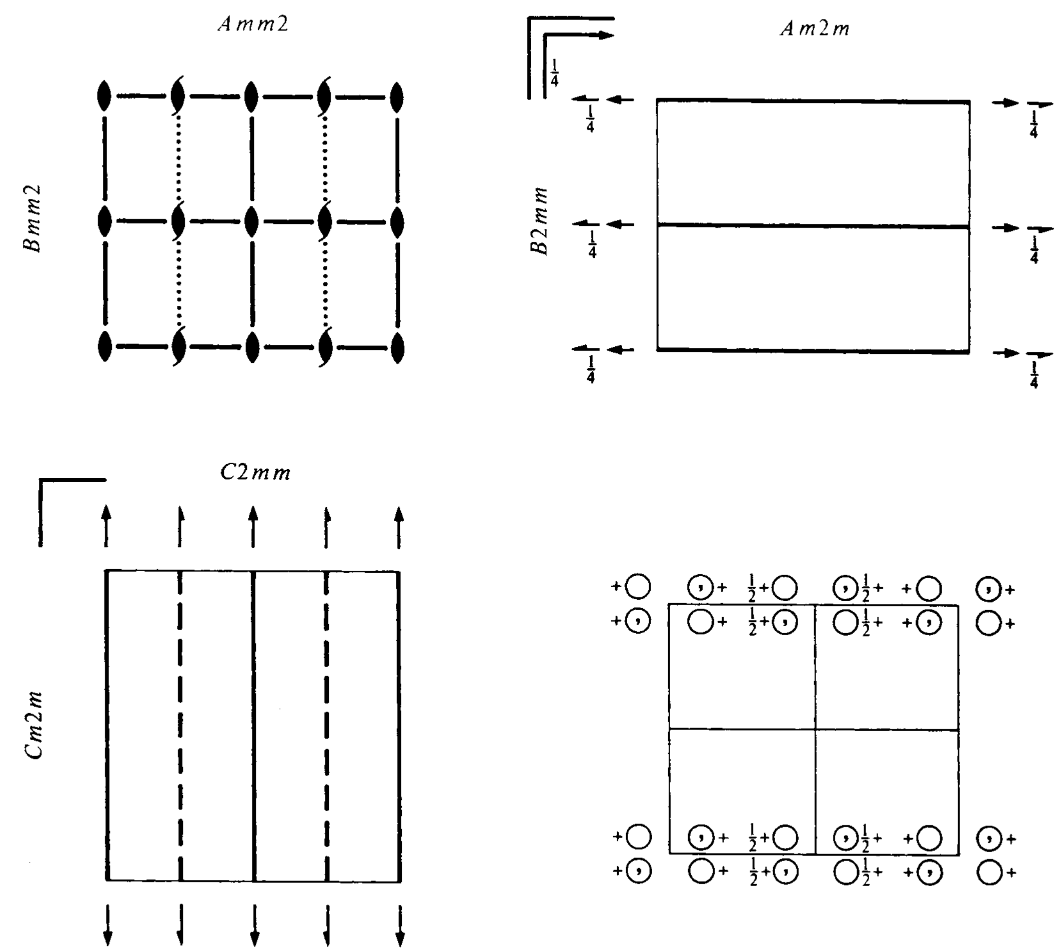
I [2] $Cccm$ (66); [2] $Ccce$ (68); [2] $P4cc$ (103); [2] $P4nc$ (104); [2] $P4_2mc$ (105); [2] $P4_2bc$ (106); [2] $P\bar{4}2c$ (112); [2] $P\bar{4}2_1c$ (114); [3] $P6cc$ (184)

II [2] $Fmm2$ (42); [2] $Pcc2$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (27); [2] $Cmm2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (35)

International Tables for Crystallography (2006). Vol. A, Space group 38, pp. 244–245.

$Amm2$ $\quad C_{2v}^{14}$ $\quad mm2$ $\quad$ Orthorhombic

No. 38 $\quad Amm2$ $\quad$ Patterson symmetry $Ammm$ ($Cmmm$)



Origin on $mm2$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 $\quad$ (2) $2 \quad 0,0,z$ $\quad$ (3) $m \quad x,0,z$ $\quad$ (4) $m \quad 0,y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ $\quad$ (2) $2(0,0,\frac{1}{2}) \quad 0,\frac{1}{4},z$ $\quad$ (3) $c \quad x,\frac{1}{4},z$ $\quad$ (4) $n(0,\frac{1}{2},\frac{1}{2}) \quad 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$				General:
8	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	hkl : $k+l=2n$ $0kl$: $k+l=2n$ $h0l$: $l=2n$ $hk0$: $k=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: no extra conditions
4	e	$m\,.\,.$	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$			
4	d	$m\,.\,.$	$0,y,z$	$0,\bar{y},z$			
4	c	$.\,m\,.$	$x,0,z$	$\bar{x},0,z$			
2	b	$m\,m\,2$	$\frac{1}{2},0,z$				
2	a	$m\,m\,2$	$0,0,z$				

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $A1m1$ (Cm, 8)	(1; 3)+
	[2] $Am11$ (Pm, 6)	(1; 4)+
	[2] $A112$ ($C2$, 5)	(1; 2)+
IIa	[2] $Pnm2_1$ ($Pmn2_1$, 31)	1; 3; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$
	[2] $Pnc2$ (30)	1; 2; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$
	[2] $Pmc2_1$ (26)	1; 4; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$
	[2] $Pmm2$ (25)	1; 2; 3; 4

IIb [2] $Ima2$ ($\mathbf{a}'=2\mathbf{a}$) (46); [2] $Imm2$ ($\mathbf{a}'=2\mathbf{a}$) (44); [2] $Ama2$ ($\mathbf{a}'=2\mathbf{a}$) (40)

Maximal isomorphic subgroups of lowest index

IIc [2] $Amm2$ ($\mathbf{a}'=2\mathbf{a}$) (38); [3] $Amm2$ ($\mathbf{b}'=3\mathbf{b}$) (38); [3] $Amm2$ ($\mathbf{c}'=3\mathbf{c}$) (38)

Minimal non-isomorphic supergroups

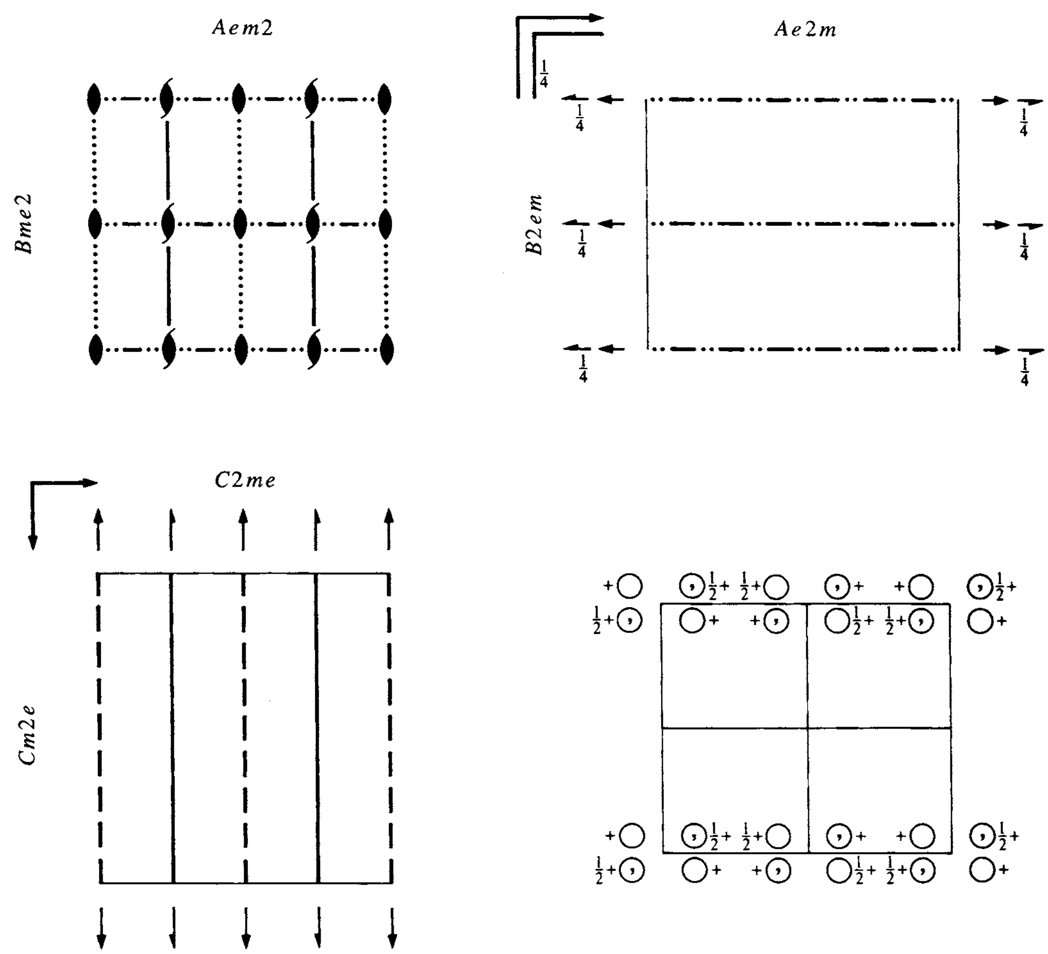
I [2] $Cmcm$ (63); [2] $Cmmm$ (65); [3] $P\bar{6}m2$ (187); [3] $P\bar{6}2m$ (189)

II [2] $Fmm2$ (42); [2] $Pmm2$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (25)

$Aem2$ $\quad C_{2v}^{15}$ $\quad mm2$ $\quad$ Orthorhombic

No. 39 $\quad Aem2$ $\quad$ Patterson symmetry $Ammm$ ($Cmmm$)

Former space-group symbol $Abm2$; *cf.* Chapter 1.3



Origin on $ec2$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2 \quad 0,0,z$	(3) $m \quad x,\frac{1}{4},z$	(4) $b \quad 0,y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2}) \quad 0,\frac{1}{4},z$	(3) $c \quad x,0,z$	(4) $c \quad 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$			General:
8	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y}+\frac{1}{2},z$	(4) $\bar{x},y+\frac{1}{2},z$	$hkl: k+l=2n$ $0kl: k,l=2n$ $h0l: l=2n$ $hk0: k=2n$ $0k0: k=2n$ $00l: l=2n$
							Special: as above, plus
4	c	$.m.$	$x,\frac{1}{4},z$	$\bar{x},\frac{3}{4},z$			no extra conditions
4	b	$..2$	$\frac{1}{2},0,z$	$\frac{1}{2},\frac{1}{2},z$			$hkl: k=2n$
4	a	$..2$	$0,0,z$	$0,\frac{1}{2},z$			$hkl: k=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $A1m1$ (Cm, 8) (1; 3)+
[2] $Ae11$ (Pc, 7) (1; 4)+
[2] $A112$ ($C2$, 5) (1; 2)+

IIa [2] $Pbc2_1$ ($Pca2_1$, 29) 1; 4; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$
[2] $Pbm2$ ($Pma2$, 28) 1; 2; 3; 4
[2] $Pcc2$ (27) 1; 2; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$
[2] $Pcm2_1$ ($Pmc2_1$, 26) 1; 3; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$

IIb [2] $Ibm2$ ($\mathbf{a}'=2\mathbf{a}$) ($Ima2$, 46); [2] $Iba2$ ($\mathbf{a}'=2\mathbf{a}$) (45); [2] $Aea2$ ($\mathbf{a}'=2\mathbf{a}$) (41)

Maximal isomorphic subgroups of lowest index

IIc [2] $Aem2$ ($\mathbf{a}'=2\mathbf{a}$) (39); [3] $Aem2$ ($\mathbf{b}'=3\mathbf{b}$) (39); [3] $Aem2$ ($\mathbf{c}'=3\mathbf{c}$) (39)

Minimal non-isomorphic supergroups

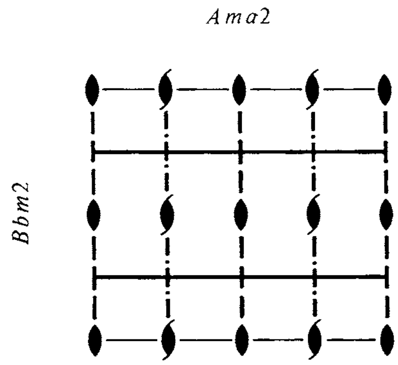
I [2] $Cmce$ (64); [2] $Cmme$ (67)

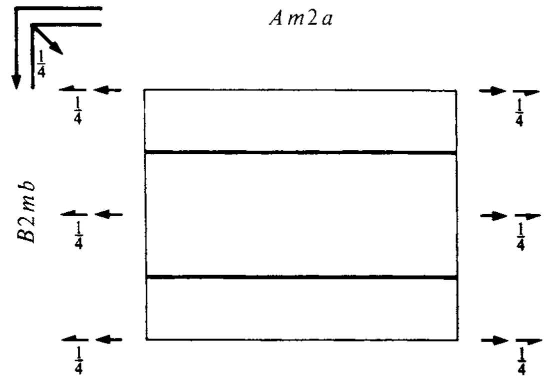
II [2] $Fmm2$ (42); [2] $Pmm2$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (25)

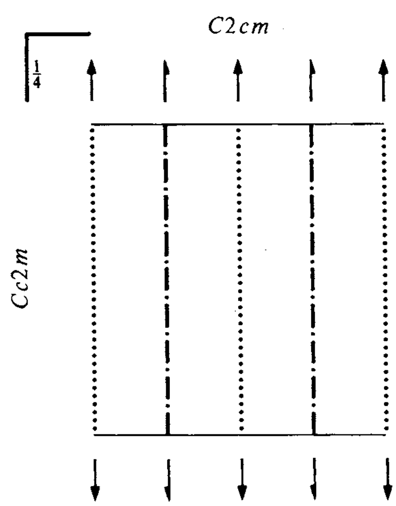
International Tables for Crystallography (2006). Vol. A, Space group 40, pp. 248–249.

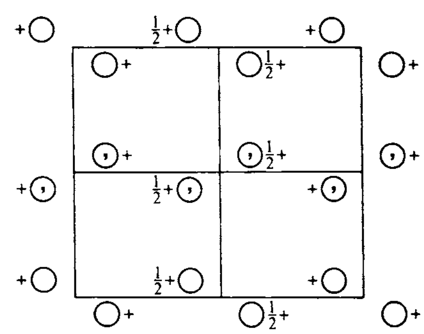
*Ama*2 C_{2v}^{16} *mm*2 Orthorhombic

No. 40 *Ama*2 Patterson symmetry *Ammm* (*Cmmm*)









Origin on 1*a*2

Asymmetric unit $0 \le x \le \frac{1}{4};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) a $x,0,z$	(4) m $\frac{1}{4},y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$	(3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(4) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$				General:
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y},z$	(4) $\bar{x}+\frac{1}{2},y,z$	hkl : $k+l=2n$ $0kl$: $k+l=2n$ $h0l$: $h,l=2n$ $hk0$: $k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	b	$m\,.\,.$	$\frac{1}{4},y,z$	$\frac{3}{4},\bar{y},z$			no extra conditions
4	a	$.\,.\,2$	$0,0,z$	$\frac{1}{2},0,z$			hkl : $h=2n$

Symmetry of special projections

Along [001] $p2mg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $A1a1$ (Cc, 9) (1; 3)+
[2] $Am11$ (Pm, 6) (1; 4)+
[2] $A112$ ($C2$, 5) (1; 2)+

IIa [2] $Pnn2$ (34) 1; 2; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$
[2] $Pna2_1$ (33) 1; 3; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$
[2] $Pmn2_1$ (31) 1; 4; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$
[2] $Pma2$ (28) 1; 2; 3; 4

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Ama2$ ($\mathbf{a}'=3\mathbf{a}$) (40); [3] $Ama2$ ($\mathbf{b}'=3\mathbf{b}$) (40); [3] $Ama2$ ($\mathbf{c}'=3\mathbf{c}$) (40)

Minimal non-isomorphic supergroups

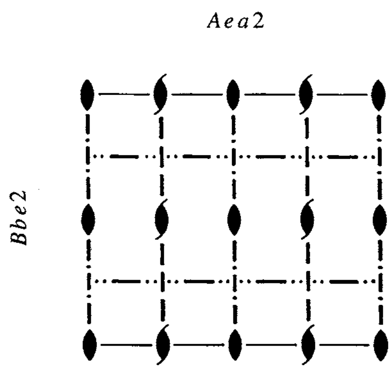
I [2] $Cmcm$ (63); [2] $Cccm$ (66); [3] $P\bar{6}c2$ (188); [3] $P\bar{6}2c$ (190)

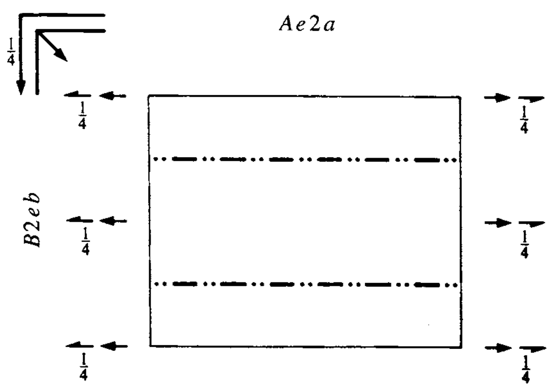
II [2] $Fmm2$ (42); [2] $Pma2$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (28); [2] $Amm2$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (38)

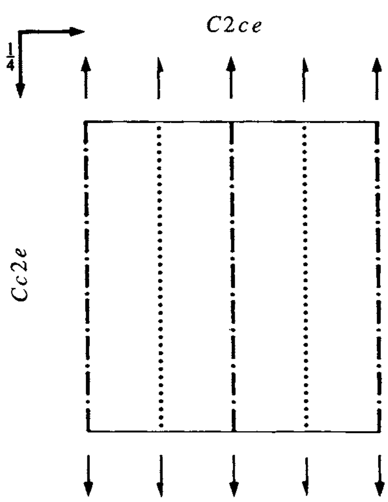
*Aea*2 C_{2v}^{17} *mm*2 Orthorhombic

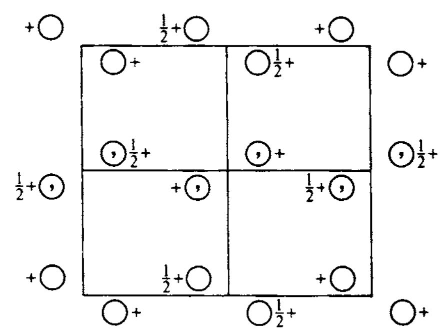
No. 41 *Aea*2 Patterson symmetry *Ammm* (*Cmmm*)

Former space-group symbol *Aba*2; *cf.* Chapter 1.3









Origin on $1n2$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) $2\ \ 0,0,z$ (3) $a\ \ x,\frac{1}{4},z$ (4) $b\ \ \frac{1}{4},y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})\ \ 0,\frac{1}{4},z$ (3) $n(\frac{1}{2},0,\frac{1}{2})\ \ x,0,z$ (4) $c\ \ \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$				General:
8 b 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	hkl : $k+l=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
					Special: as above, plus
4 a ..2	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p2mg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $A1a1$ (Cc, 9)	(1; 3)+
	[2] $Ae11$ (Pc, 7)	(1; 4)+
	[2] $A112$ ($C2$, 5)	(1; 2)+
IIa	[2] $Pbn2_1$ ($Pna2_1$, 33)	1; 4; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$
	[2] $Pba2$ (32)	1; 2; 3; 4
	[2] $Pcn2$ ($Pnc2$, 30)	1; 2; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$
	[2] $Pca2_1$ (29)	1; 3; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Aea2$ ($\mathbf{a}'=3\mathbf{a}$) (41); [3] $Aea2$ ($\mathbf{b}'=3\mathbf{b}$) (41); [3] $Aea2$ ($\mathbf{c}'=3\mathbf{c}$) (41)

Minimal non-isomorphic supergroups

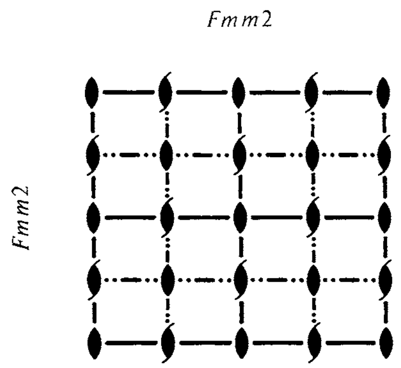
I [2] $Cmce$ (64); [2] $Ccce$ (68)

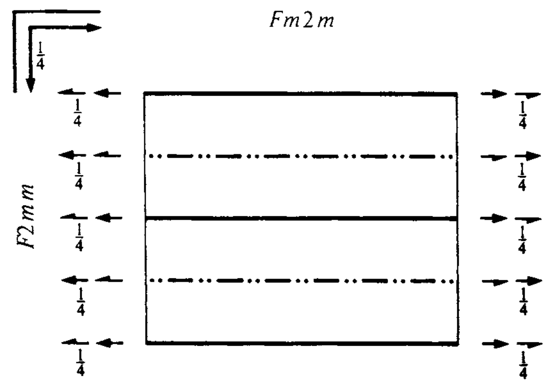
II [2] $Fmm2$ (42); [2] $Pma2$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (28); [2] $Aem2$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (39)

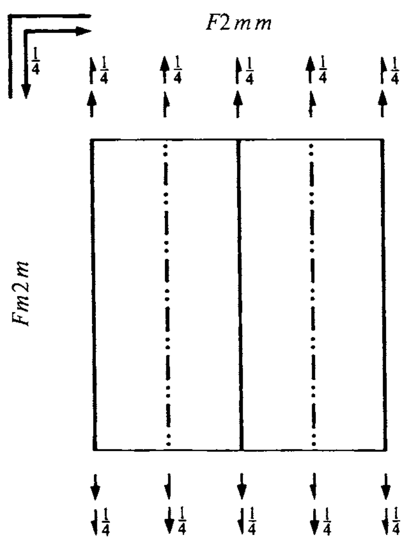
International Tables for Crystallography (2006). Vol. A, Space group 42, pp. 252–253.

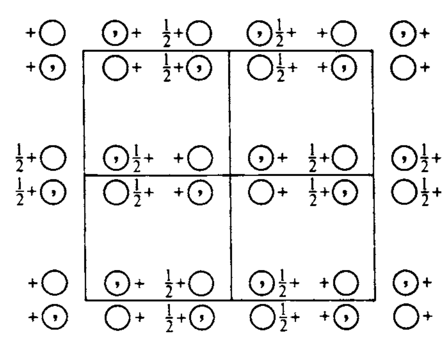
$Fmm2$ C_{2v}^{18} $mm2$ Orthorhombic

No. 42 $Fmm2$ Patterson symmetry $Fmmm$









Origin on $mm2$

Asymmetric unit $0 \le x \le \frac{1}{4};\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $m\quad x,0,z$	(4) $m\quad 0,y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad 0,\frac{1}{4},z$	(3) $c\quad x,\frac{1}{4},z$	(4) $n(0,\frac{1}{2},\frac{1}{2})\quad 0,y,z$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $n(\frac{1}{2},0,\frac{1}{2})\quad x,0,z$	(4) $c\quad \frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $a\quad x,\frac{1}{4},z$	(4) $b\quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	General:
16	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	hkl : $h+k,h+l,k+l=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	d	$.m.$	$x,0,z$	$\bar{x},0,z$			no extra conditions
8	c	$m..$	$0,y,z$	$0,\bar{y},z$			no extra conditions
8	b	$..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$			hkl : $h=2n$
4	a	$mm2$	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $F1m1$ (Cm, 8)	(1; 3)+
	[2] $Fm11$ (Cm, 8)	(1; 4)+
	[2] $F112$ ($C2$, 5)	(1; 2)+
IIa	[2] $Aea2$ (41)	1; 2; (1; 2) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 4) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Bbe2$ ($Aea2$, 41)	1; 2; (1; 2) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Ama2$ (40)	1; 4; (1; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 3) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Bbm2$ ($Ama2$, 40)	1; 3; (1; 3) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Bme2$ ($Aem2$, 39)	1; 4; (1; 4) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Aem2$ (39)	1; 3; (1; 3) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 4) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Amm2$ (38)	1; 2; 3; 4; (1; 2; 3; 4) + $(0,\frac{1}{2},\frac{1}{2})$
	[2] $Bmm2$ ($Amm2$, 38)	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2},0,\frac{1}{2})$
	[2] $Ccc2$ (37)	1; 2; (1; 2) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 4) + $(\frac{1}{2},0,\frac{1}{2})$
	[2] $Ccm2_1$ ($Cmc2_1$, 36)	1; 3; (1; 3) + $(\frac{1}{2},\frac{1}{2},0)$; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 4) + $(\frac{1}{2},0,\frac{1}{2})$
	[2] $Cmc2_1$ (36)	1; 4; (1; 4) + $(\frac{1}{2},\frac{1}{2},0)$; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 3) + $(\frac{1}{2},0,\frac{1}{2})$
	[2] $Cmm2$ (35)	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Fmm2$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (42); [3] $Fmm2$ ($\mathbf{c}'=3\mathbf{c}$) (42)

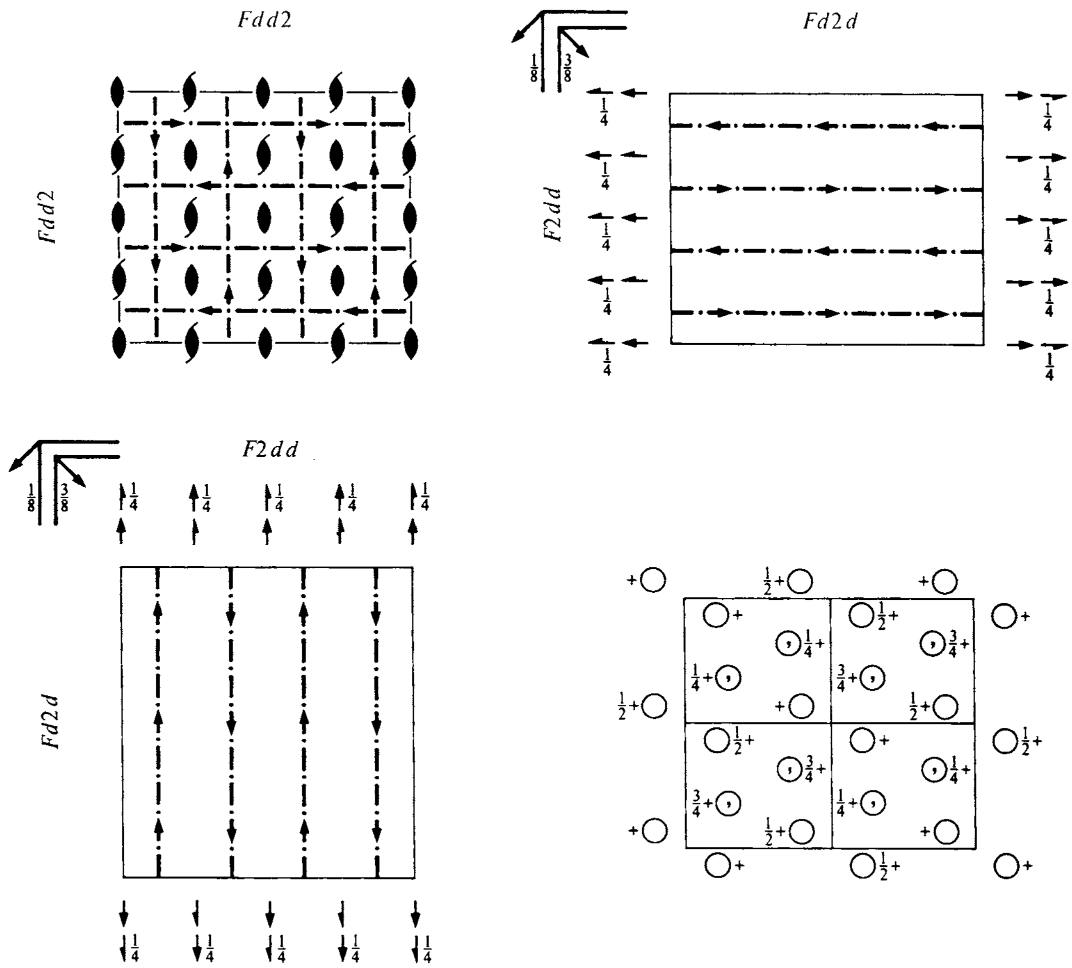
Minimal non-isomorphic supergroups

I [2] $Fmmm$ (69); [2] $I4mm$ (107); [2] $I4cm$ (108); [2] $I\bar{4}2m$ (121)

II [2] $Pmm2$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (25)

$Fdd2$ $\quad C_{2v}^{19}$ $\quad mm2$ $\quad$ Orthorhombic

No. 43 $\quad Fdd2$ $\quad$ Patterson symmetry $Fmmm$



Origin on 1 1 2

Asymmetric unit $\quad 0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2 \quad 0,0,z$	(3) $d(\frac{1}{4},0,\frac{1}{4}) \quad x,\frac{1}{8},z$	(4) $d(0,\frac{1}{4},\frac{1}{4}) \quad \frac{1}{8},y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2}) \quad 0,\frac{1}{4},z$	(3) $d(\frac{1}{4},0,\frac{3}{4}) \quad x,\frac{3}{8},z$	(4) $d(0,\frac{3}{4},\frac{3}{4}) \quad \frac{1}{8},y,z$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4},0,z$	(3) $d(\frac{3}{4},0,\frac{3}{4}) \quad x,\frac{1}{8},z$	(4) $d(0,\frac{1}{4},\frac{3}{4}) \quad \frac{3}{8},y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2 \quad \frac{1}{4},\frac{1}{4},z$	(3) $d(\frac{3}{4},0,\frac{1}{4}) \quad x,\frac{3}{8},z$	(4) $d(0,\frac{3}{4},\frac{1}{4}) \quad \frac{3}{8},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$				General:
16	b	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{4},\bar{y}+\frac{1}{4},z+\frac{1}{4}$	(4) $\bar{x}+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	hkl : $h+k,h+l,k+l=2n$ $0kl$: $k+l=4n,\ k,l=2n$ $h0l$: $h+l=4n,\ h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=4n$ $0k0$: $k=4n$ $00l$: $l=4n$
							Special: as above, plus
8	a	..2	$0,0,z$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{4}$			hkl : $h=2n+1$ or $h+k+l=4n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $c11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $F1d1$ (Cc, 9) (1; 3)+
[2] $Fd11$ (Cc, 9) (1; 4)+
[2] $F112$ ($C2$, 5) (1; 2)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Fdd2$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (43); [3] $Fdd2$ ($\mathbf{c}'=3\mathbf{c}$) (43)

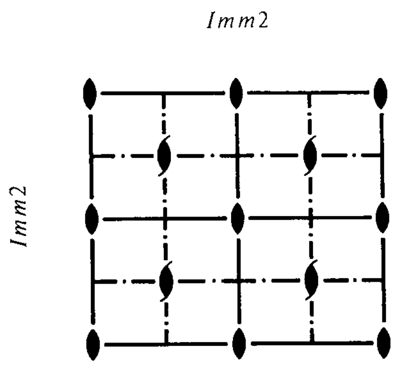
Minimal non-isomorphic supergroups

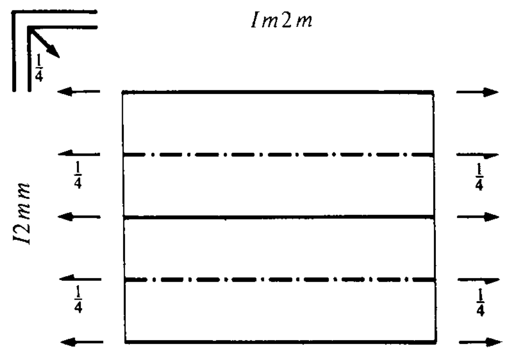
I [2] $Fddd$ (70); [2] $I4_1md$ (109); [2] $I4_1cd$ (110); [2] $I\bar{4}2d$ (122)

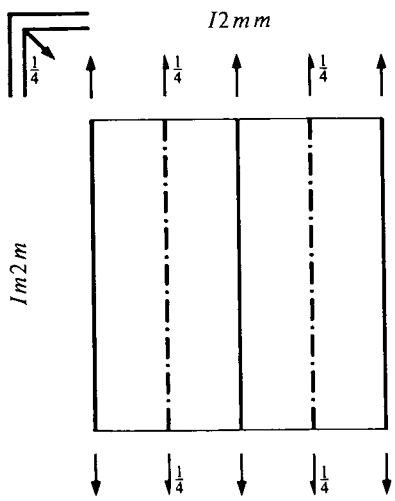
II [2] $Pnn2$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (34)

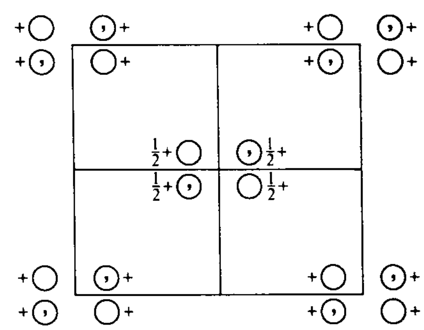
$Imm2$ $\qquad C_{2v}^{20}$ $\qquad mm2$ $\qquad$ Orthorhombic

No. 44 $\qquad Imm2$ $\qquad$ Patterson symmetry $Immm$









Origin on $mm2$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $m\quad x,0,z$	(4) $m\quad 0,y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},\frac{1}{4},z$	(3) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(4) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
8	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	hkl : $h+k+l=2n$ $0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: no extra conditions
4	d	$m\,.\,.$	$0,y,z$	$0,\bar{y},z$			
4	c	$.\,m\,.$	$x,0,z$	$\bar{x},0,z$			
2	b	$m\,m\,2$	$0,\frac{1}{2},z$				
2	a	$m\,m\,2$	$0,0,z$				

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $c11m$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $I1m1$ (Cm, 8) (1; 3)+
[2] $Im11$ (Cm, 8) (1; 4)+
[2] $I112$ ($C2$, 5) (1; 2)+

IIa [2] $Pnn2$ (34) 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $Pnm2_1$ ($Pmn2_1$, 31) 1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $Pmn2_1$ (31) 1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $Pmm2$ (25) 1; 2; 3; 4

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Imm2$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (44); [3] $Imm2$ ($\mathbf{c}'=3\mathbf{c}$) (44)

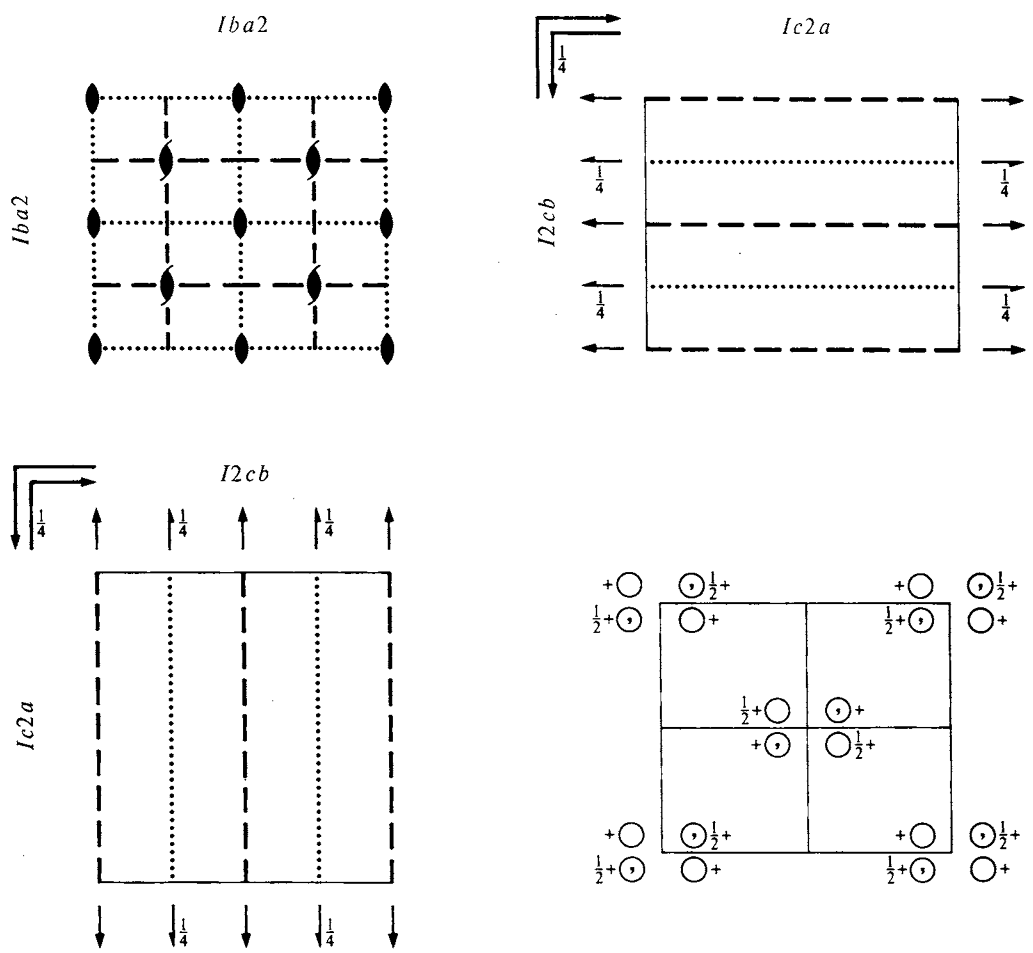
Minimal non-isomorphic supergroups

I [2] $Immm$ (71); [2] $Imma$ (74); [2] $I4mm$ (107); [2] $I4_1md$ (109); [2] $I\bar{4}m2$ (119)

II [2] $Cmm2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (35); [2] $Amm2$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (38); [2] $Bmm2$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Amm2$, 38)

$Iba2$ $\quad$ C_{2v}^{21} $\quad$ $mm2$ $\quad$ Orthorhombic

No. 45 $\quad$ $Iba2$ $\quad$ Patterson symmetry $Immm$



Origin on $cc2$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 $\quad$ (2) $2 \quad 0,0,z$ $\quad$ (3) $a \quad x,\frac{1}{4},z$ $\quad$ (4) $b \quad \frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ $\quad$ (2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4},\frac{1}{4},z$ $\quad$ (3) $c \quad x,0,z$ $\quad$ (4) $c \quad 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	hkl : $h+k+l=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	b	..2	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			hkl : $l=2n$
4	a	..2	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$			hkl : $l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $I1a1$ (Cc, 9)	(1; 3)+
	[2] $Ib11$ (Cc, 9)	(1; 4)+
	[2] $I112$ ($C2$, 5)	(1; 2)+
IIa	[2] $Pba2$ (32)	1; 2; 3; 4
	[2] $Pca2_1$ (29)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pbc2_1$ ($Pca2_1$, 29)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pcc2$ (27)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Iba2$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (45); [3] $Iba2$ ($\mathbf{c}'=3\mathbf{c}$) (45)

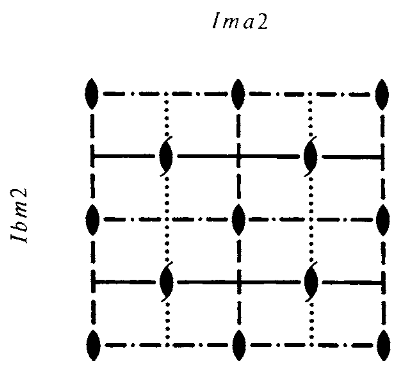
Minimal non-isomorphic supergroups

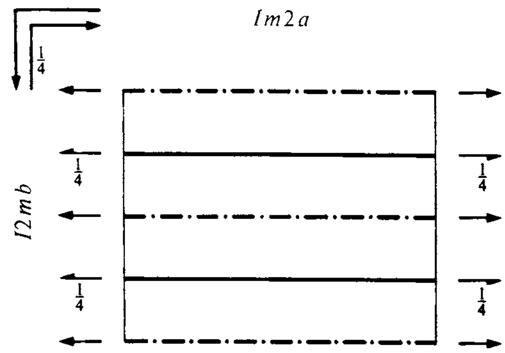
I [2] $Ibam$ (72); [2] $Ibca$ (73); [2] $I4cm$ (108); [2] $I4_1cd$ (110); [2] $I\bar{4}c2$ (120)

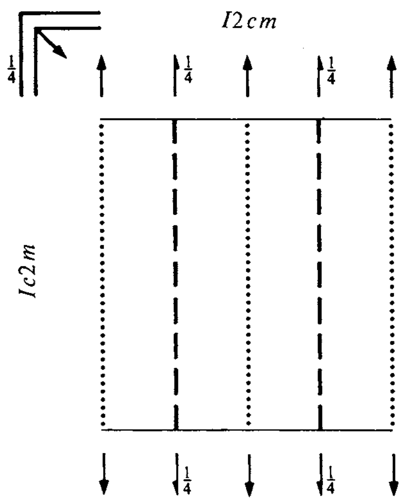
II [2] $Cmm2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (35); [2] $Aem2$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (39); [2] $Bme2$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Aem2$, 39)

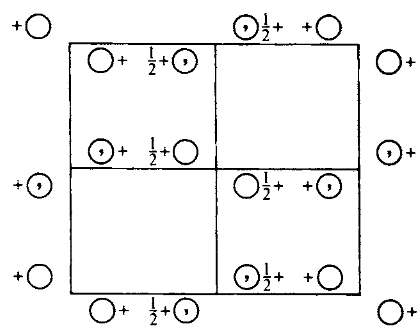
$Ima2$ $\quad C_{2v}^{22}$ $\quad mm2$ $\quad$ Orthorhombic

No. 46 $\quad Ima2$ $\quad$ Patterson symmetry $Immm$









Origin on $na2$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2 \quad 0,0,z$	(3) $a \quad x,0,z$	(4) $m \quad \frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4},\frac{1}{4},z$	(3) $c \quad x,\frac{1}{4},z$	(4) $n(0,\frac{1}{2},\frac{1}{2}) \quad 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			General:
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y},z$	(4) $\bar{x}+\frac{1}{2},y,z$	hkl : $h+k+l=2n$ $0kl$: $k+l=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	b	$m..$	$\frac{1}{4},y,z$	$\frac{3}{4},\bar{y},z$			no extra conditions
4	a	$..2$	$0,0,z$	$\frac{1}{2},0,z$			hkl : $h=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $I1a1$ (Cc, 9) (1; 3)+
[2] $Im11$ (Cm, 8) (1; 4)+
[2] $I112$ ($C2$, 5) (1; 2)+

IIa [2] $Pna2_1$ (33) 1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $Pnc2$ (30) 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $Pma2$ (28) 1; 2; 3; 4
[2] $Pmc2_1$ (26) 1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Ima2$ ($\mathbf{a}'=3\mathbf{a}$) (46); [3] $Ima2$ ($\mathbf{b}'=3\mathbf{b}$) (46); [3] $Ima2$ ($\mathbf{c}'=3\mathbf{c}$) (46)

Minimal non-isomorphic supergroups

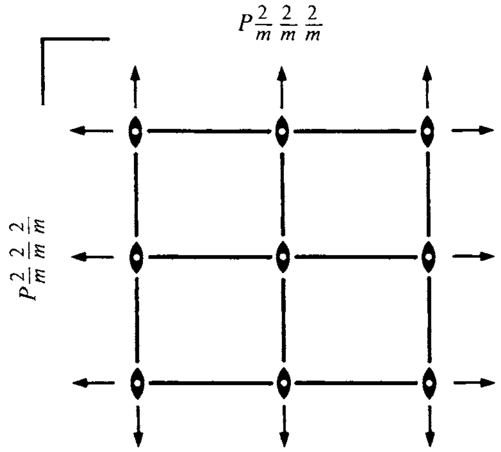
I [2] $Ibam$ (72); [2] $Imma$ (74)

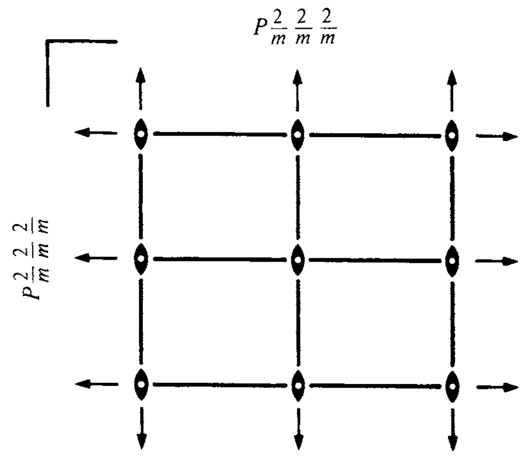
II [2] $Cmm2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (35); [2] $Amm2$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (38); [2] $Bme2$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Aem2$, 39)

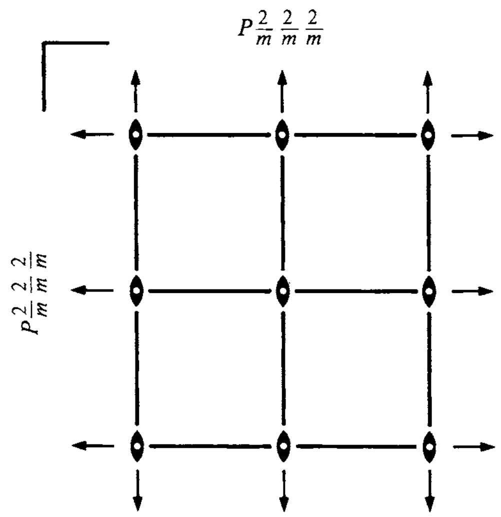
International Tables for Crystallography (2006). Vol. A, Space group 47, pp. 262–263.

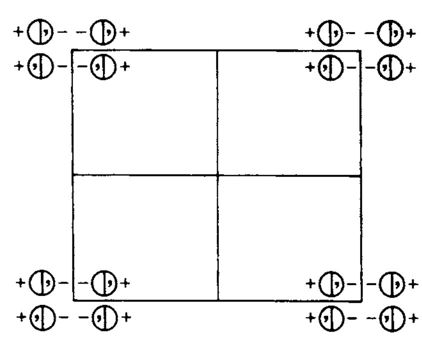
$Pmmm$ $\quad D_{2h}^{1}$ $\quad mmm$ $\quad$ Orthorhombic

No. 47 $\quad P\ 2/m\ 2/m\ 2/m$ $\quad$ Patterson symmetry $Pmmm$









Origin at centre (mmm)

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $\bar{1}\quad 0,0,0$	(6) $m\quad x,y,0$	(7) $m\quad x,0,z$	(8) $m\quad 0,y,z$

Maximal non-isomorphic subgroups *(continued)*

IIa none

IIb [2] $Pmma$ ($\mathbf{a}' = 2\mathbf{a}$) (51); [2] $Pmam$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pmma$, 51); [2] $Pmaa$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pccm$, 49); [2] $Pbmm$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pmma$, 51); [2] $Pmmb$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pmma$, 51); [2] $Pbmb$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pccm$, 49); [2] $Pcmm$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pmma$, 51); [2] $Pmcm$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pmma$, 51); [2] $Pccm$ ($\mathbf{c}' = 2\mathbf{c}$) (49); [2] $Aemm$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($Cmme$, 67); [2] $Ammm$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($Cmmm$, 65); [2] $Bmem$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Cmme$, 67); [2] $Bmmm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($Cmmm$, 65); [2] $Cmme$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (67); [2] $Cmmm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (65); [2] $Fmmm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (69)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmmm$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{c}' = 2\mathbf{c}$) (47)

Minimal non-isomorphic supergroups

I [2] $P4/mmm$ (123); [2] $P4_2/mmc$ (131); [3] $Pm\bar{3}$ (200)

II [2] $Ammm$ ($Cmmm$, 65); [2] $Bmmm$ ($Cmmm$, 65); [2] $Cmmm$ (65); [2] $Immm$ (71)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	α	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}$ (7) $x,\bar{y},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	no conditions
							Special: no extra conditions
4	z	$..m$	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	
4	y	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,0$	$x,\bar{y},0$	
4	x	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\bar{x},\frac{1}{2},\bar{z}$	$x,\frac{1}{2},\bar{z}$	
4	w	$.m.$	$x,0,z$	$\bar{x},0,z$	$\bar{x},0,\bar{z}$	$x,0,\bar{z}$	
4	v	$m..$	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$	$\frac{1}{2},y,\bar{z}$	$\frac{1}{2},\bar{y},\bar{z}$	
4	u	$m..$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	
2	t	$mm2$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			
2	s	$mm2$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$			
2	r	$mm2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			
2	q	$mm2$	$0,0,z$	$0,0,\bar{z}$			

2	p	$m2m$	$\frac{1}{2},y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\frac{1}{2}$	1	h	mmm	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$
2	o	$m2m$	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},0$	1	g	mmm	$0,\frac{1}{2},\frac{1}{2}$
2	n	$m2m$	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$	1	f	mmm	$\frac{1}{2},\frac{1}{2},0$
2	m	$m2m$	$0,y,0$	$0,\bar{y},0$	1	e	mmm	$0,\frac{1}{2},0$
2	l	$2mm$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	1	d	mmm	$\frac{1}{2},0,\frac{1}{2}$
2	k	$2mm$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	1	c	mmm	$0,0,\frac{1}{2}$
2	j	$2mm$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	1	b	mmm	$\frac{1}{2},0,0$
2	i	$2mm$	$x,0,0$	$\bar{x},0,0$	1	a	mmm	$0,0,0$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I
[2] $Pmm2$ (25) 1; 2; 7; 8
[2] $Pm2m$ ($Pmm2$, 25) 1; 3; 6; 8
[2] $P2mm$ ($Pmm2$, 25) 1; 4; 6; 7
[2] $P222$ (16) 1; 2; 3; 4
[2] $P112/m$ ($P2/m$, 10) 1; 2; 5; 6
[2] $P12/m1$ ($P2/m$, 10) 1; 3; 5; 7
[2] $P2/m11$ ($P2/m$, 10) 1; 4; 5; 8

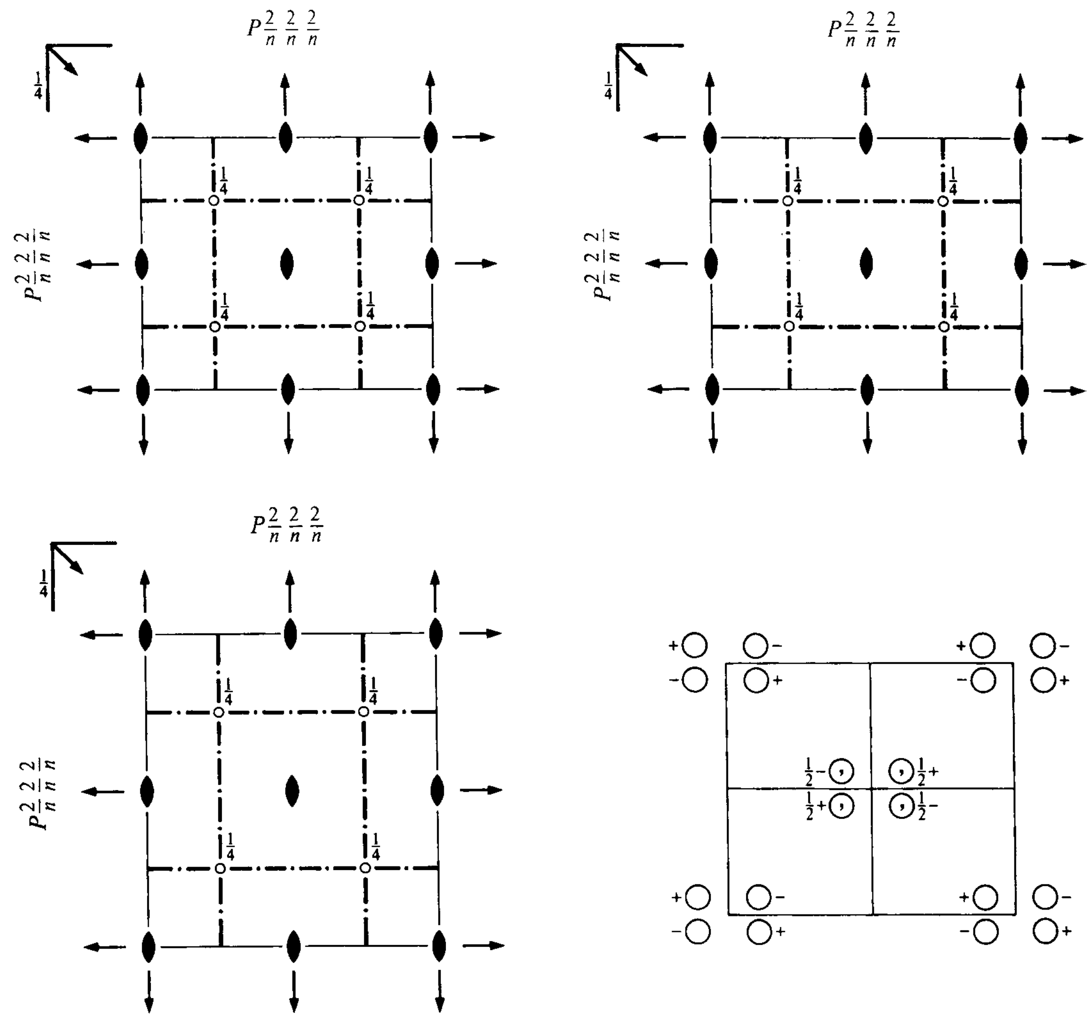
(*Continued on preceding page*)

International Tables for Crystallography (2006). Vol. A, Space group 48, pp. 264–267.

$Pnnn$ $\quad D_{2h}^{2}$ $\quad mmm$ $\quad$ Orthorhombic

No. 48 $\quad P\,2/n\,2/n\,2/n$ $\quad$ Patterson symmetry $Pmmm$

ORIGIN CHOICE 1



Origin at 222, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le 1$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$

Minimal non-isomorphic supergroups

I $\quad$ [2] $P4/nnc$ (126); [2] $P4_2/nnm$ (134); [3] $Pn\bar{3}$ (201)

II $\quad$ [2] $Immm$ (71); [2] $Amaa$ ($Cccm$, 66); [2] $Bbmb$ ($Cccm$, 66); [2] $Cccm$ (66); [2] $Pncb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pban$, 50); [2] $Pcna$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pban$, 50); [2] $Pban$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (50)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*m*	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}$ (7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*l*	. . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	hkl : $h+k+l=2n$
4	*k*	. . 2	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl : $h+k+l=2n$
4	*j*	. 2 .	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},0$	$0,\bar{y}+\frac{1}{2},\frac{1}{2}$	$0,y+\frac{1}{2},\frac{1}{2}$	hkl : $h+k+l=2n$
4	*i*	. 2 .	$0,y,0$	$0,\bar{y},0$	$\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	hkl : $h+k+l=2n$
4	*h*	2 . .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},0$	hkl : $h+k+l=2n$
4	*g*	2 . .	$x,0,0$	$\bar{x},0,0$	$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+k+l=2n$
4	*f*	$\bar{1}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	hkl : $h+k,h+l,k+l=2n$
4	*e*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	hkl : $h+k,h+l,k+l=2n$
2	*d*	2 2 2	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k+l=2n$
2	*c*	2 2 2	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k+l=2n$
2	*b*	2 2 2	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $h+k+l=2n$
2	*a*	2 2 2	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $c2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Pnn2$ (34)	1; 2; 7; 8
	[2] $Pn2n$ ($Pnn2$, 34)	1; 3; 6; 8
	[2] $P2nn$ ($Pnn2$, 34)	1; 4; 6; 7
	[2] $P222$ (16)	1; 2; 3; 4
	[2] $P112/n$ ($P2/c$, 13)	1; 2; 5; 6
	[2] $P12/n1$ ($P2/c$, 13)	1; 3; 5; 7
	[2] $P2/n11$ ($P2/c$, 13)	1; 4; 5; 8

IIa none

IIb [2] $Fddd$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (70)

Maximal isomorphic subgroups of lowest index

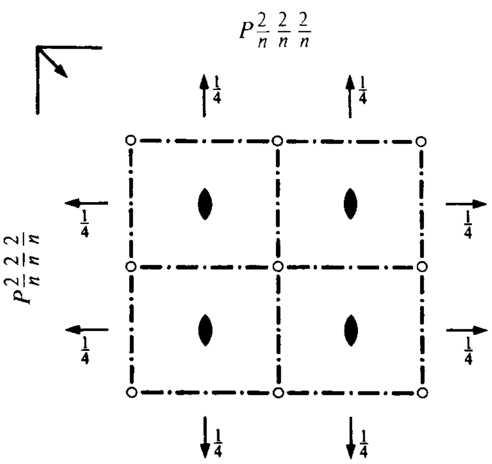
IIc [3] $Pnnn$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$ or $\mathbf{c}'=3\mathbf{c}$) (48)

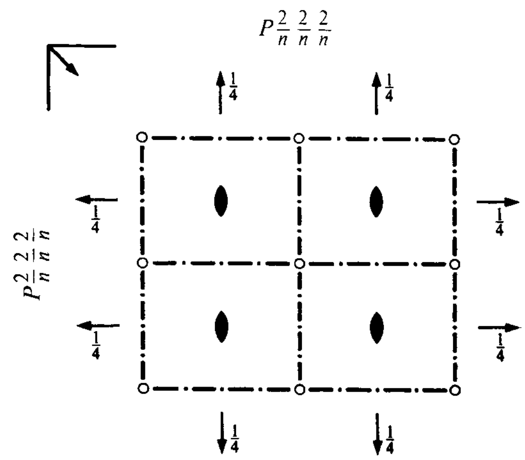
(*Continued on preceding page*)

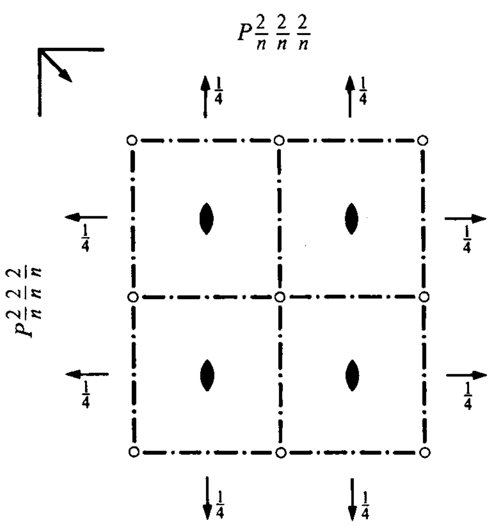
Pnnn D_{2h}^{2} *mmm* Orthorhombic

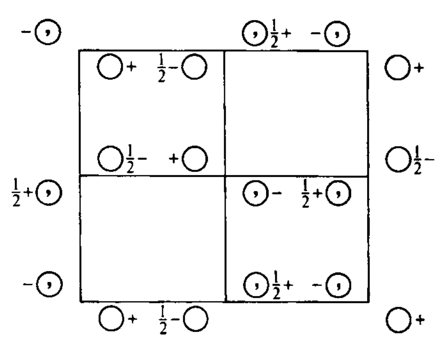
No. 48 $P\ 2/n\ 2/n\ 2/n$ Patterson symmetry *Pmmm*

ORIGIN CHOICE 2









Origin at $\bar{1}$ at nnn, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from 222

Asymmetric unit $0 \le x \le \frac{1}{4}$; $-\frac{1}{4} \le y \le \frac{1}{4}$; $0 \le z \le 1$

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) 2 $\frac{1}{4},y,\frac{1}{4}$	(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ 0,0,0	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$

Maximal isomorphic subgroups of lowest index

IIc [3] *Pnnn* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (48)

Minimal non-isomorphic supergroups

I [2] $P4/nnc$ (126); [2] $P4_2/nnm$ (134); [3] $Pn\bar{3}$ (201)

II [2] *Immm* (71); [2] *Amaa* (*Cccm*, 66); [2] *Bbmb* (*Cccm*, 66); [2] *Cccm* (66); [2] *Pncb* ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (*Pban*, 50); [2] *Pcna* ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (*Pban*, 50); [2] *Pban* ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (50)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	m	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$ (7) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	l	..2	$\frac{1}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},z+\frac{1}{2}$	hkl : $h+k+l=2n$
4	k	..2	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},z+\frac{1}{2}$	hkl : $h+k+l=2n$
4	j	.2.	$\frac{3}{4},y,\frac{1}{4}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\bar{y},\frac{3}{4}$	$\frac{1}{4},y+\frac{1}{2},\frac{3}{4}$	hkl : $h+k+l=2n$
4	i	.2.	$\frac{1}{4},y,\frac{1}{4}$	$\frac{1}{4},\bar{y}+\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},\bar{y},\frac{3}{4}$	$\frac{3}{4},y+\frac{1}{2},\frac{3}{4}$	hkl : $h+k+l=2n$
4	h	2..	$x,\frac{1}{4},\frac{3}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	hkl : $h+k+l=2n$
4	g	2..	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$	hkl : $h+k+l=2n$
4	f	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl : $h+k,h+l,k+l=2n$
4	e	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	hkl : $h+k,h+l,k+l=2n$
2	d	222	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$			hkl : $h+k+l=2n$
2	c	222	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$			hkl : $h+k+l=2n$
2	b	222	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$			hkl : $h+k+l=2n$
2	a	222	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [010] $c2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $\frac{1}{4},y,\frac{1}{4}$

Maximal non-isomorphic subgroups

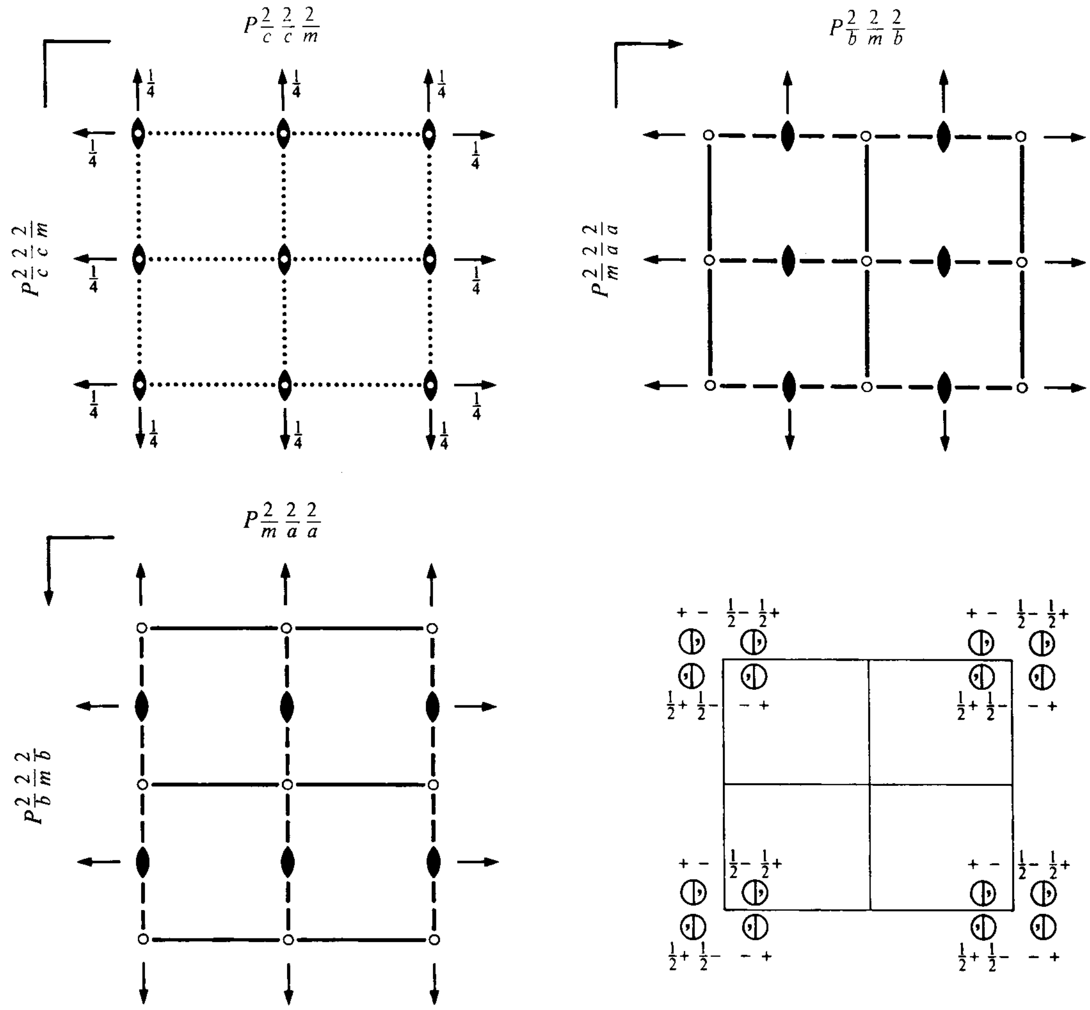
I	[2] $Pnn2$ (34)	1; 2; 7; 8
	[2] $Pn2n$ ($Pnn2$, 34)	1; 3; 6; 8
	[2] $P2nn$ ($Pnn2$, 34)	1; 4; 6; 7
	[2] $P222$ (16)	1; 2; 3; 4
	[2] $P112/n$ ($P2/c$, 13)	1; 2; 5; 6
	[2] $P12/n1$ ($P2/c$, 13)	1; 3; 5; 7
	[2] $P2/n11$ ($P2/c$, 13)	1; 4; 5; 8
IIa	none	
IIb	[2] $Fddd$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (70)	

(*Continued on preceding page*)

International Tables for Crystallography (2006). Vol. A, Space group 49, pp. 268–269.

$Pccm$ $\quad D_{2h}^{3}$ $\quad mmm$ $\quad$ Orthorhombic

No. 49 $\quad P\ 2/c\ 2/c\ 2/m$ $\quad$ Patterson symmetry $Pmmm$



Origin at centre $(2/m)$ at $cc2/m$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,\frac{1}{4}$	(4) $2\quad x,0,\frac{1}{4}$
(5) $\bar{1}\quad 0,0,0$	(6) $m\quad x,y,0$	(7) $c\quad x,0,z$	(8) $c\quad 0,y,z$

Maximal non-isomorphic subgroups *(continued)*

IIa none

IIb [2] $Pcca$ ($\mathbf{a}' = 2\mathbf{a}$) (54); [2] $Pcnm$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pmna$, 53); [2] $Pcna$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pban$, 50); [2] $Pccb$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pcca$, 54); [2] $Pncm$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pmna$, 53); [2] $Pncb$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pban$, 50); [2] $Ccce$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (68); [2] $Cccm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (66)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pccm$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$) (49); [3] $Pccm$ ($\mathbf{c}' = 3\mathbf{c}$) (49)

Minimal non-isomorphic supergroups

I [2] $P4/mcc$ (124); [2] $P4_2/mcm$ (132)

II [2] $Cccm$ (66); [2] $Aemm$ ($Cmme$, 67); [2] $Bmem$ ($Cmme$, 67); [2] $Ibam$ (72); [2] $Pmmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (47)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*r*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}+\frac{1}{2}$ (8) $\bar{x},y,z+\frac{1}{2}$	$0kl$: $l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*q*	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditions
4	*p*	$..2$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z+\frac{1}{2}$	hkl : $l=2n$
4	*o*	$..2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl : $l=2n$
4	*n*	$..2$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl : $l=2n$
4	*m*	$..2$	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl : $l=2n$
4	*l*	$.2.$	$\frac{1}{2},y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{3}{4}$	$\frac{1}{2},y,\frac{3}{4}$	hkl : $l=2n$
4	*k*	$.2.$	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	hkl : $l=2n$
4	*j*	$2..$	$x,\frac{1}{2},\frac{1}{4}$	$\bar{x},\frac{1}{2},\frac{1}{4}$	$\bar{x},\frac{1}{2},\frac{3}{4}$	$x,\frac{1}{2},\frac{3}{4}$	hkl : $l=2n$
4	*i*	$2..$	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	hkl : $l=2n$
2	*h*	222	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl : $l=2n$
2	*g*	222	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl : $l=2n$
2	*f*	222	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$			hkl : $l=2n$
2	*e*	222	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl : $l=2n$
2	*d*	$..2/m$	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $l=2n$
2	*c*	$..2/m$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
2	*b*	$..2/m$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
2	*a*	$..2/m$	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $Pc2m$ ($Pma2$, 28) 1; 3; 6; 8
[2] $P2cm$ ($Pma2$, 28) 1; 4; 6; 7
[2] $Pcc2$ (27) 1; 2; 7; 8
[2] $P222$ (16) 1; 2; 3; 4
[2] $P12/c1$ ($P2/c$, 13) 1; 3; 5; 7
[2] $P2/c11$ ($P2/c$, 13) 1; 4; 5; 8
[2] $P112/m$ ($P2/m$, 10) 1; 2; 5; 6

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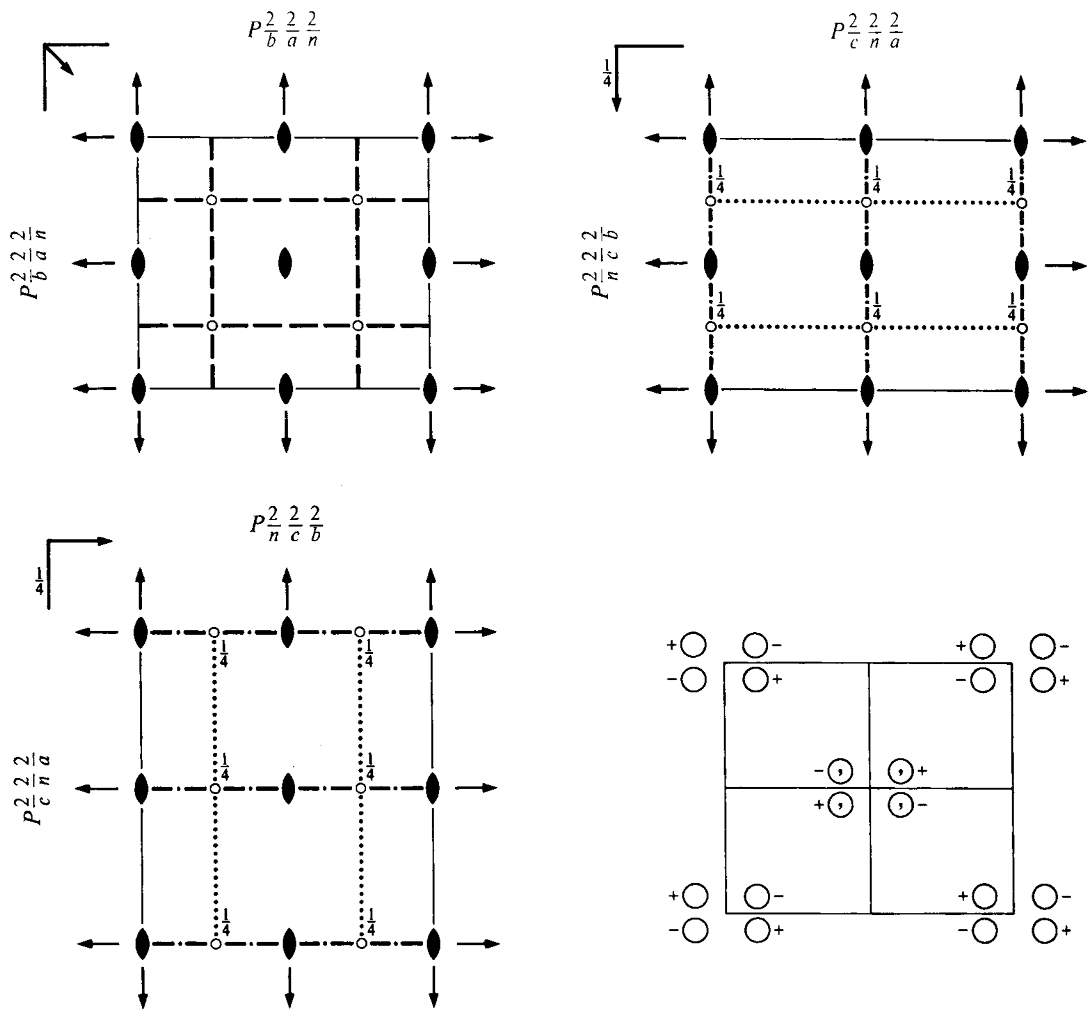
International Tables for Crystallography (2006). Vol. A, Space group 50, pp. 270–273.

$Pban$ $\quad D_{2h}^4$ $\quad mmm$ $\quad$ Orthorhombic

No. 50 $\quad P\ 2/b\ 2/a\ 2/n$ $\quad$ Patterson symmetry $Pmmm$

ORIGIN CHOICE 1



Origin at $222/n$, at $\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},0$	(6) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,0$	(7) $a\quad x,\frac{1}{4},z$	(8) $b\quad \frac{1}{4},y,z$

Minimal non-isomorphic supergroups

I $\quad$ [2] $P4/nbm$ (125); [2] $P4_2/nbc$ (133)

II $\quad$ [2] $Cmmm$ (65); [2] $Aeaa$ ($Ccce$, 68); [2] $Bbeb$ ($Ccce$, 68); [2] $Ibam$ (72); [2] $Pbmb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pccm$, 49); [2] $Pmaa$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pccm$, 49)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	m	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x},y,\bar{z}$ (7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	l	..2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z$	hkl : $h+k=2n$
4	k	..2	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl : $h+k=2n$
4	j	.2.	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	hkl : $h+k=2n$
4	i	.2.	$0,y,0$	$0,\bar{y},0$	$\frac{1}{2},\bar{y}+\frac{1}{2},0$	$\frac{1}{2},y+\frac{1}{2},0$	hkl : $h+k=2n$
4	h	2..	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+k=2n$
4	g	2..	$x,0,0$	$\bar{x},0,0$	$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},0$	hkl : $h+k=2n$
4	f	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	hkl : $h,k=2n$
4	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$	hkl : $h,k=2n$
2	d	222	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	c	222	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	b	222	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			hkl : $h+k=2n$
2	a	222	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Pba2$ (32)	1; 2; 7; 8
	[2] $Pb2n$ ($Pnc2$, 30)	1; 3; 6; 8
	[2] $P2an$ ($Pnc2$, 30)	1; 4; 6; 7
	[2] $P222$ (16)	1; 2; 3; 4
	[2] $P112/n$ ($P2/c$, 13)	1; 2; 5; 6
	[2] $P12/a1$ ($P2/c$, 13)	1; 3; 5; 7
	[2] $P2/b11$ ($P2/c$, 13)	1; 4; 5; 8

IIa none

IIb [2] $Pnan$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnna$, 52); [2] $Pbnn$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnna$, 52); [2] $Pnnn$ ($\mathbf{c}'=2\mathbf{c}$) (48)

Maximal isomorphic subgroups of lowest index

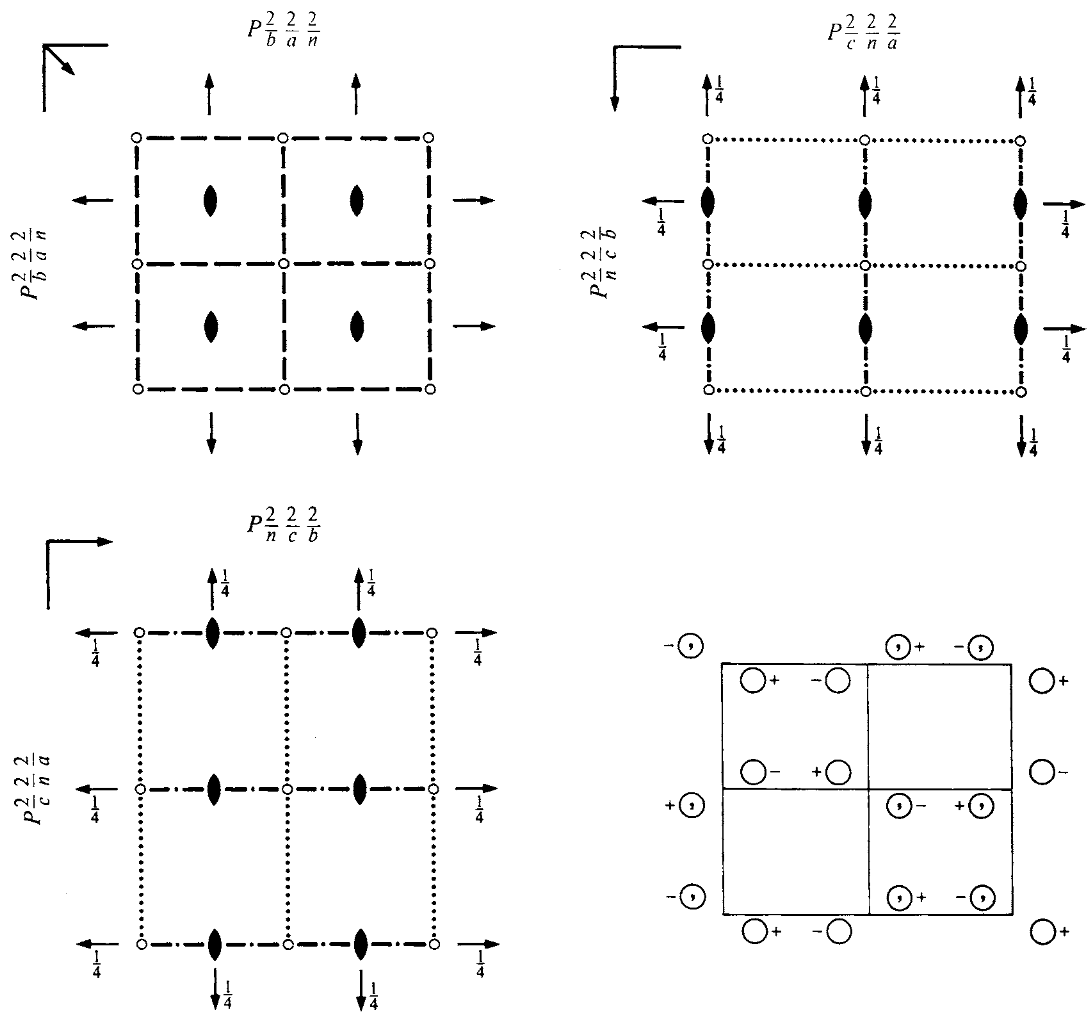
IIc [2] $Pban$ ($\mathbf{c}'=2\mathbf{c}$) (50); [3] $Pban$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (50)

(*Continued on preceding page*)

$Pban$ D_{2h}^{4} mmm Orthorhombic

No. 50 $P\ 2/b\ 2/a\ 2/n$ Patterson symmetry $Pmmm$

ORIGIN CHOICE 2



Origin at $\bar{1}$ at ban, at $-\frac{1}{4},-\frac{1}{4},0$ from 222

Asymmetric unit $\quad 0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) 2 $\frac{1}{4},y,0$	(4) 2 $x,\frac{1}{4},0$
(5) $\bar{1}$ $0,0,0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(7) a $x,0,z$	(8) b $0,y,z$

Minimal non-isomorphic supergroups

I [2] $P4/nbm$ (125); [2] $P4_2/nbc$ (133)

II [2] $Cmmm$ (65); [2] $Aeaa$ ($Ccce$, 68); [2] $Bbeb$ ($Ccce$, 68); [2] $Ibam$ (72); [2] $Pbmb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pccm$, 49); [2] $Pmaa$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pccm$, 49)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	m	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}$ (7) $x+\frac{1}{2},\bar{y},z$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x},y+\frac{1}{2},z$	$0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	l	..2	$\frac{1}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},z$	hkl : $h+k=2n$
4	k	..2	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},z$	hkl : $h+k=2n$
4	j	.2.	$\frac{1}{4},y,\frac{1}{2}$	$\frac{1}{4},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\frac{3}{4},\bar{y},\frac{1}{2}$	$\frac{3}{4},y+\frac{1}{2},\frac{1}{2}$	hkl : $h+k=2n$
4	i	.2.	$\frac{1}{4},y,0$	$\frac{1}{4},\bar{y}+\frac{1}{2},0$	$\frac{3}{4},\bar{y},0$	$\frac{3}{4},y+\frac{1}{2},0$	hkl : $h+k=2n$
4	h	2..	$x,\frac{1}{4},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{2}$	$\bar{x},\frac{3}{4},\frac{1}{2}$	$x+\frac{1}{2},\frac{3}{4},\frac{1}{2}$	hkl : $h+k=2n$
4	g	2..	$x,\frac{1}{4},0$	$\bar{x}+\frac{1}{2},\frac{1}{4},0$	$\bar{x},\frac{3}{4},0$	$x+\frac{1}{2},\frac{3}{4},0$	hkl : $h+k=2n$
4	f	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl : $h,k=2n$
4	e	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hkl : $h,k=2n$
2	d	222	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			hkl : $h+k=2n$
2	c	222	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$			hkl : $h+k=2n$
2	b	222	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$			hkl : $h+k=2n$
2	a	222	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $Pba2$ (32) 1; 2; 7; 8
[2] $Pb2n$ ($Pnc2$, 30) 1; 3; 6; 8
[2] $P2an$ ($Pnc2$, 30) 1; 4; 6; 7
[2] $P222$ (16) 1; 2; 3; 4
[2] $P112/n$ ($P2/c$, 13) 1; 2; 5; 6
[2] $P12/a1$ ($P2/c$, 13) 1; 3; 5; 7
[2] $P2/b11$ ($P2/c$, 13) 1; 4; 5; 8

IIa none

IIb [2] $Pnan$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnna$, 52); [2] $Pbnn$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnna$, 52); [2] $Pnnn$ ($\mathbf{c}'=2\mathbf{c}$) (48)

Maximal isomorphic subgroups of lowest index

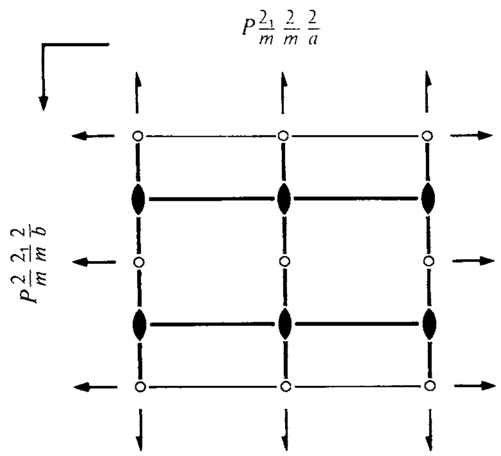
IIc [2] $Pban$ ($\mathbf{c}'=2\mathbf{c}$) (50); [3] $Pban$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (50)

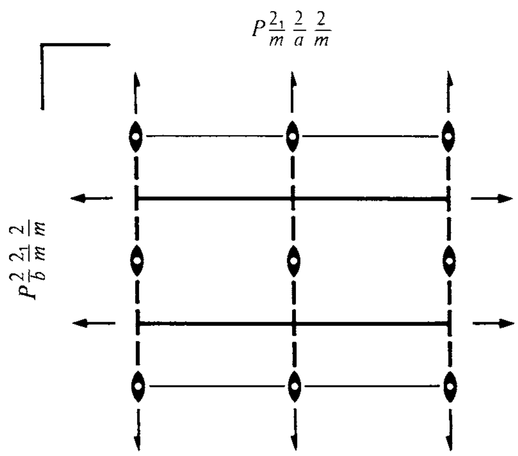
(*Continued on preceding page*)

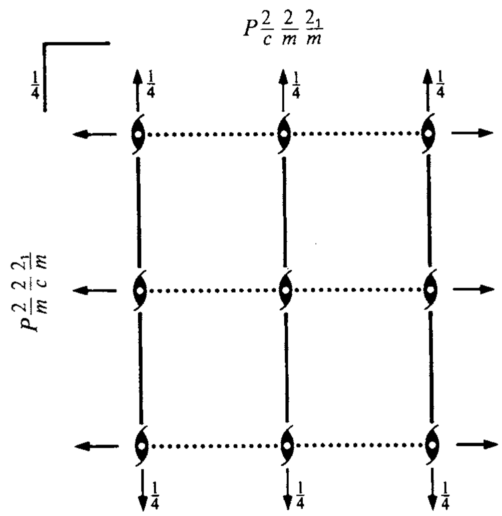
International Tables for Crystallography (2006). Vol. A, Space group 51, pp. 274–275.

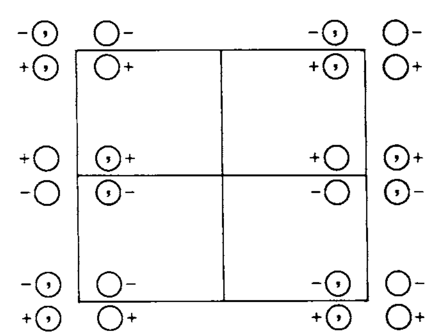
$Pmma$ $\quad D_{2h}^{5}$ $\quad mmm$ $\quad$ Orthorhombic

No. 51 $\quad P\ 2_1/m\ 2/m\ 2/a$ $\quad$ Patterson symmetry $Pmmm$









Origin at centre $(2/m)$ at $2_1 2/ma$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le 1$

Symmetry operations

(1) 1	(2) $2\quad \frac{1}{4},0,z$	(3) $2\quad 0,y,0$	(4) $2(\frac{1}{2},0,0)\quad x,0,0$
(5) $\bar{1}\quad 0,0,0$	(6) $a\quad x,y,0$	(7) $m\quad x,0,z$	(8) $m\quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	l	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z$ (6) $x+\frac{1}{2},y,\bar{z}$	(3) $\bar{x},y,\bar{z}$ (7) $x,\bar{y},z$	(4) $x+\frac{1}{2},\bar{y},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y,z$	$hk0$: $h=2n$ $h00$: $h=2n$
							Special: as above, plus
4	k	$m\,.\,.$	$\frac{1}{4},y,z$	$\frac{1}{4},\bar{y},z$	$\frac{3}{4},y,\bar{z}$	$\frac{3}{4},\bar{y},\bar{z}$	no extra conditions
4	j	$.\,m\,.$	$x,\frac{1}{2},z$	$\bar{x}+\frac{1}{2},\frac{1}{2},z$	$\bar{x},\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\frac{1}{2},\bar{z}$	no extra conditions
4	i	$.\,m\,.$	$x,0,z$	$\bar{x}+\frac{1}{2},0,z$	$\bar{x},0,\bar{z}$	$x+\frac{1}{2},0,\bar{z}$	no extra conditions
4	h	$.\,2\,.$	$0,y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$	$\frac{1}{2},y,\frac{1}{2}$	hkl : $h=2n$
4	g	$.\,2\,.$	$0,y,0$	$\frac{1}{2},\bar{y},0$	$0,\bar{y},0$	$\frac{1}{2},y,0$	hkl : $h=2n$
2	f	$m\,m\,2$	$\frac{1}{4},\frac{1}{2},z$	$\frac{3}{4},\frac{1}{2},\bar{z}$			no extra conditions
2	e	$m\,m\,2$	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}$			no extra conditions
2	d	$.\,2/m\,.$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h=2n$
2	c	$.\,2/m\,.$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h=2n$
2	b	$.\,2/m\,.$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h=2n$
2	a	$.\,2/m\,.$	$0,0,0$	$\frac{1}{2},0,0$			hkl : $h=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I
[2] $Pm2a$ ($Pma2$, 28) 1; 3; 6; 8
[2] $P2_1ma$ ($Pmc2_1$, 26) 1; 4; 6; 7
[2] $Pmm2$ (25) 1; 2; 7; 8
[2] $P2_122$ ($P222_1$, 17) 1; 2; 3; 4
[2] $P112/a$ ($P2/c$, 13) 1; 2; 5; 6
[2] $P2_1/m11$ ($P2_1/m$, 11) 1; 4; 5; 8
[2] $P12/m1$ ($P2/m$, 10) 1; 3; 5; 7

IIa none

IIb [2] $Pmmn$ ($\mathbf{b}'=2\mathbf{b}$) (59); [2] $Pbma$ ($\mathbf{b}'=2\mathbf{b}$) ($Pbcm$, 57); [2] $Pbmn$ ($\mathbf{b}'=2\mathbf{b}$) ($Pmna$, 53); [2] $Pmca$ ($\mathbf{c}'=2\mathbf{c}$) ($Pbcm$, 57); [2] $Pcma$ ($\mathbf{c}'=2\mathbf{c}$) ($Pbam$, 55); [2] $Pcca$ ($\mathbf{c}'=2\mathbf{c}$) (54); [2] $Aema$ ($\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($Cmce$, 64); [2] $Amma$ ($\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($Cmcm$, 63)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmma$ ($\mathbf{b}'=2\mathbf{b}$) (51); [2] $Pmma$ ($\mathbf{c}'=2\mathbf{c}$) (51); [3] $Pmma$ ($\mathbf{a}'=3\mathbf{a}$) (51)

Minimal non-isomorphic supergroups

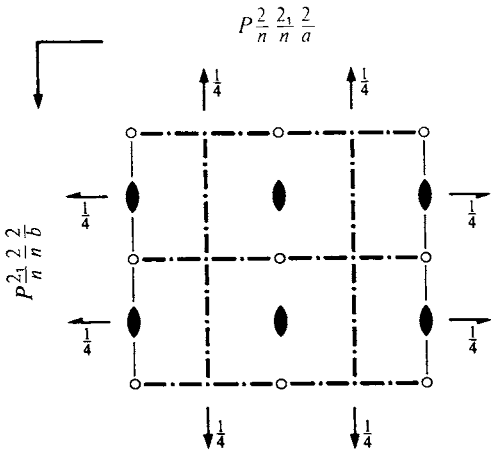
I none

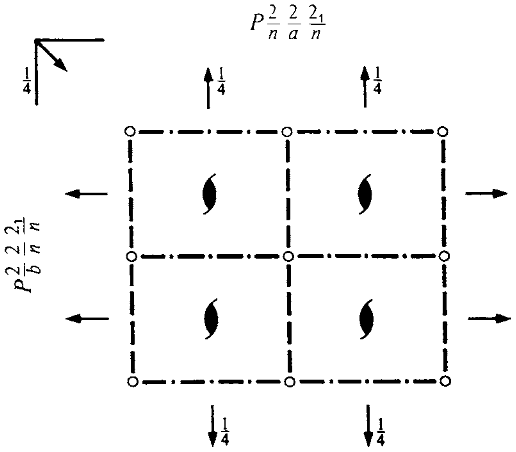
II [2] $Amma$ ($Cmcm$, 63); [2] $Bmmm$ ($Cmmm$, 65); [2] $Cmme$ (67); [2] $Imma$ (74); [2] $Pmmm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (47)

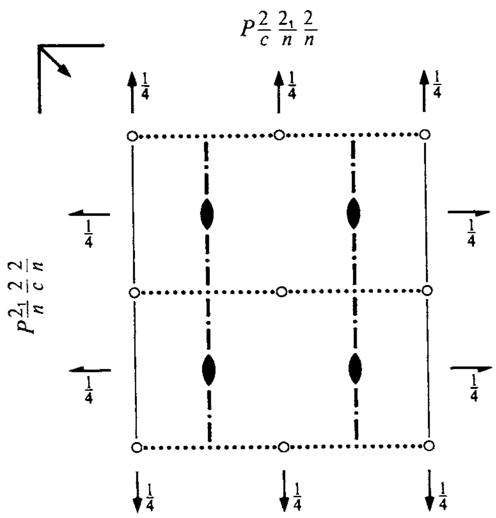
International Tables for Crystallography (2006). Vol. A, Space group 52, pp. 276–277.

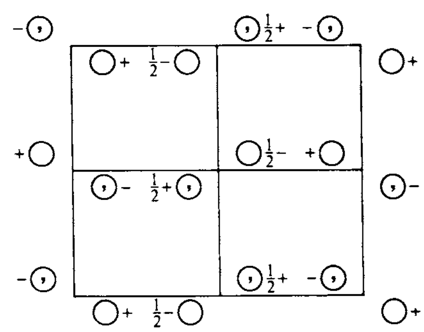
Pnna D_{2h}^{6} *mmm* Orthorhombic

No. 52 $P\ 2/n\ 2_1/n\ 2/a$ Patterson symmetry *Pmmm*









Origin at $\bar{1}$ on $n\,1\,a$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2\quad \frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2\quad x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}\quad 0,0,0$	(6) $a\quad x,y,0$	(7) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})\quad 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*e*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z$ (6) $x+\frac{1}{2},y,\bar{z}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $hk0$: $h=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*d*	$2\,.\,.$	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	hkl : $h+l=2n$
4	*c*	$.\,.\,2$	$\frac{1}{4},0,z$	$\frac{1}{4},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{3}{4},0,\bar{z}$	$\frac{3}{4},\frac{1}{2},z+\frac{1}{2}$	hkl : $h+k+l=2n$
4	*b*	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},0$	hkl : $h,k+l=2n$
4	*a*	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl : $h,k+l=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $c2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $\frac{1}{4},y,\frac{1}{4}$

Maximal non-isomorphic subgroups

I
[2] $Pnn2$ (34) 1; 2; 7; 8
[2] $Pn2_1a$ ($Pna2_1$, 33) 1; 3; 6; 8
[2] $P2na$ ($Pnc2$, 30) 1; 4; 6; 7
[2] $P22_12$ ($P222_1$, 17) 1; 2; 3; 4
[2] $P12_1/n1$ ($P2_1/c$, 14) 1; 3; 5; 7
[2] $P112/a$ ($P2/c$, 13) 1; 2; 5; 6
[2] $P2/n11$ ($P2/c$, 13) 1; 4; 5; 8

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pnna$ ($\mathbf{a}'=3\mathbf{a}$) (52); [3] $Pnna$ ($\mathbf{b}'=3\mathbf{b}$) (52); [3] $Pnna$ ($\mathbf{c}'=3\mathbf{c}$) (52)

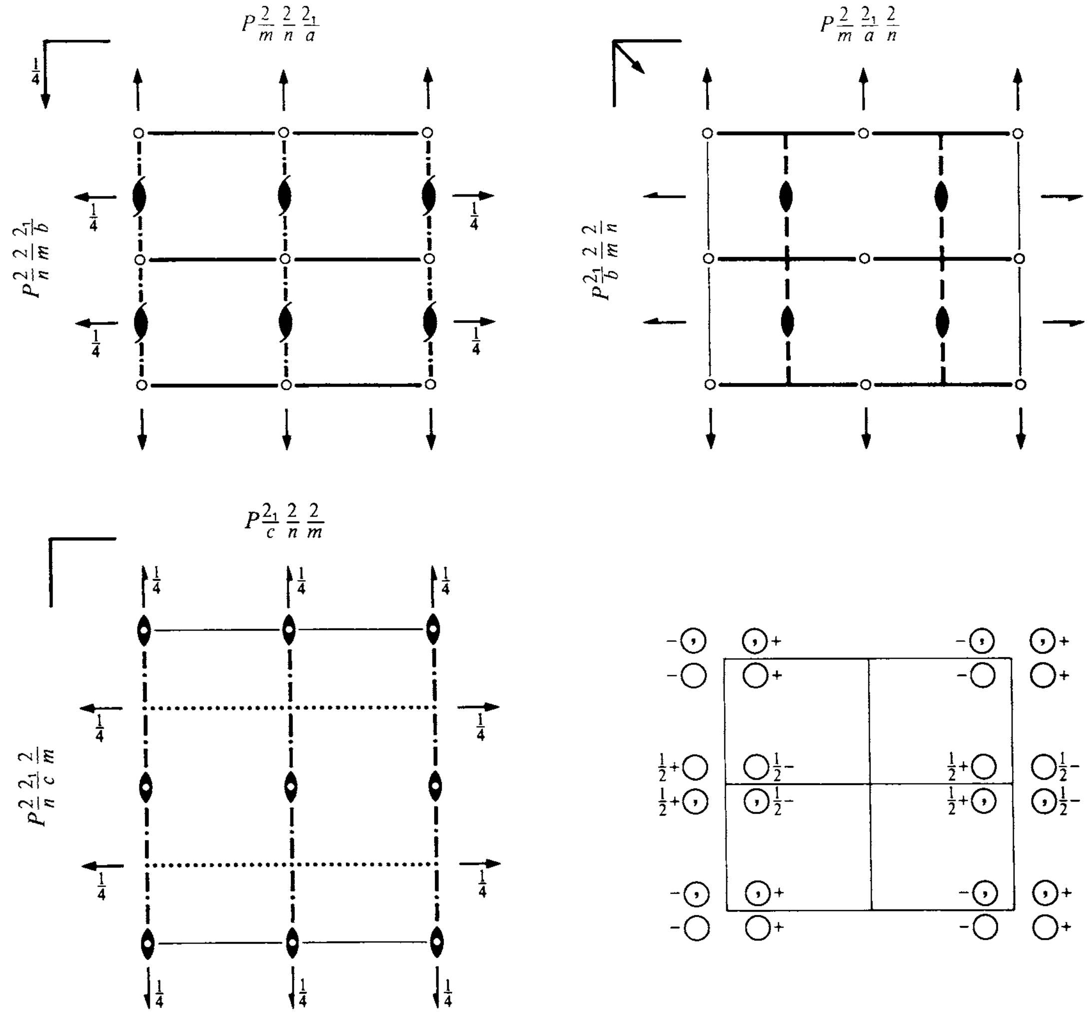
Minimal non-isomorphic supergroups

I none

II [2] $Bbmm$ ($Cmcm$, 63); [2] $Amaa$ ($Cccm$, 66); [2] $Ccce$ (68); [2] $Imma$ (74); [2] $Pncm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Pmna$, 53); [2] $Pcna$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Pban$, 50); [2] $Pbaa$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($Pcca$, 54)

Pmna D_{2h}^{7} *mmm* Orthorhombic

No. 53 $P\ 2/m\ 2/n\ 2_1/a$ Patterson symmetry *Pmmm*



Origin at centre $(2/m)$ at $2/mn1$

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2\quad x,0,0$
(5) $\bar{1}\quad 0,0,0$	(6) $a\quad x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})\quad x,0,z$	(8) $m\quad 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	i	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$ (7) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	$h0l$: $h+l=2n$ $hk0$: $h=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus
4	h	$m\,.\,.$	$0,y,z$	$\frac{1}{2},\bar{y},z+\frac{1}{2}$	$\frac{1}{2},y,\bar{z}+\frac{1}{2}$	$0,\bar{y},\bar{z}$	no extra conditions
4	g	$.\,2\,.$	$\frac{1}{4},y,\frac{1}{4}$	$\frac{1}{4},\bar{y},\frac{3}{4}$	$\frac{3}{4},\bar{y},\frac{3}{4}$	$\frac{3}{4},y,\frac{1}{4}$	hkl : $h=2n$
4	f	$2\,.\,.$	$x,\frac{1}{2},0$	$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+l=2n$
4	e	$2\,.\,.$	$x,0,0$	$\bar{x}+\frac{1}{2},0,\frac{1}{2}$	$\bar{x},0,0$	$x+\frac{1}{2},0,\frac{1}{2}$	hkl : $h+l=2n$
2	d	$2/m\,.\,.$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+l=2n$
2	c	$2/m\,.\,.$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $h+l=2n$
2	b	$2/m\,.\,.$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$			hkl : $h+l=2n$
2	a	$2/m\,.\,.$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+l=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $c2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Pmn2_1$ (31)	1; 2; 7; 8
	[2] $P2na$ ($Pnc2$, 30)	1; 4; 6; 7
	[2] $Pm2a$ ($Pma2$, 28)	1; 3; 6; 8
	[2] $P222_1$ (17)	1; 2; 3; 4
	[2] $P112_1/a$ ($P2_1/c$, 14)	1; 2; 5; 6
	[2] $P12/n1$ ($P2/c$, 13)	1; 3; 5; 7
	[2] $P2/m11$ ($P2/m$, 10)	1; 4; 5; 8

IIa none

IIb [2] $Pbna$ ($\mathbf{b}'=2\mathbf{b}$) ($Pbcn$, 60); [2] $Pmnn$ ($\mathbf{b}'=2\mathbf{b}$) ($Pnnm$, 58); [2] $Pbnn$ ($\mathbf{b}'=2\mathbf{b}$) ($Pnna$, 52)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmna$ ($\mathbf{b}'=2\mathbf{b}$) (53); [3] $Pmna$ ($\mathbf{a}'=3\mathbf{a}$) (53); [3] $Pmna$ ($\mathbf{c}'=3\mathbf{c}$) (53)

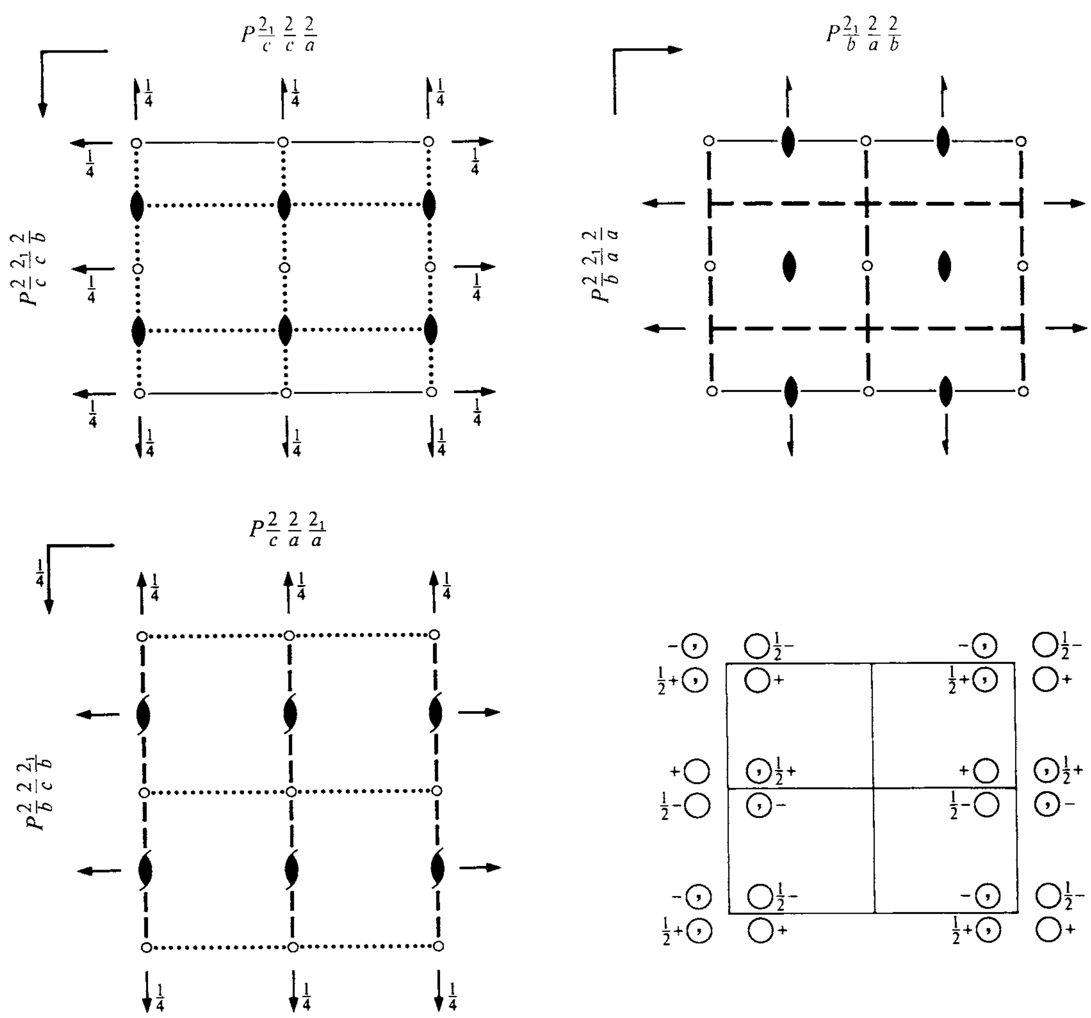
Minimal non-isomorphic supergroups

I none

II [2] $Cmce$ (64); [2] $Bmmm$ ($Cmmm$, 65); [2] $Amaa$ ($Cccm$, 66); [2] $Imma$ (74); [2] $Pmaa$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($Pccm$, 49); [2] $Pmcm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Pmma$, 51)

Pcca D_{2h}^{8} *mmm* Orthorhombic

No. 54 $P\ 2_1/c\ 2/c\ 2/a$ Patterson symmetry *Pmmm*



Origin at $\bar{1}$ on $1ca$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4},0,z$	(3) 2 $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$
(5) $\bar{1}$ $0,0,0$	(6) a $x,y,0$	(7) c $x,0,z$	(8) c $\frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	f	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z$ (6) $x+\frac{1}{2},y,\bar{z}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	$0kl$: $l=2n$ $h0l$: $l=2n$ $hk0$: $h=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus
4	e	$..2$	$\frac{1}{4},\frac{1}{2},z$	$\frac{3}{4},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{1}{2},\bar{z}$	$\frac{1}{4},\frac{1}{2},z+\frac{1}{2}$	hkl : $l=2n$
4	d	$..2$	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}+\frac{1}{2}$	$\frac{3}{4},0,\bar{z}$	$\frac{1}{4},0,z+\frac{1}{2}$	hkl : $l=2n$
4	c	$.2.$	$0,y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$\frac{1}{2},y,\frac{3}{4}$	hkl : $h+l=2n$
4	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h,l=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl : $h,l=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Pc2a$ ($Pba2$, 32)	1; 3; 6; 8
	[2] $P2_1ca$ ($Pca2_1$, 29)	1; 4; 6; 7
	[2] $Pcc2$ (27)	1; 2; 7; 8
	[2] $P2_122$ ($P222_1$, 17)	1; 2; 3; 4
	[2] $P2_1/c11$ ($P2_1/c$, 14)	1; 4; 5; 8
	[2] $P112/a$ ($P2/c$, 13)	1; 2; 5; 6
	[2] $P12/c1$ ($P2/c$, 13)	1; 3; 5; 7

IIa none

IIb [2] $Pnca$ ($\mathbf{b}'=2\mathbf{b}$) ($Pbcn$, 60); [2] $Pccn$ ($\mathbf{b}'=2\mathbf{b}$) (56); [2] $Pncn$ ($\mathbf{b}'=2\mathbf{b}$) ($Pnna$, 52)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pcca$ ($\mathbf{b}'=2\mathbf{b}$) (54); [3] $Pcca$ ($\mathbf{a}'=3\mathbf{a}$) (54); [3] $Pcca$ ($\mathbf{c}'=3\mathbf{c}$) (54)

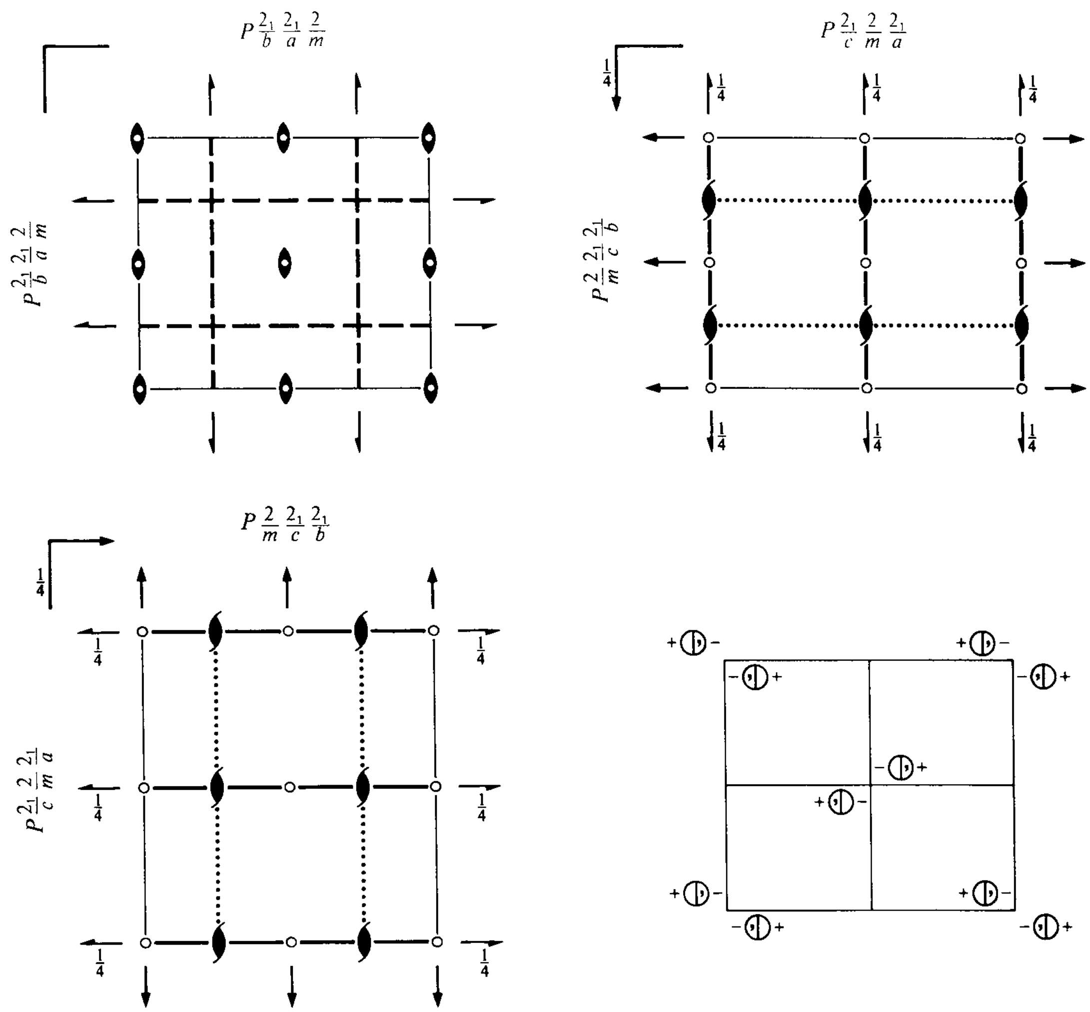
Minimal non-isomorphic supergroups

I none

II [2] $Aema$ ($Cmce$, 64); [2] $Bmem$ ($Cmme$, 67); [2] $Ccce$ (68); [2] $Ibca$ (73); [2] $Pccm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (49); [2] $Pmma$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (51)

International Tables for Crystallography (2006). Vol. A, Space group 55, pp. 282–283.

$Pbam$	D_{2h}^{9}	mmm	Orthorhombic
No. 55	$P\ 2_1/b\ 2_1/a\ 2/m$		Patterson symmetry $Pmmm$



Origin at centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $\bar{1}\quad 0,0,0$	(6) $m\quad x,y,0$	(7) $a\quad x,\frac{1}{4},z$	(8) $b\quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	i	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$0kl$: $k=2n$ $h0l$: $h=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	h	$..m$	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	no extra conditions
4	g	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	no extra conditions
4	f	$..2$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$	hkl : $h+k=2n$
4	e	$..2$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl : $h+k=2n$
2	d	$..2/m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k=2n$
2	c	$..2/m$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $h+k=2n$
2	b	$..2/m$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	a	$..2/m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I
- [2] $Pba2$ (32) 1; 2; 7; 8
- [2] $Pb2_1m$ ($Pmc2_1$, 26) 1; 3; 6; 8
- [2] $P2_1am$ ($Pmc2_1$, 26) 1; 4; 6; 7
- [2] $P2_12_12$ (18) 1; 2; 3; 4
- [2] $P12_1/a1$ ($P2_1/c$, 14) 1; 3; 5; 7
- [2] $P2_1/b11$ ($P2_1/c$, 14) 1; 4; 5; 8
- [2] $P112/m$ ($P2/m$, 10) 1; 2; 5; 6

IIa none

IIb [2] $Pnam$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnma$, 62); [2] $Pbnm$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnma$, 62); [2] $Pnnm$ ($\mathbf{c}'=2\mathbf{c}$) (58)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pbam$ ($\mathbf{c}'=2\mathbf{c}$) (55); [3] $Pbam$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (55)

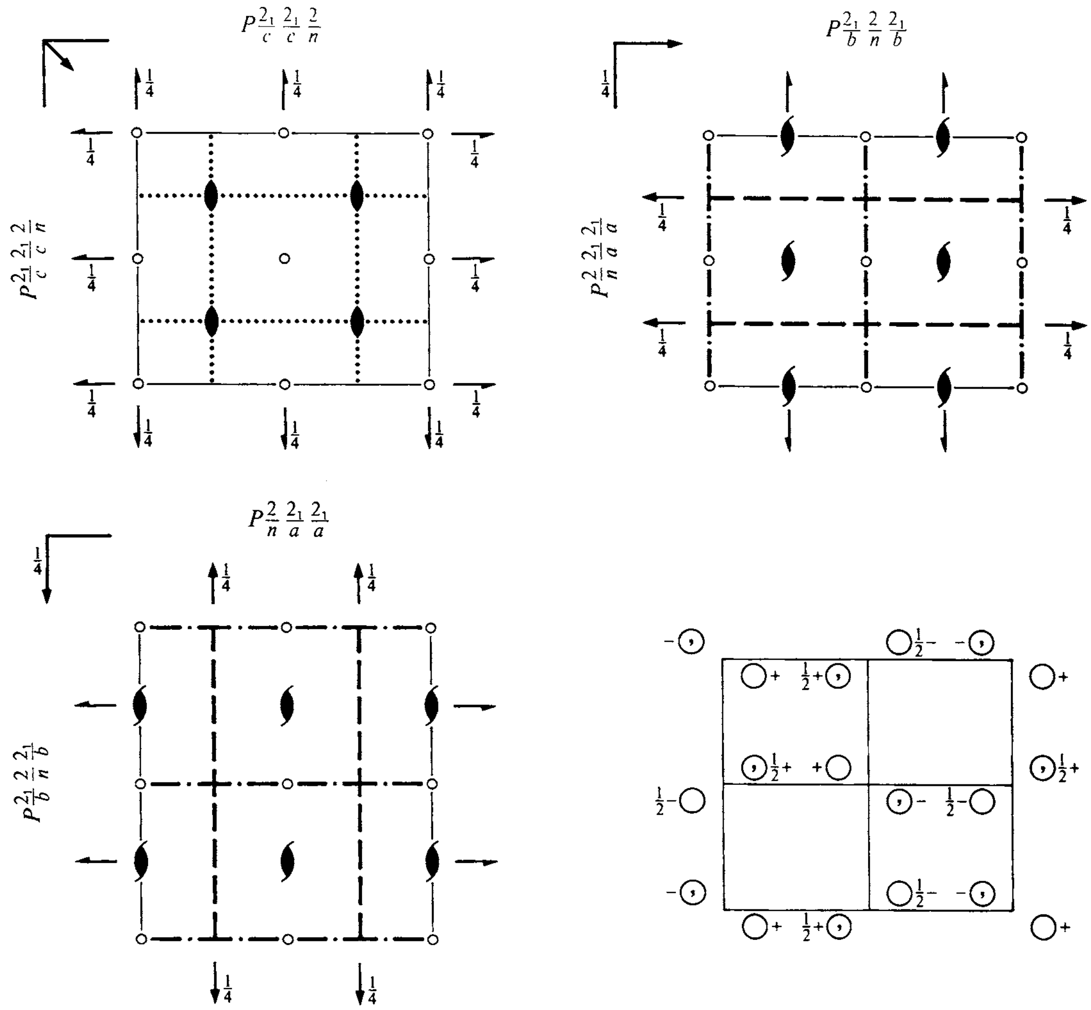
Minimal non-isomorphic supergroups

I [2] $P4/mbm$ (127); [2] $P4_2/mbc$ (135)

II [2] $Aeam$ ($Cmce$, 64); [2] $Bbem$ ($Cmce$, 64); [2] $Cmmm$ (65); [2] $Ibam$ (72); [2] $Pbmm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Pmma$, 51); [2] $Pmam$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Pmma$, 51)

$Pccn$ $\quad$ D_{2h}^{10} $\quad$ mmm $\quad$ Orthorhombic

No. 56 $\quad$ $P\ 2_1/c\ 2_1/c\ 2/n$ $\quad$ Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $1\,1\,n$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4};\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,0,\frac{1}{4}$
(5) $\bar{1}\quad 0,0,0$	(6) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,0$	(7) $c\quad x,\frac{1}{4},z$	(8) $c\quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$	$0kl$: $l=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	$h0l$: $l=2n$
							$hk0$: $h+k=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
							Special: as above, plus
4	d	. . 2	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl : $l=2n$
4	c	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$	hkl : $l=2n$
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	hkl : $h+k,h+l,k+l=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl : $h+k,h+l,k+l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Pc2_1n$ ($Pna2_1$, 33)	1; 3; 6; 8
	[2] $P2_1cn$ ($Pna2_1$, 33)	1; 4; 6; 7
	[2] $Pcc2$ (27)	1; 2; 7; 8
	[2] $P2_12_12$ (18)	1; 2; 3; 4
	[2] $P12_1/c1$ ($P2_1/c$, 14)	1; 3; 5; 7
	[2] $P2_1/c11$ ($P2_1/c$, 14)	1; 4; 5; 8
	[2] $P112/n$ ($P2/c$, 13)	1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pccn$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (56); [3] $Pccn$ ($\mathbf{c}'=3\mathbf{c}$) (56)

Minimal non-isomorphic supergroups

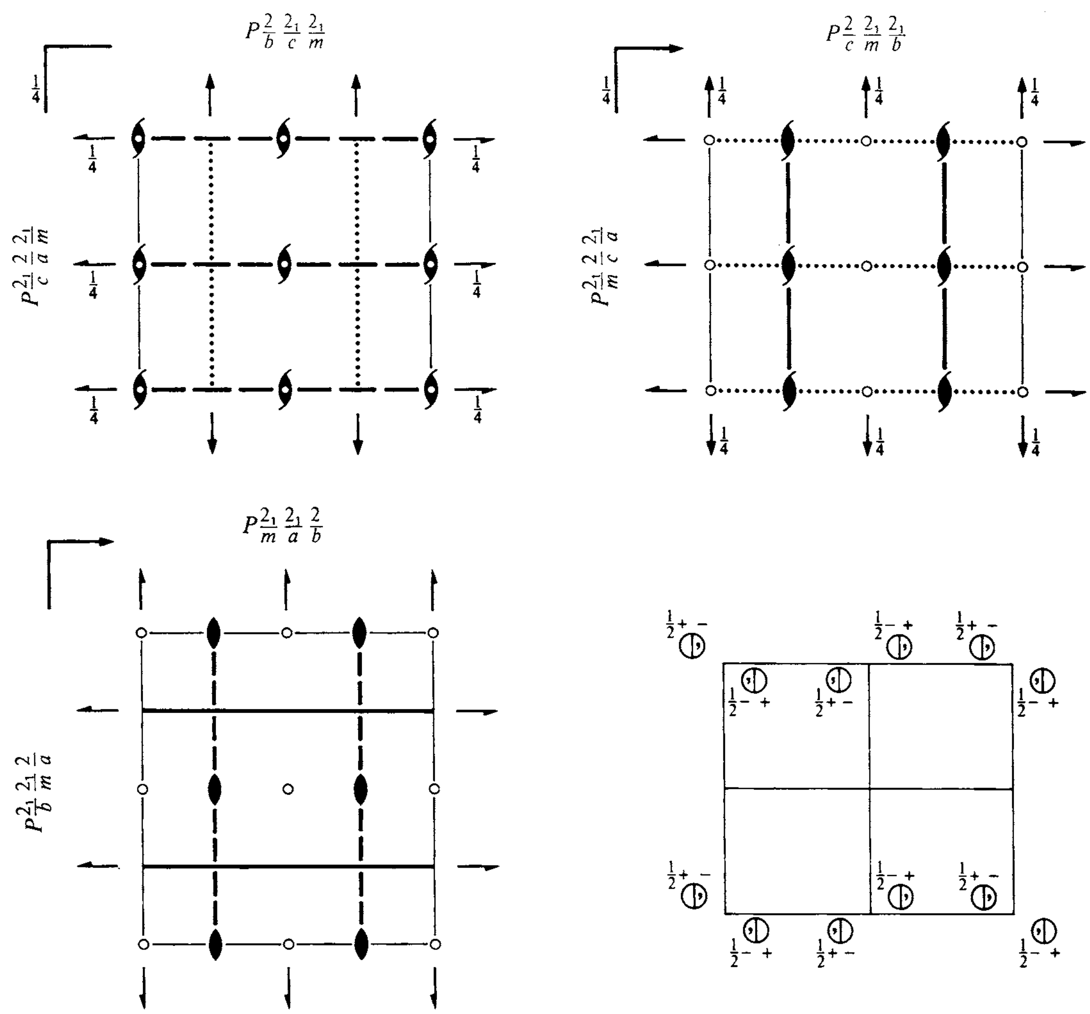
I [2] $P4/ncc$ (130); [2] $P4_2/ncm$ (138)

II [2] $Aema$ ($Cmce$, 64); [2] $Bmeb$ ($Cmce$, 64); [2] $Cccm$ (66); [2] $Ibam$ (72); [2] $Pccb$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Pcca$, 54); [2] $Pcca$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (54); [2] $Pmmn$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (59)

International Tables for Crystallography (2006). Vol. A, Space group 57, pp. 286–287.

$Pbcm$ D_{2h}^{11} mmm Orthorhombic

No. 57 $P\ 2/b\ 2_1/c\ 2_1/m$ Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $b12_1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $0,0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) 2 $x,\frac{1}{4},0$
(5) $\bar{1}$ $0,0,0$	(6) m $x,y,\frac{1}{4}$	(7) c $x,\frac{1}{4},z$	(8) b $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*e*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}$	$0kl$: $k=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(8) $\bar{x},y+\frac{1}{2},z$	$h0l$: $l=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
							Special: as above, plus
4	*d*	$..m$	$x,y,\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$\bar{x},y+\frac{1}{2},\frac{1}{4}$	$x,\bar{y}+\frac{1}{2},\frac{3}{4}$	no extra conditions
4	*c*	$2..$	$x,\frac{1}{4},0$	$\bar{x},\frac{3}{4},\frac{1}{2}$	$\bar{x},\frac{3}{4},0$	$x,\frac{1}{4},\frac{1}{2}$	hkl : $l=2n$
4	*b*	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl : $k,l=2n$
4	*a*	$\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	hkl : $k,l=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $Pbc2_1$ ($Pca2_1$, 29) 1; 2; 7; 8
[2] $P2cm$ ($Pma2$, 28) 1; 4; 6; 7
[2] $Pb2_1m$ ($Pmc2_1$, 26) 1; 3; 6; 8
[2] $P22_12_1$ ($P2_12_12$, 18) 1; 2; 3; 4
[2] $P12_1/c1$ ($P2_1/c$, 14) 1; 3; 5; 7
[2] $P2/b11$ ($P2/c$, 13) 1; 4; 5; 8
[2] $P112_1/m$ ($P2_1/m$, 11) 1; 2; 5; 6

IIa none

IIb [2] $Pbnm$ ($\mathbf{a}'=2\mathbf{a}$) ($Pnma$, 62); [2] $Pbca$ ($\mathbf{a}'=2\mathbf{a}$) (61); [2] $Pbna$ ($\mathbf{a}'=2\mathbf{a}$) ($Pbcn$, 60)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pbcm$ ($\mathbf{a}'=2\mathbf{a}$) (57); [3] $Pbcm$ ($\mathbf{b}'=3\mathbf{b}$) (57); [3] $Pbcm$ ($\mathbf{c}'=3\mathbf{c}$) (57)

Minimal non-isomorphic supergroups

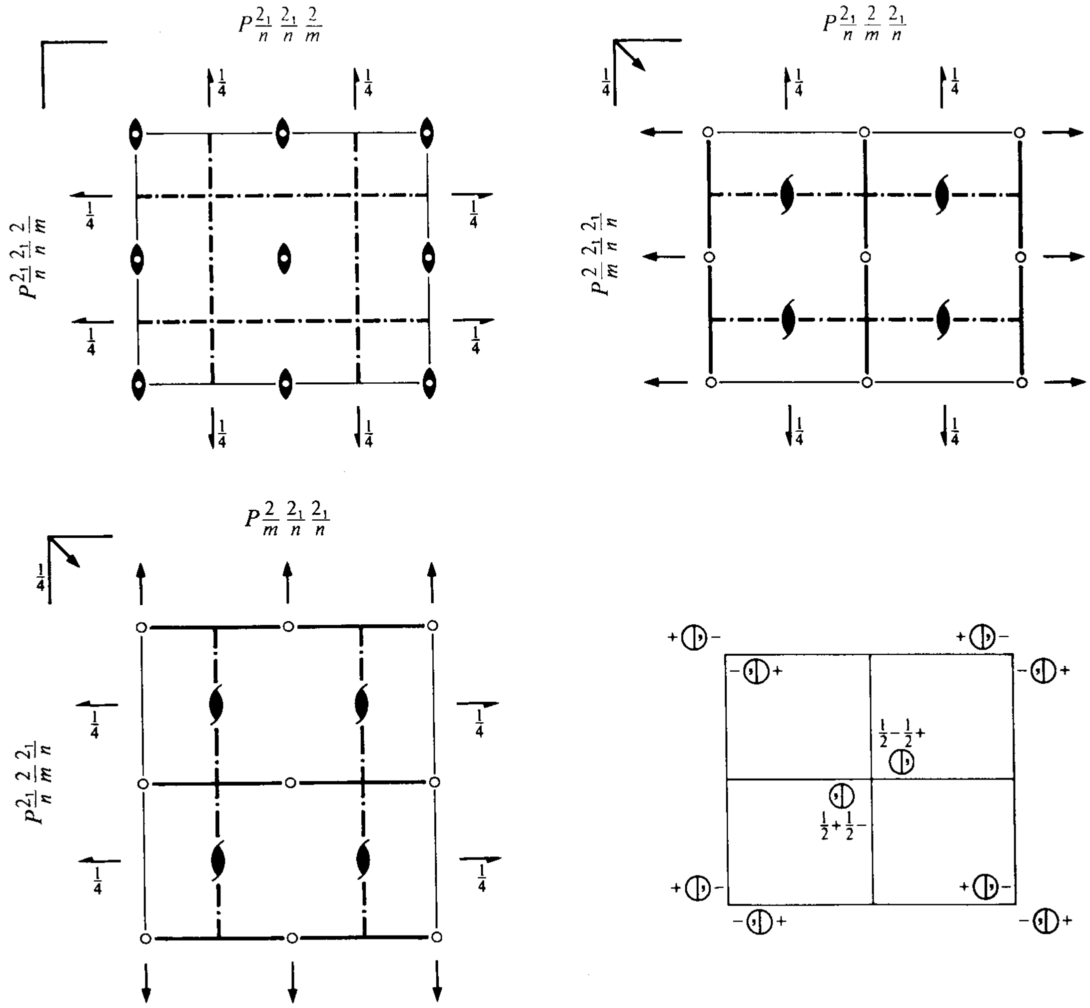
I none

II [2] $Cmcm$ (63); [2] $Bbem$ ($Cmce$, 64); [2] $Aemm$ ($Cmme$, 67); [2] $Ibam$ (72); [2] $Pmcm$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Pmma$, 51); [2] $Pbmm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($Pmma$, 51)

International Tables for Crystallography (2006). Vol. A, Space group 58, pp. 288–289.

$Pnnm$ $\quad D_{2h}^{12}$ $\quad mmm$ $\quad$ Orthorhombic

No. 58 $\quad P\ 2_1/n\ 2_1/n\ 2/m$ $\quad$ Patterson symmetry $Pmmm$



Origin at centre $(2/m)$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}\quad 0,0,0$	(6) $m\quad x,y,0$	(7) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	h	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	g	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	no extra conditions
4	f	$..2$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z+\frac{1}{2}$	hkl : $h+k+l=2n$
4	e	$..2$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl : $h+k+l=2n$
2	d	$..2/m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$			hkl : $h+k+l=2n$
2	c	$..2/m$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k+l=2n$
2	b	$..2/m$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k+l=2n$
2	a	$..2/m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $c2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Pnn2$ (34)	1; 2; 7; 8
	[2] $Pn2_1m$ ($Pmn2_1$, 31)	1; 3; 6; 8
	[2] $P2_1nm$ ($Pmn2_1$, 31)	1; 4; 6; 7
	[2] $P2_12_12$ (18)	1; 2; 3; 4
	[2] $P12_1/n1$ ($P2_1/c$, 14)	1; 3; 5; 7
	[2] $P2_1/n11$ ($P2_1/c$, 14)	1; 4; 5; 8
	[2] $P112/m$ ($P2/m$, 10)	1; 2; 5; 6
IIa	none	
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Pnnm$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (58); [3] $Pnnm$ ($\mathbf{c}'=3\mathbf{c}$) (58)

Minimal non-isomorphic supergroups

I [2] $P4/mnc$ (128); [2] $P4_2/mnm$ (136)

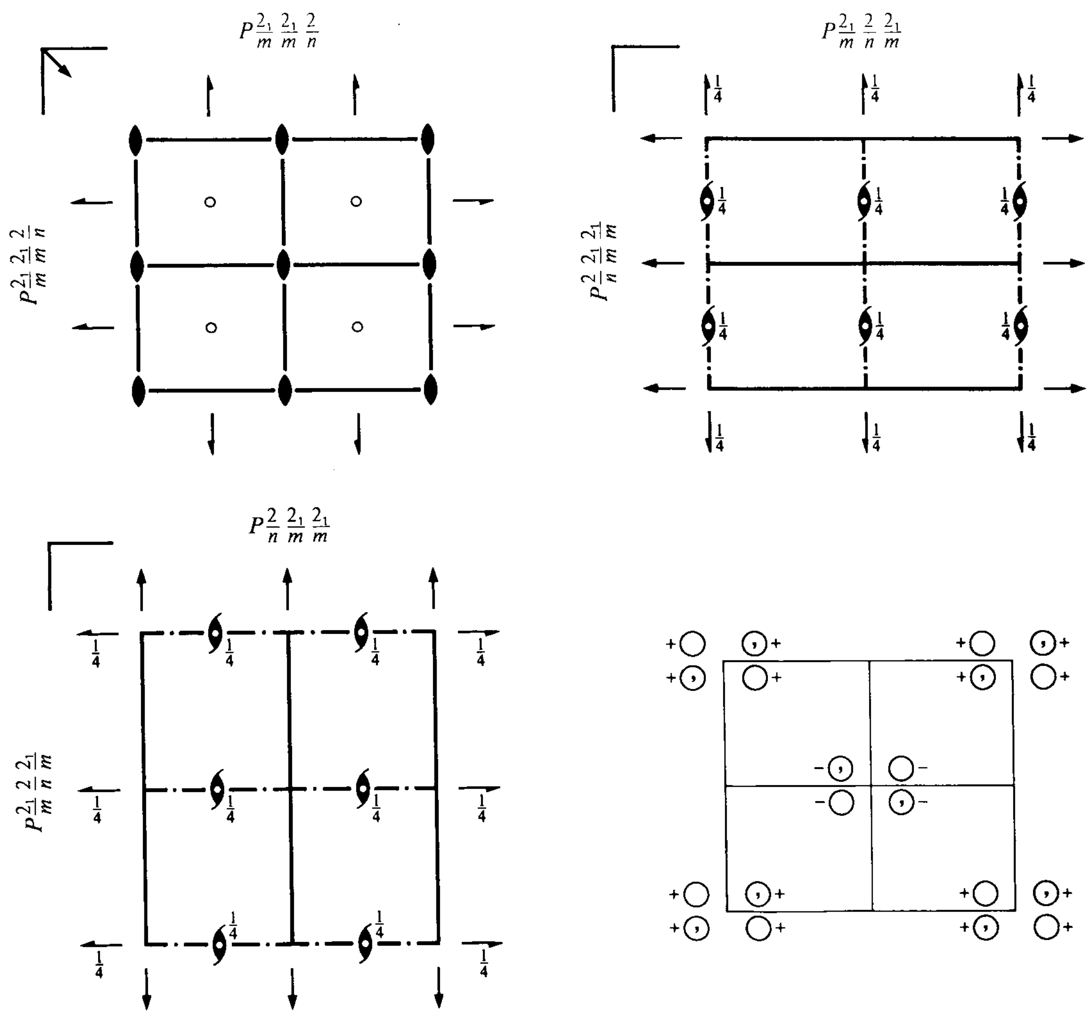
II [2] $Amam$ ($Cmcm$, 63); [2] $Bbmm$ ($Cmcm$, 63); [2] $Cccm$ (66); [2] $Immm$ (71); [2] $Pncm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Pmna$, 53); [2] $Pcnm$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Pmna$, 53); [2] $Pbam$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (55)

International Tables for Crystallography (2006). Vol. A, Space group 59, pp. 290–293.

$Pmmn$ D_{2h}^{13} mmm Orthorhombic

No. 59 $P\ 2_1/m\ 2_1/m\ 2/n$ Patterson symmetry $Pmmm$

ORIGIN CHOICE 1



Origin at $mm2/n$, at $\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},0$	(6) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,0$	(7) $m\quad x,0,z$	(8) $m\quad 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y},z$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x},y,z$	$hk0: h+k=2n$ $h00: h=2n$ $0k0: k=2n$
							Special: as above, plus
4	f	$.m.$	$x,0,z$	$\bar{x},0,z$	$\bar{x}+\frac{1}{2},\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\frac{1}{2},\bar{z}$	no extra conditions
4	e	$m..$	$0,y,z$	$0,\bar{y},z$	$\frac{1}{2},y+\frac{1}{2},\bar{z}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	no extra conditions
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$hkl: h,k=2n$
4	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	$hkl: h,k=2n$
2	b	$mm2$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			no extra conditions
2	a	$mm2$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions

Symmetry of special projections

Along [001] $c2mm$	Along [100] $p2mg$	Along [010] $p2gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$	$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$	$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,0,z$	Origin at $x,\frac{1}{4},0$	Origin at $\frac{1}{4},y,0$

Maximal non-isomorphic subgroups

I	[2] $Pm2_1n$ ($Pmn2_1$, 31)	1; 3; 6; 8
	[2] $P2_1mn$ ($Pmn2_1$, 31)	1; 4; 6; 7
	[2] $Pmm2$ (25)	1; 2; 7; 8
	[2] $P2_12_12$ (18)	1; 2; 3; 4
	[2] $P112/n$ ($P2/c$, 13)	1; 2; 5; 6
	[2] $P12_1/m1$ ($P2_1/m$, 11)	1; 3; 5; 7
	[2] $P2_1/m11$ ($P2_1/m$, 11)	1; 4; 5; 8

IIa none

IIb [2] $Pcmn$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnma$, 62); [2] $Pmcn$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnma$, 62); [2] $Pccn$ ($\mathbf{c}'=2\mathbf{c}$) (56)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmmn$ ($\mathbf{c}'=2\mathbf{c}$) (59); [3] $Pmmn$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (59)

Minimal non-isomorphic supergroups

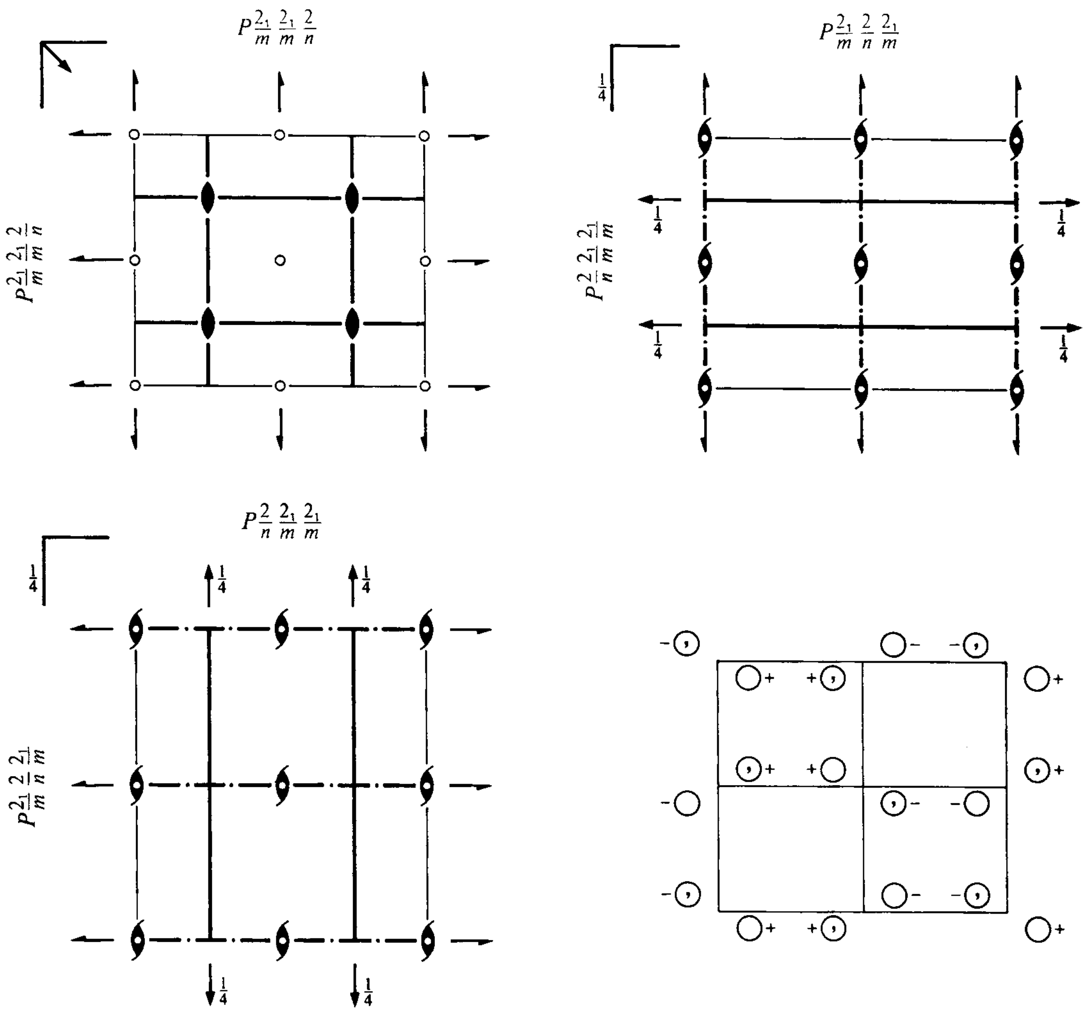
I [2] $P4/nmm$ (129); [2] $P4_2/nmc$ (137)

II [2] $Amma$ ($Cmcm$, 63); [2] $Bmmb$ ($Cmcm$, 63); [2] $Cmmm$ (65); [2] $Immm$ (71); [2] $Pmmb$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Pmma$, 51); [2] $Pmma$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (51)

$Pmmn$ $\quad D_{2h}^{13}$ $\quad mmm$ $\quad$ Orthorhombic

No. 59 $\quad P\ 2_1/m\ 2_1/m\ 2/n$ $\quad$ Patterson symmetry $Pmmm$

ORIGIN CHOICE 2



Origin at $\bar{1}$ at $2_1 2_1 n$, at $-\frac{1}{4},-\frac{1}{4},0$ from $mm2$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4}; \quad -\frac{1}{4} \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1	(2) $2\ \ \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\ \ 0,y,0$	(4) $2(\frac{1}{2},0,0)\ \ x,0,0$
(5) $\bar{1}\ \ 0,0,0$	(6) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$	(7) $m\ \ x,\frac{1}{4},z$	(8) $m\ \ \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*g*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x+\frac{1}{2},\bar{y},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y,z$	$hk0:\ h+k=2n$ $h00:\ h=2n$ $0k0:\ k=2n$
							Special: as above, plus
4	*f*	$.\,m\,.$	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{1}{4},z$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{3}{4},\bar{z}$	no extra conditions
4	*e*	$m\,.\,.$	$\frac{1}{4},y,z$	$\frac{1}{4},\bar{y}+\frac{1}{2},z$	$\frac{3}{4},y+\frac{1}{2},\bar{z}$	$\frac{3}{4},\bar{y},\bar{z}$	no extra conditions
4	*d*	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$hkl:\ h,k=2n$
4	*c*	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$hkl:\ h,k=2n$
2	*b*	$m\,m\,2$	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$			no extra conditions
2	*a*	$m\,m\,2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}$			no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Pm2_1n$ ($Pmn2_1$, 31)	1; 3; 6; 8
	[2] $P2_1mn$ ($Pmn2_1$, 31)	1; 4; 6; 7
	[2] $Pmm2$ (25)	1; 2; 7; 8
	[2] $P2_12_12$ (18)	1; 2; 3; 4
	[2] $P112/n$ ($P2/c$, 13)	1; 2; 5; 6
	[2] $P12_1/m1$ ($P2_1/m$, 11)	1; 3; 5; 7
	[2] $P2_1/m11$ ($P2_1/m$, 11)	1; 4; 5; 8

IIa none

IIb [2] $Pcmn$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnma$, 62); [2] $Pmcn$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnma$, 62); [2] $Pccn$ ($\mathbf{c}'=2\mathbf{c}$) (56)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pmmn$ ($\mathbf{c}'=2\mathbf{c}$) (59); [3] $Pmmn$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (59)

Minimal non-isomorphic supergroups

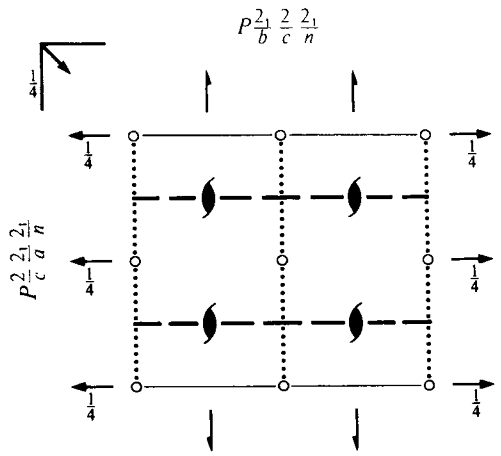
I [2] $P4/nmm$ (129); [2] $P4_2/nmc$ (137)

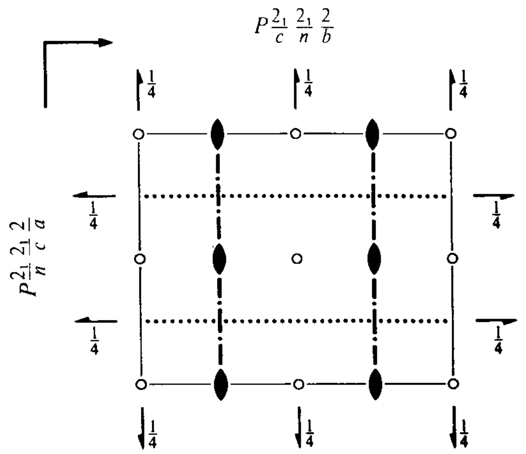
II [2] $Amma$ ($Cmcm$, 63); [2] $Bmmb$ ($Cmcm$, 63); [2] $Cmmm$ (65); [2] $Immm$ (71); [2] $Pmmb$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Pmma$, 51); [2] $Pmma$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (51)

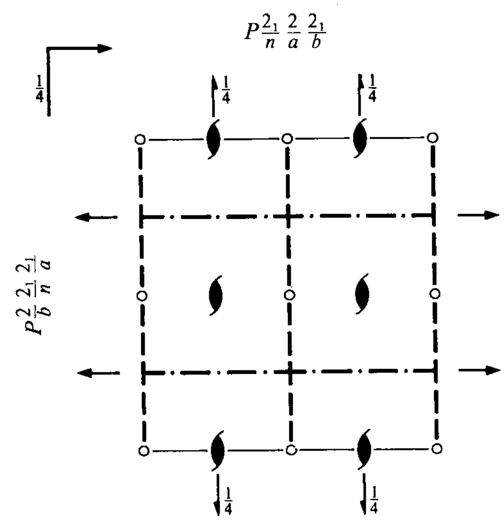
International Tables for Crystallography (2006). Vol. A, Space group 60, pp. 294–295.

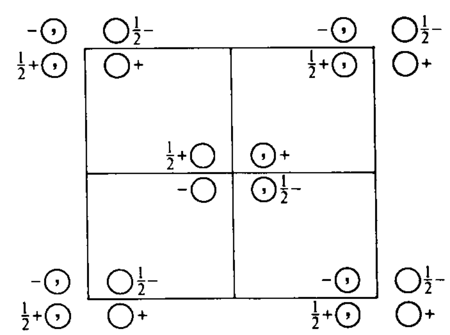
Pbcn D_{2h}^{14} *mmm* Orthorhombic

No. 60 $P\ 2_1/b\ 2/c\ 2_1/n$ Patterson symmetry *Pmmm*









Origin at $\bar{1}$ on $1c1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) 2 $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $\bar{1}$ $0,0,0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(7) c $x,0,z$	(8) b $\frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$0kl$: $k=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$h0l$: $l=2n$
							$hk0$: $h+k=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
							Special: as above, plus
4	c	. 2 .	$0,y,\frac{1}{4}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\frac{3}{4}$	$0,\bar{y},\frac{3}{4}$	$\frac{1}{2},y+\frac{1}{2},\frac{1}{4}$	hkl : $h+k=2n$
4	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$	hkl : $h+k,l=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl : $h+k,l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $P2_1cn$ ($Pna2_1$, 33)	1; 4; 6; 7
	[2] $Pb2n$ ($Pnc2$, 30)	1; 3; 6; 8
	[2] $Pbc2_1$ ($Pca2_1$, 29)	1; 2; 7; 8
	[2] $P2_122_1$ ($P2_12_12$, 18)	1; 2; 3; 4
	[2] $P112_1/n$ ($P2_1/c$, 14)	1; 2; 5; 6
	[2] $P2_1/b11$ ($P2_1/c$, 14)	1; 4; 5; 8
	[2] $P12/c1$ ($P2/c$, 13)	1; 3; 5; 7

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pbcn$ ($\mathbf{a}'=3\mathbf{a}$) (60); [3] $Pbcn$ ($\mathbf{b}'=3\mathbf{b}$) (60); [3] $Pbcn$ ($\mathbf{c}'=3\mathbf{c}$) (60)

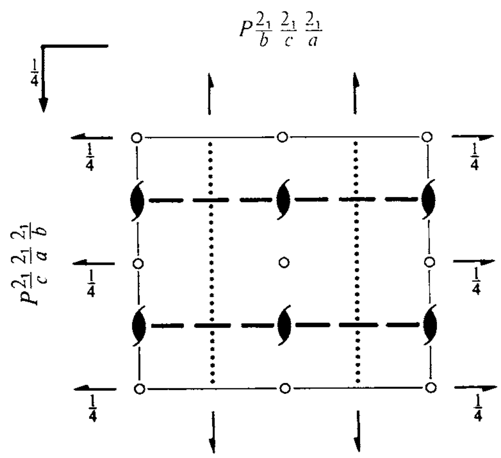
Minimal non-isomorphic supergroups

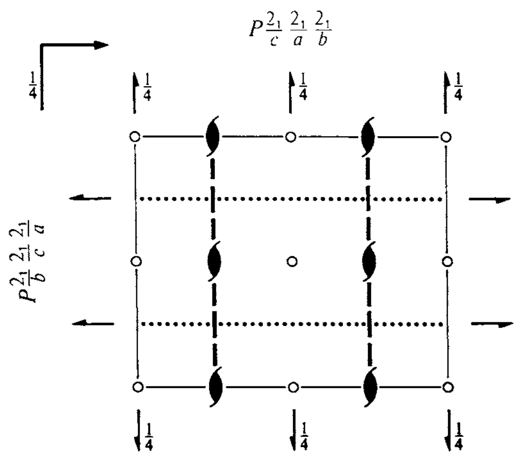
I none

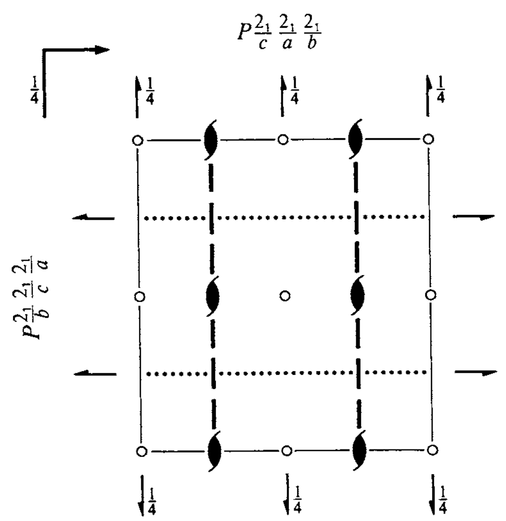
II [2] $Cmcm$ (63); [2] $Aema$ ($Cmce$, 64); [2] $Bbeb$ ($Ccce$, 68); [2] $Ibam$ (72); [2] $Pbmn$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($Pmna$, 53); [2] $Pbcb$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Pcca$, 54); [2] $Pmca$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Pbcm$, 57)

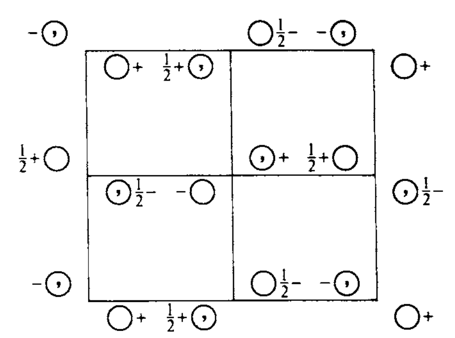
$Pbca$ $\quad D_{2h}^{15}$ $\quad mmm$ $\quad$ Orthorhombic

No. 61 $\quad P\ 2_1/b\ 2_1/c\ 2_1/a$ $\quad$ Patterson symmetry $Pmmm$









Origin at $\bar{1}$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $\bar{1}\quad 0,0,0$	(6) $a\quad x,y,\frac{1}{4}$	(7) $c\quad x,\frac{1}{4},z$	(8) $b\quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	c	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$0kl$: $k=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$h0l$: $l=2n$
							$hk0$: $h=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
							Special: as above, plus
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+k,h+l,k+l=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl : $h+k,h+l,k+l=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $Pbc2_1$ ($Pca2_1$, 29) 1; 2; 7; 8
[2] $Pb2_1a$ ($Pca2_1$, 29) 1; 3; 6; 8
[2] $P2_1ca$ ($Pca2_1$, 29) 1; 4; 6; 7
[2] $P2_12_12_1$ (19) 1; 2; 3; 4
[2] $P112_1/a$ ($P2_1/c$, 14) 1; 2; 5; 6
[2] $P12_1/c1$ ($P2_1/c$, 14) 1; 3; 5; 7
[2] $P2_1/b11$ ($P2_1/c$, 14) 1; 4; 5; 8

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pbca$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$ or $\mathbf{c}'=3\mathbf{c}$) (61)

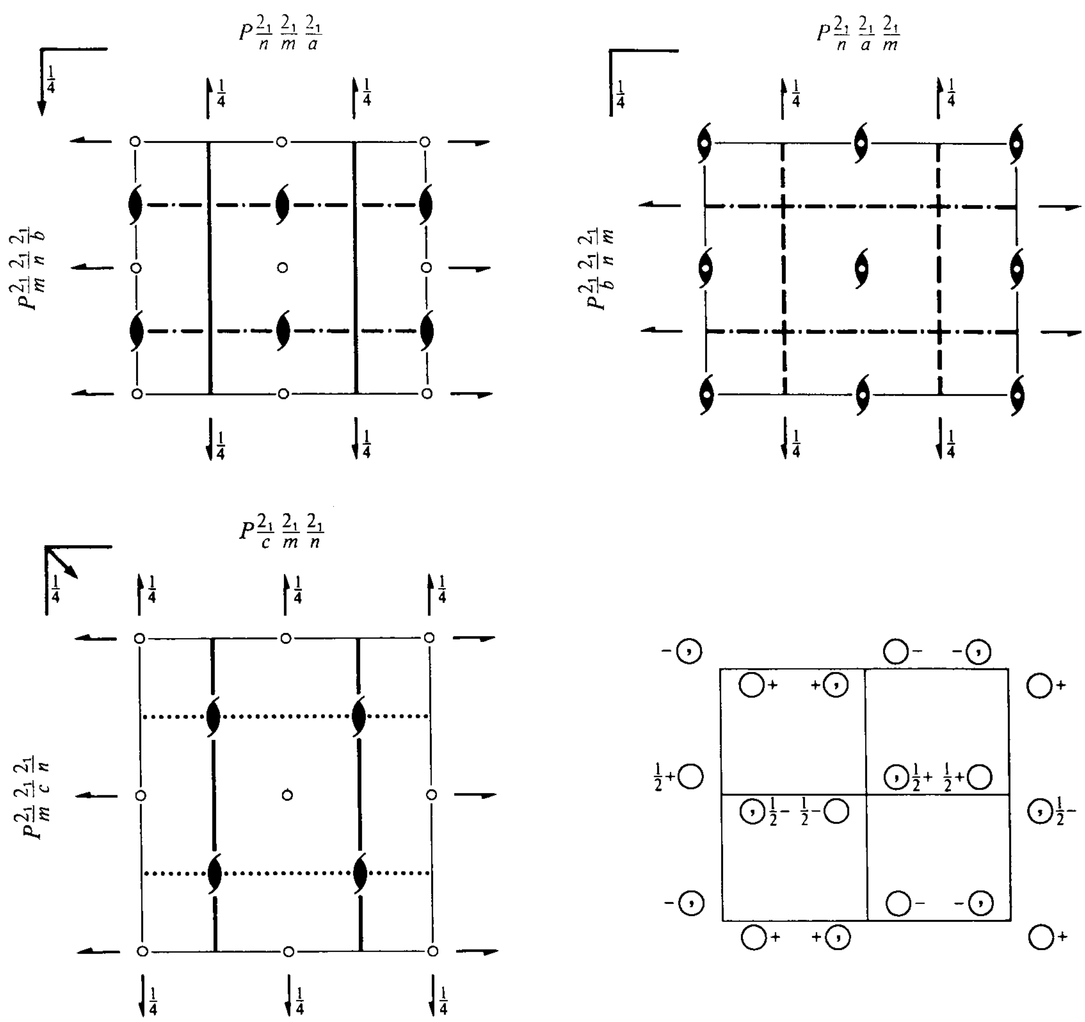
Minimal non-isomorphic supergroups

I [3] $Pa\bar{3}$ (205)

II [2] $Aema$ ($Cmce$, 64); [2] $Bbem$ ($Cmce$, 64); [2] $Cmce$ (64); [2] $Ibca$ (73); [2] $Pbcm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) (57); [2] $Pmca$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Pbcm$, 57); [2] $Pbma$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($Pbcm$, 57)

Pnma D_{2h}^{16} *mmm* Orthorhombic

No. 62 $P\ 2_1/n\ 2_1/m\ 2_1/a$ Patterson symmetry *Pmmm*



Origin at $\bar{1}$ on $1\,2_1\,1$

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}\quad 0,0,0$	(6) $a\quad x,y,\frac{1}{4}$	(7) $m\quad x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0kl$: $k+l=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
							Special: as above, plus
4	c	$.m.$	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$	no extra conditions
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl : $h+l,k=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+l,k=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [010] $p2gg$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Pn2_1a$ ($Pna2_1$, 33)	1; 3; 6; 8
	[2] $Pnm2_1$ ($Pmn2_1$, 31)	1; 2; 7; 8
	[2] $P2_1ma$ ($Pmc2_1$, 26)	1; 4; 6; 7
	[2] $P2_12_12_1$ (19)	1; 2; 3; 4
	[2] $P112_1/a$ ($P2_1/c$, 14)	1; 2; 5; 6
	[2] $P2_1/n11$ ($P2_1/c$, 14)	1; 4; 5; 8
	[2] $P12_1/m1$ ($P2_1/m$, 11)	1; 3; 5; 7

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pnma$ ($\mathbf{a}'=3\mathbf{a}$) (62); [3] $Pnma$ ($\mathbf{b}'=3\mathbf{b}$) (62); [3] $Pnma$ ($\mathbf{c}'=3\mathbf{c}$) (62)

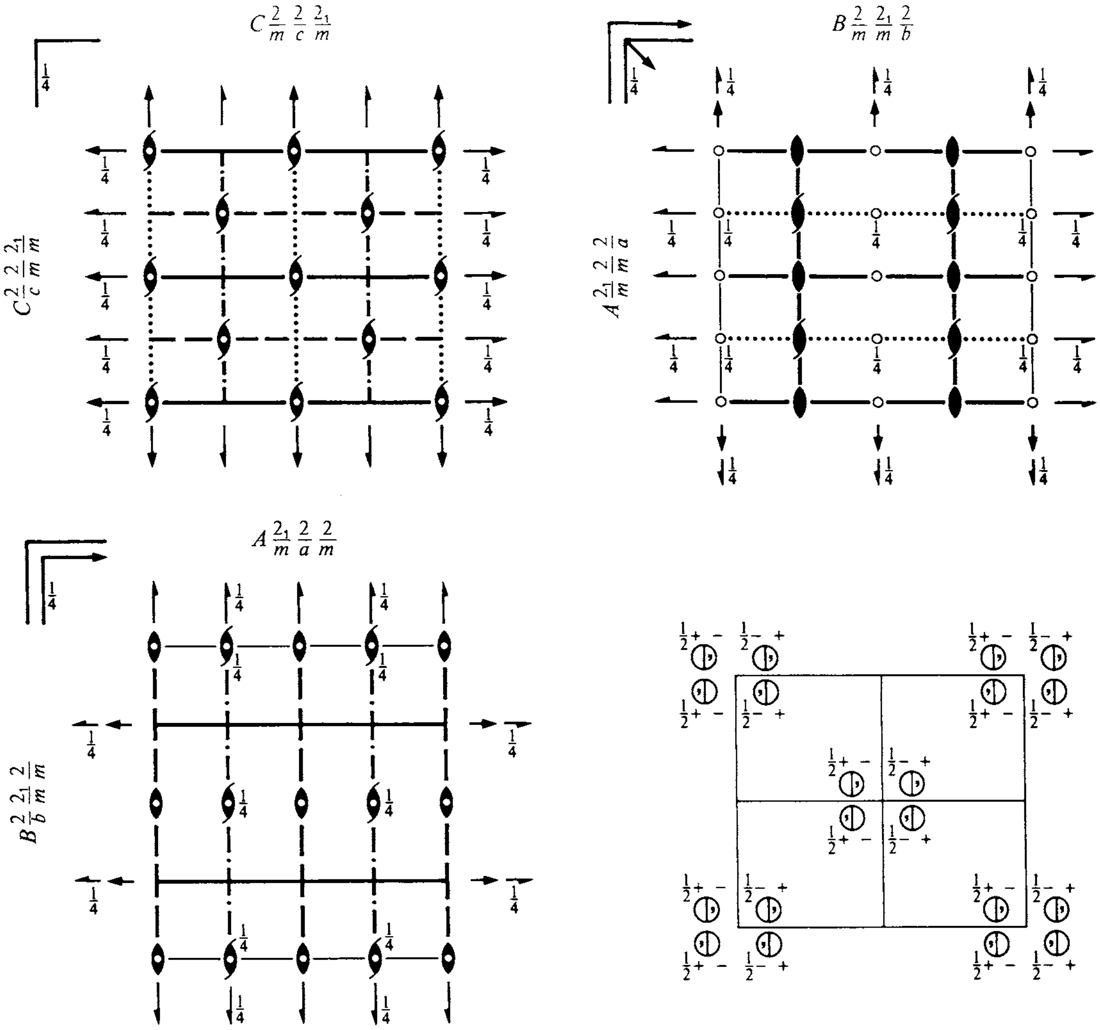
Minimal non-isomorphic supergroups

I none

II [2] $Amma$ ($Cmcm$, 63); [2] $Bbmm$ ($Cmcm$, 63); [2] $Ccme$ ($Cmce$, 64); [2] $Imma$ (74); [2] $Pcma$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Pbam$, 55); [2] $Pbma$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($Pbcm$, 57); [2] $Pnmm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Pmmn$, 59)

Cmcm D_{2h}^{17} *mmm* Orthorhombic

No. 63 $C\ 2/m\ 2/c\ 2_1/m$ Patterson symmetry $Cmmm$



Origin at centre $(2/m)$ at $2/mc2_1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $0,0,z$	(3) 2 $0,y,\frac{1}{4}$	(4) 2 $x,0,0$
(5) $\bar{1}$ $0,0,0$	(6) m $x,y,\frac{1}{4}$	(7) c $x,0,z$	(8) m $0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(8) b $\frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
16	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$	hkl : $h+k=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x},y,z$	$0kl$: $k=2n$
							$h0l$: $h,l=2n$
							$hk0$: $h+k=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
							Special: as above, plus
8	g	$..m$	$x,y,\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$\bar{x},y,\frac{1}{4}$	$x,\bar{y},\frac{3}{4}$	no extra conditions
8	f	$m..$	$0,y,z$	$0,\bar{y},z+\frac{1}{2}$	$0,y,\bar{z}+\frac{1}{2}$	$0,\bar{y},\bar{z}$	no extra conditions
8	e	$2..$	$x,0,0$	$\bar{x},0,\frac{1}{2}$	$\bar{x},0,0$	$x,0,\frac{1}{2}$	hkl : $l=2n$
8	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	hkl : $k,l=2n$
4	c	$m2m$	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			no extra conditions
4	b	$2/m..$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
4	a	$2/m..$	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}\quad \mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}\quad \mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}\quad \mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $C2cm$ ($Ama2$, 40)	(1; 4; 6; 7)+
	[2] $Cm2m$ ($Amm2$, 38)	(1; 3; 6; 8)+
	[2] $Cmc2_1$ (36)	(1; 2; 7; 8)+
	[2] $C222_1$ (20)	(1; 2; 3; 4)+
	[2] $C12/c1$ ($C2/c$, 15)	(1; 3; 5; 7)+
	[2] $C2/m11$ ($C2/m$, 12)	(1; 4; 5; 8)+
	[2] $C112_1/m$ ($P2_1/m$, 11)	(1; 2; 5; 6)+
IIa	[2] $Pbnm$ ($Pnma$, 62)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmcn$ ($Pnma$, 62)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbcn$ (60)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmnm$ ($Pmmn$, 59)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmnn$ ($Pnnm$, 58)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbcm$ (57)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbnn$ ($Pnna$, 52)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmcm$ ($Pmma$, 51)	1; 2; 3; 4; 5; 6; 7; 8
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Cmcm$ ($\mathbf{a}'=3\mathbf{a}$) (63); [3] $Cmcm$ ($\mathbf{b}'=3\mathbf{b}$) (63); [3] $Cmcm$ ($\mathbf{c}'=3\mathbf{c}$) (63)

Minimal non-isomorphic supergroups

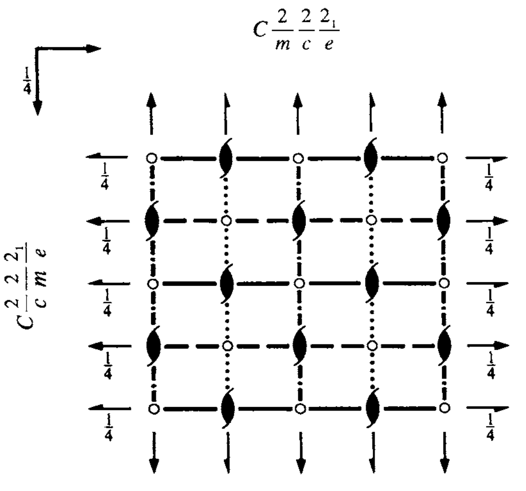
I [3] $P6_3/mcm$ (193); [3] $P6_3/mmc$ (194)

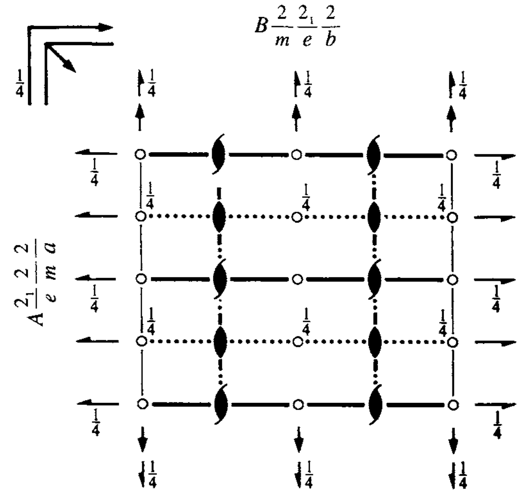
II [2] $Fmmm$ (69); [2] $Pmcm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Pmma$, 51); [2] $Cmmm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (65)

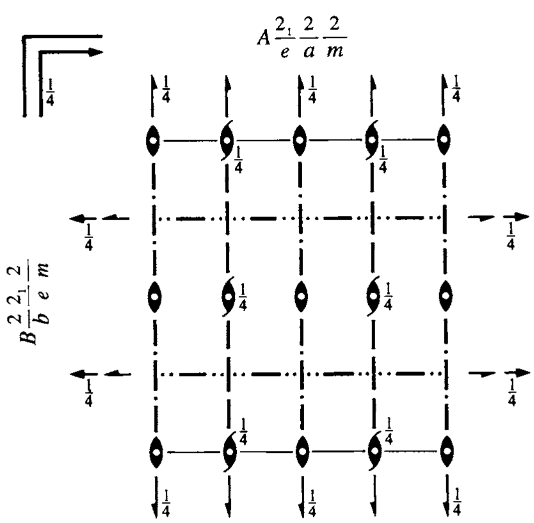
$Cmce$ $\quad D_{2h}^{18}$ $\quad mmm$ $\quad$ Orthorhombic

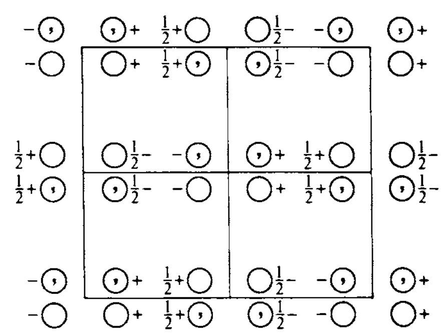
No. 64 $\quad C\ 2/m\ 2/c\ 2_1/e$ $\quad$ Patterson symmetry $Cmmm$

Former space-group symbol $Cmca$; *cf.* Chapter 1.3









Origin at centre $(2/m)$ at $2/mn1$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\quad 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2\quad x,0,0$
(5) $\bar{1}\quad 0,0,0$	(6) $b\quad x,y,\frac{1}{4}$	(7) $c\quad x,\frac{1}{4},z$	(8) $m\quad 0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},0$	(6) $a\quad x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})\quad x,0,z$	(8) $b\quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$			General:
16	g	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (6) $x,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	hkl : $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	f	$m..$	$0,y,z$	$0,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$0,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\bar{y},\bar{z}$	no extra conditions
8	e	$.2.$	$\frac{1}{4},y,\frac{1}{4}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\bar{y},\frac{3}{4}$	$\frac{1}{4},y+\frac{1}{2},\frac{1}{4}$	hkl : $h=2n$
8	d	$2..$	$x,0,0$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\bar{x},0,0$	$x,\frac{1}{2},\frac{1}{2}$	hkl : $k+l=2n$
8	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	hkl : $k,l=2n$
4	b	$2/m..$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$
4	a	$2/m..$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $C2ce$ ($Aea2$, 41)	(1; 4; 6; 7)+
	[2] $Cm2e$ ($Aem2$, 39)	(1; 3; 6; 8)+
	[2] $Cmc2_1$ (36)	(1; 2; 7; 8)+
	[2] $C222_1$ (20)	(1; 2; 3; 4)+
	[2] $C12/c1$ ($C2/c$, 15)	(1; 3; 5; 7)+
	[2] $C112_1/e$ ($P2_1/c$, 14)	(1; 2; 5; 6)+
	[2] $C2/m11$ ($C2/m$, 12)	(1; 4; 5; 8)+
IIa	[2] $Pmnb$ ($Pnma$, 62)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbca$ (61)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbna$ ($Pbcn$, 60)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmca$ ($Pbcm$, 57)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbnb$ ($Pccn$, 56)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmcb$ ($Pbam$, 55)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $Pbcb$ ($Pcca$, 54)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmna$ (53)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Cmce$ ($\mathbf{a}'=3\mathbf{a}$) (64); [3] $Cmce$ ($\mathbf{b}'=3\mathbf{b}$) (64); [3] $Cmce$ ($\mathbf{c}'=3\mathbf{c}$) (64)

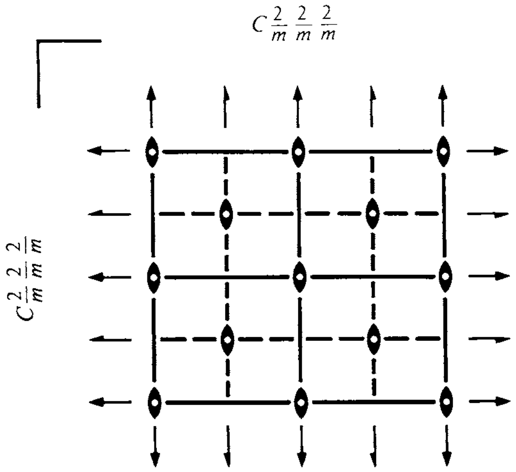
Minimal non-isomorphic supergroups

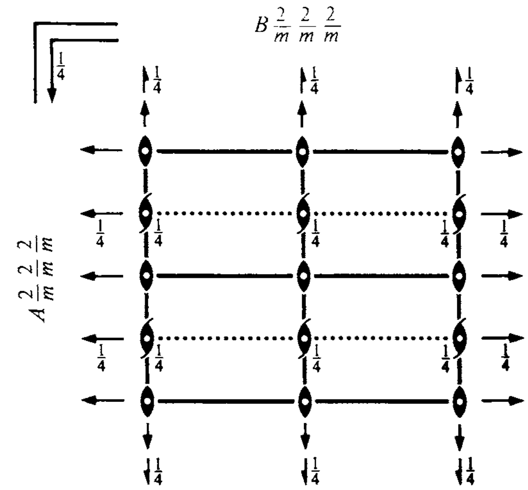
I none

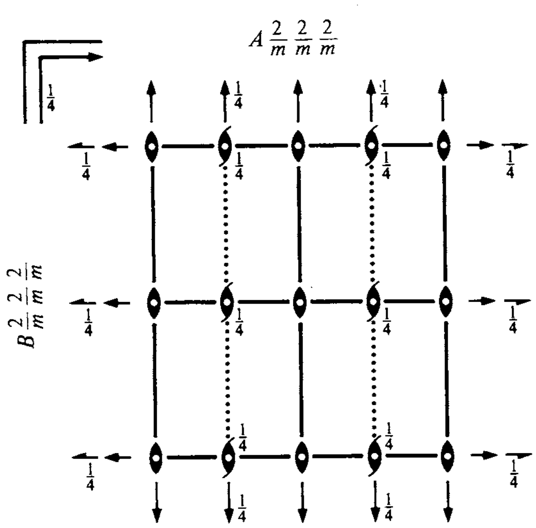
II [2] $Fmmm$ (69); [2] $Pmcm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Pmma$, 51); [2] $Cmme$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (67)

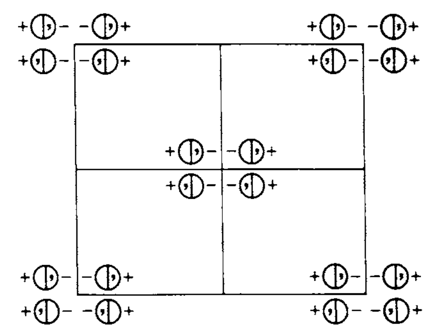
Cmmm D_{2h}^{19} *mmm* Orthorhombic

No. 65 $C\ 2/m\ 2/m\ 2/m$ Patterson symmetry *Cmmm*









Origin at centre (mmm)

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $\bar{1}\quad 0,0,0$	(6) $m\quad x,y,0$	(7) $m\quad x,0,z$	(8) $m\quad 0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},0$	(6) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,0$	(7) $a\quad x,\frac{1}{4},z$	(8) $b\quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
16	r	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}$ (7) $x,\bar{y},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	hkl : $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
8	q	$..m$	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditions
8	p	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,0$	$x,\bar{y},0$	no extra conditions
8	o	$.m.$	$x,0,z$	$\bar{x},0,z$	$\bar{x},0,\bar{z}$	$x,0,\bar{z}$	no extra conditions
8	n	$m..$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	no extra conditions
8	m	$..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z$	hkl : $h=2n$
4	l	$mm2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			no extra conditions
4	k	$mm2$	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	j	$m2m$	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			no extra conditions
4	i	$m2m$	$0,y,0$	$0,\bar{y},0$			no extra conditions
4	h	$2mm$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$			no extra conditions
4	g	$2mm$	$x,0,0$	$\bar{x},0,0$			no extra conditions
4	f	$..2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl : $h=2n$
4	e	$..2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$			hkl : $h=2n$
2	d	mmm	$0,0,\frac{1}{2}$				no extra conditions
2	c	mmm	$\frac{1}{2},0,\frac{1}{2}$				no extra conditions
2	b	mmm	$\frac{1}{2},0,0$				no extra conditions
2	a	mmm	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}\quad \mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}\quad \mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\mathbf{c}\quad \mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Cm2m$ ($Amm2$, 38)	(1; 3; 6; 8)+
	[2] $C2mm$ ($Amm2$, 38)	(1; 4; 6; 7)+
	[2] $Cmm2$ (35)	(1; 2; 7; 8)+
	[2] $C222$ (21)	(1; 2; 3; 4)+
	[2] $C12/m1$ ($C2/m$, 12)	(1; 3; 5; 7)+
	[2] $C2/m11$ ($C2/m$, 12)	(1; 4; 5; 8)+
	[2] $C112/m$ ($P2/m$, 10)	(1; 2; 5; 6)+
IIa	[2] $Pmmn$ (59)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbam$ (55)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbmn$ ($Pmna$, 53)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pman$ ($Pmna$, 53)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmam$ ($Pmma$, 51)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbmm$ ($Pmma$, 51)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pban$ (50)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmmm$ (47)	1; 2; 3; 4; 5; 6; 7; 8

IIb [2] $Cccm$ ($\mathbf{c}' = 2\mathbf{c}$) (66); [2] $Ccmm$ ($\mathbf{c}' = 2\mathbf{c}$) ($Cmcm$, 63); [2] $Cmcm$ ($\mathbf{c}' = 2\mathbf{c}$) (63); [2] $Ibmm$ ($\mathbf{c}' = 2\mathbf{c}$) ($Imma$, 74); [2] $Imam$ ($\mathbf{c}' = 2\mathbf{c}$) ($Imma$, 74); [2] $Ibam$ ($\mathbf{c}' = 2\mathbf{c}$) (72); [2] $Immm$ ($\mathbf{c}' = 2\mathbf{c}$) (71)

Maximal isomorphic subgroups of lowest index

IIc [2] $Cmmm$ ($\mathbf{c}' = 2\mathbf{c}$) (65); [3] $Cmmm$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (65)

Minimal non-isomorphic supergroups

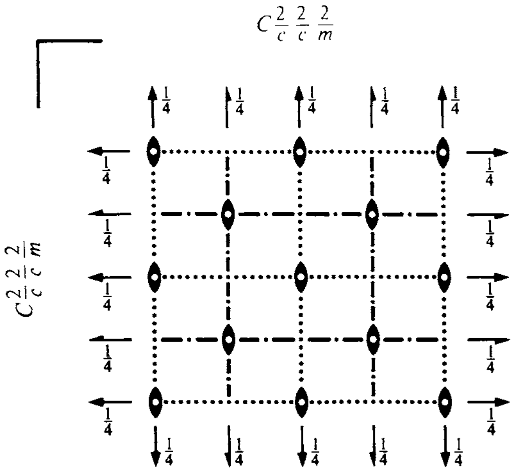
I [2] $P4/mmm$ (123); [2] $P4/mbm$ (127); [2] $P4_2/mcm$ (132); [2] $P4_2/mnm$ (136); [3] $P6/mmm$ (191)

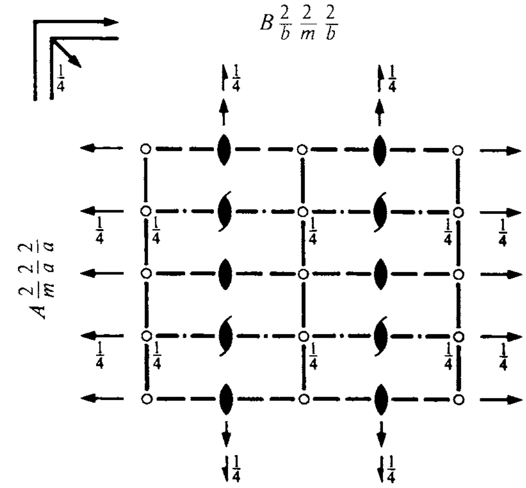
II [2] $Fmmm$ (69); [2] $Pmmm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) (47)

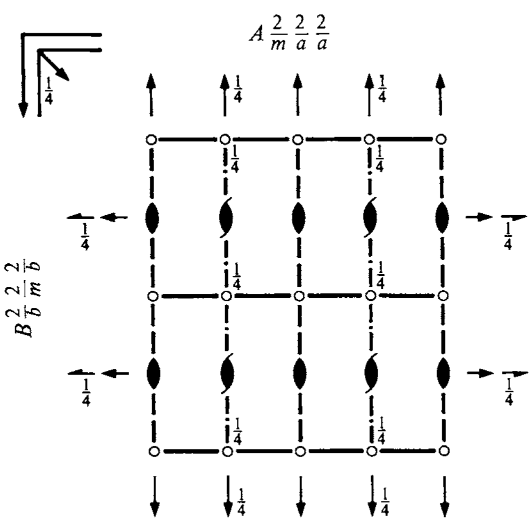
International Tables for Crystallography (2006). Vol. A, Space group 66, pp. 308–309.

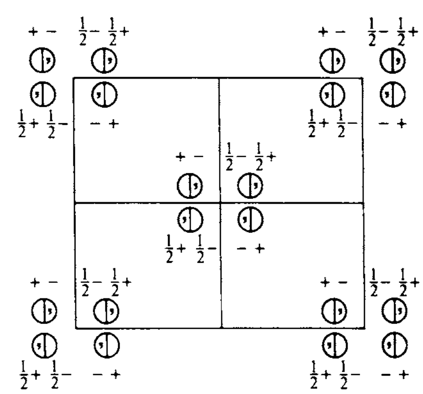
Cccm D_{2h}^{20} *mmm* Orthorhombic

No. 66 $C\ 2/c\ 2/c\ 2/m$ Patterson symmetry *Cmmm*









Origin at centre ($2/m$) at $cc2/m$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,\frac{1}{4}$	(4) 2 $x,0,\frac{1}{4}$
(5) $\bar{1}$ $0,0,0$	(6) m $x,y,0$	(7) c $x,0,z$	(8) c $0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

Maximal isomorphic subgroups of lowest index

IIc [3] *Cccm* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (66); [3] *Cccm* ($\mathbf{c}' = 3\mathbf{c}$) (66)

Minimal non-isomorphic supergroups

I [2] $P4/mcc$ (124); [2] $P4/mnc$ (128); [2] $P4_2/mmc$ (131); [2] $P4_2/mbc$ (135); [3] $P6/mcc$ (192)

II [2] $Fmmm$ (69); [2] $Pccm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) (49); [2] $Cmmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (65)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
16	m	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}+\frac{1}{2}$ (8) $\bar{x},y,z+\frac{1}{2}$	hkl : $h+k=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	l	. . m	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditions
8	k	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl : $k+l=2n$
8	j	. . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl : $l=2n$
8	i	. . 2	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl : $l=2n$
8	h	. 2 .	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	hkl : $l=2n$
8	g	2 . .	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	hkl : $l=2n$
4	f	. . $2/m$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			hkl : $k+l=2n$
4	e	. . $2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl : $k+l=2n$
4	d	. . $2/m$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
4	c	. . $2/m$	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$
4	b	2 2 2	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl : $l=2n$
4	a	2 2 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Cc2m$ ($Ama2$, 40)	(1; 3; 6; 8)+
	[2] $C2cm$ ($Ama2$, 40)	(1; 4; 6; 7)+
	[2] $Ccc2$ (37)	(1; 2; 7; 8)+
	[2] $C222$ (21)	(1; 2; 3; 4)+
	[2] $C12/c1$ ($C2/c$, 15)	(1; 3; 5; 7)+
	[2] $C2/c11$ ($C2/c$, 15)	(1; 4; 5; 8)+
	[2] $C112/m$ ($P2/m$, 10)	(1; 2; 5; 6)+
IIa	[2] $Pnnm$ (58)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pccn$ (56)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pcnm$ ($Pmna$, 53)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pncm$ ($Pmna$, 53)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pncn$ ($Pnna$, 52)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pcnn$ ($Pnna$, 52)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pccm$ (49)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $Pnnn$ (48)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	none	

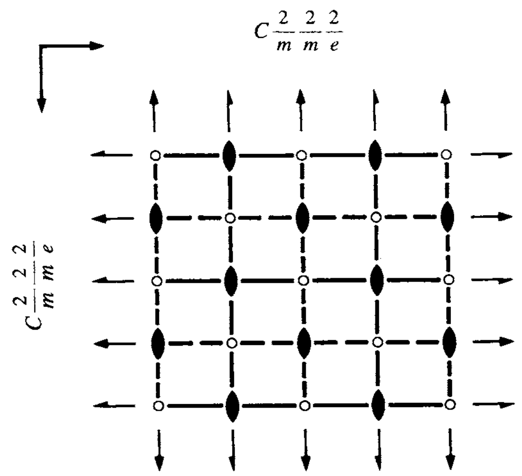
(*Continued on preceding page*)

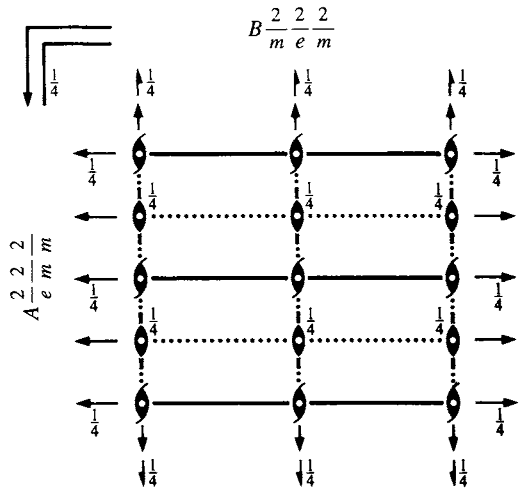
International Tables for Crystallography (2006). Vol. A, Space group 67, pp. 310–311.

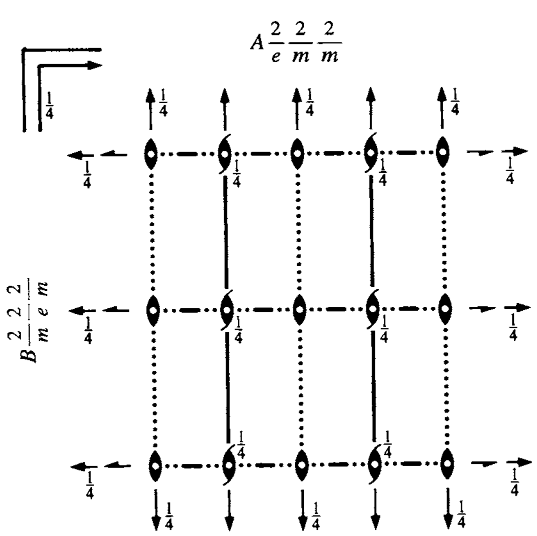
$Cmme$ $\quad D_{2h}^{21}$ $\quad mmm$ $\quad$ Orthorhombic

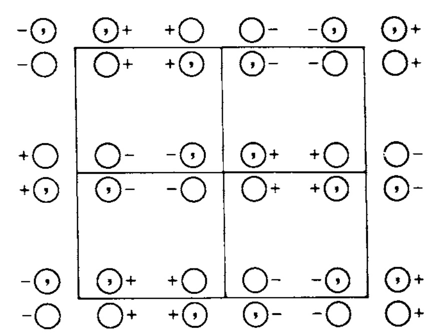
No. 67 $\quad C\ 2/m\ 2/m\ 2/e$ $\quad$ Patterson symmetry $Cmmm$

Former space-group symbol $Cmma$; *cf.* Chapter 1.3









Origin at centre $(2/m)$ at $2/m2_1/ae$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $\bar{1}\quad 0,0,0$	(6) $b\quad x,y,0$	(7) $m\quad x,\frac{1}{4},z$	(8) $m\quad 0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad \frac{1}{4},0,z$	(3) $2\quad \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},0$	(6) $a\quad x,y,0$	(7) $a\quad x,0,z$	(8) $b\quad \frac{1}{4},y,z$

Maximal isomorphic subgroups of lowest index

IIc $\quad$ [2] $Cmme$ ($\mathbf{c}' = 2\mathbf{c}$) (67); [3] $Cmme$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (67)

Minimal non-isomorphic supergroups

I $\quad$ [2] $P4/nbm$ (125); [2] $P4/nmm$ (129); [2] $P4_2/nnm$ (134); [2] $P4_2/ncm$ (138)

II $\quad$ [2] $Fmmm$ (69); [2] $Pmmm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) (47)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},0)+$				General:
16	*o*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y}+\frac{1}{2},z$ (6) $x,y+\frac{1}{2},\bar{z}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	hkl : $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
8	*n*	. *m* .	$x,\frac{1}{4},z$	$\bar{x},\frac{1}{4},z$	$\bar{x},\frac{3}{4},\bar{z}$	$x,\frac{3}{4},\bar{z}$	no extra conditions
8	*m*	*m* . .	$0,y,z$	$0,\bar{y}+\frac{1}{2},z$	$0,y+\frac{1}{2},\bar{z}$	$0,\bar{y},\bar{z}$	no extra conditions
8	*l*	. . 2	$\frac{1}{4},0,z$	$\frac{3}{4},\frac{1}{2},\bar{z}$	$\frac{3}{4},0,\bar{z}$	$\frac{1}{4},\frac{1}{2},z$	hkl : $h=2n$
8	*k*	. 2 .	$\frac{1}{4},y,\frac{1}{2}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\frac{3}{4},\bar{y},\frac{1}{2}$	$\frac{1}{4},y+\frac{1}{2},\frac{1}{2}$	hkl : $h=2n$
8	*j*	. 2 .	$\frac{1}{4},y,0$	$\frac{3}{4},\bar{y}+\frac{1}{2},0$	$\frac{3}{4},\bar{y},0$	$\frac{1}{4},y+\frac{1}{2},0$	hkl : $h=2n$
8	*i*	2 . .	$x,0,\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$x,\frac{1}{2},\frac{1}{2}$	hkl : $h=2n$
8	*h*	2 . .	$x,0,0$	$\bar{x},\frac{1}{2},0$	$\bar{x},0,0$	$x,\frac{1}{2},0$	hkl : $h=2n$
4	*g*	*m m* 2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}$			no extra conditions
4	*f*	. 2/*m* .	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl : $h=2n$
4	*e*	. 2/*m* .	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$			hkl : $h=2n$
4	*d*	2/*m* . .	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $h=2n$
4	*c*	2/*m* . .	$0,0,0$	$0,\frac{1}{2},0$			hkl : $h=2n$
4	*b*	2 2 2	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$			hkl : $h=2n$
4	*a*	2 2 2	$\frac{1}{4},0,0$	$\frac{3}{4},0,0$			hkl : $h=2n$

Symmetry of special projections

Along [001] *p*2*mm*
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] *p*2*mm*
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] *p*2*mm*
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] *Cm*2*e* (*Aem*2, 39)	(1; 3; 6; 8)+
	[2] *C*2*me* (*Aem*2, 39)	(1; 4; 6; 7)+
	[2] *Cmm*2 (35)	(1; 2; 7; 8)+
	[2] *C*222 (21)	(1; 2; 3; 4)+
	[2] *C*112/*e* (*P*2/*c*, 13)	(1; 2; 5; 6)+
	[2] *C*12/*m*1 (*C*2/*m*, 12)	(1; 3; 5; 7)+
	[2] *C*2/*m*11 (*C*2/*m*, 12)	(1; 4; 5; 8)+

IIa	[2] *Pbma* (*Pbcm*, 57)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] *Pmab* (*Pbcm*, 57)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] *Pbaa* (*Pcca*, 54)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] *Pbab* (*Pcca*, 54)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] *Pmmb* (*Pmma*, 51)	1; 2; 3; 4; 5; 6; 7; 8
	[2] *Pmma* (51)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] *Pmaa* (*Pccm*, 49)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] *Pbmb* (*Pccm*, 49)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$

IIb [2] *Ccce* ($\mathbf{c}'=2\mathbf{c}$) (68); [2] *Ccme* ($\mathbf{c}'=2\mathbf{c}$) (*Cmce*, 64); [2] *Cmce* ($\mathbf{c}'=2\mathbf{c}$) (64); [2] *Imma* ($\mathbf{c}'=2\mathbf{c}$) (74); [2] *Ibca* ($\mathbf{c}'=2\mathbf{c}$) (73); [2] *Ibmb* ($\mathbf{c}'=2\mathbf{c}$) (*Ibam*, 72); [2] *Imaa* ($\mathbf{c}'=2\mathbf{c}$) (*Ibam*, 72)

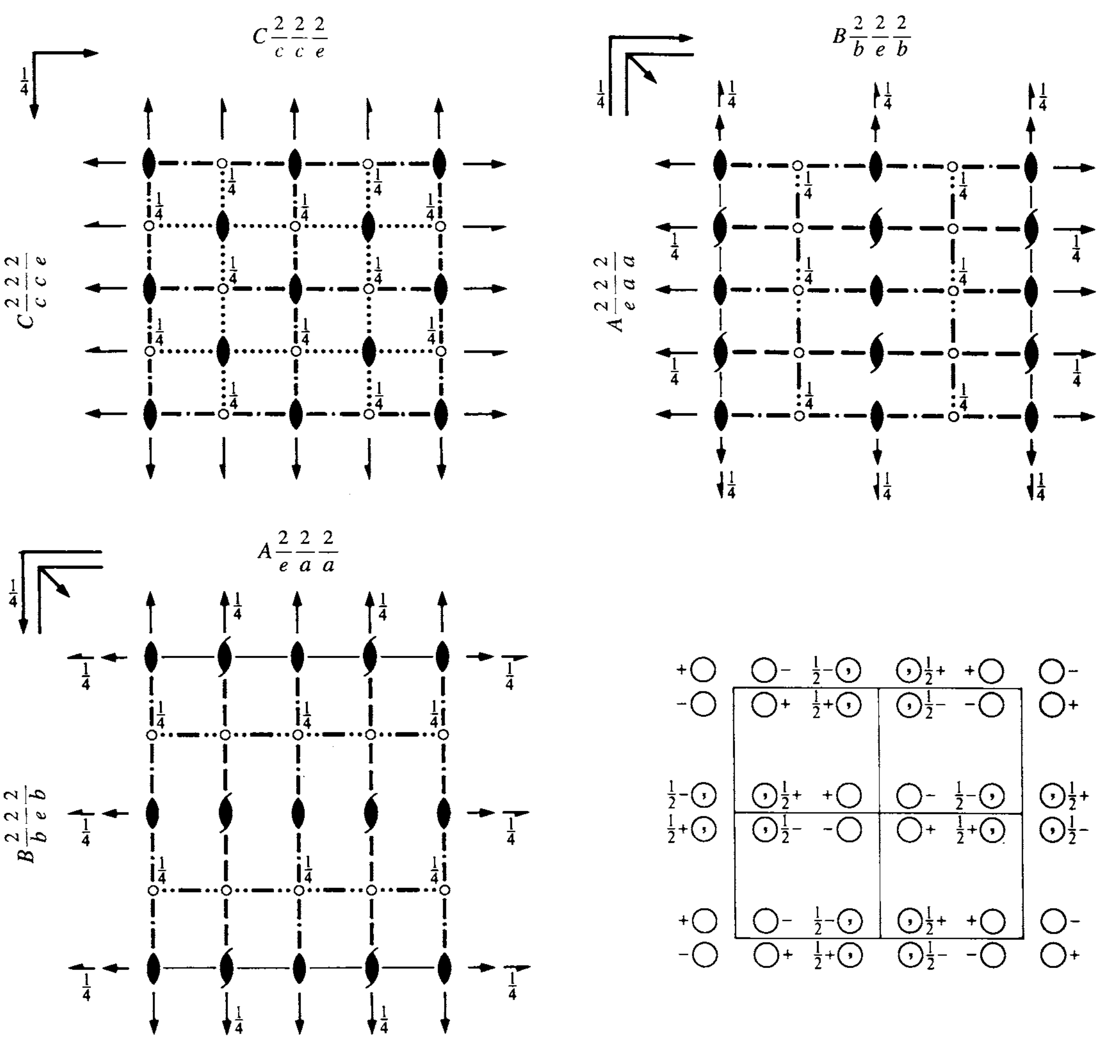
(*Continued on preceding page*)

$Ccce$ $\quad D_{2h}^{22}$ $\quad mmm$ $\quad$ Orthorhombic

No. 68 $\quad C\ 2/c\ 2/c\ 2/e$ $\quad$ Patterson symmetry $Cmmm$

Former space-group symbol $Ccca$; *cf.* Chapter 1.3

ORIGIN CHOICE 1



Origin at 222 at $2/n2/n2$, at $0, \frac{1}{4}, \frac{1}{4}$ from $\bar{1}$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $2\quad 0,y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $\bar{1}\quad 0,\frac{1}{4},\frac{1}{4}$	(6) $a\quad x,y,\frac{1}{4}$	(7) $c\quad x,\frac{1}{4},z$	(8) $c\quad \frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad 0,0,z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(4) $2\quad x,0,0$
(5) $\bar{1}\quad \frac{1}{4},0,\frac{1}{4}$	(6) $b\quad x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})\quad x,0,z$	(8) $n(0,\frac{1}{2},\frac{1}{2})\quad 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates $(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},0)+$ — Reflection conditions

								General:
16	i	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x},y,\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$		hkl : $h+k=2n$
			(5) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$		$0kl$: $k,l=2n$
								$h0l$: $h,l=2n$
								$hk0$: $h,k=2n$
								$h00$: $h=2n$
								$0k0$: $k=2n$
								$00l$: $l=2n$
								Special: as above, plus
8	h	..2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$		hkl : $l=2n$
8	g	..2	$0,0,z$	$0,0,\bar{z}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$		hkl : $k+l=2n$
8	f	.2.	$0,y,0$	$\frac{1}{2},\bar{y}+\frac{1}{2},0$	$0,\bar{y}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},y,\frac{1}{2}$		hkl : $k+l=2n$
8	e	2..	$x,0,0$	$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},0,\frac{1}{2}$		hkl : $k+l=2n$
8	d	$\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$0,\frac{1}{4},\frac{3}{4}$	$\frac{1}{2},\frac{1}{4},\frac{3}{4}$		hkl : $k,l=2n$
8	c	$\bar{1}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},0,\frac{3}{4}$	$\frac{3}{4},\frac{1}{2},\frac{3}{4}$		hkl : $k,l=2n$
4	b	222	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$				hkl : $k+l=2n$
4	a	222	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$				hkl : $k+l=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\quad \mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\quad \mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\quad \mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Cc2e$ ($Aea2$, 41)	(1; 3; 6; 8)+
	[2] $C2ce$ ($Aea2$, 41)	(1; 4; 6; 7)+
	[2] $Ccc2$ (37)	(1; 2; 7; 8)+
	[2] $C222$ (21)	(1; 2; 3; 4)+
	[2] $C12/c1$ ($C2/c$, 15)	(1; 3; 5; 7)+
	[2] $C2/c11$ ($C2/c$, 15)	(1; 4; 5; 8)+
	[2] $C112/e$ ($P2/c$, 13)	(1; 2; 5; 6)+
IIa	[2] $Pcnb$ ($Pbcn$, 60)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pnca$ ($Pbcn$, 60)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pcca$ (54)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $Pccb$ ($Pcca$, 54)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pnnb$ ($Pnna$, 52)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pnna$ (52)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pncb$ ($Pban$, 50)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pcna$ ($Pban$, 50)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Ccce$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (68); [3] $Ccce$ ($\mathbf{c}'=3\mathbf{c}$) (68)

Minimal non-isomorphic supergroups

I [2] $P4/nnc$ (126); [2] $P4/ncc$ (130); [2] $P4_2/nbc$ (133); [2] $P4_2/nmc$ (137)

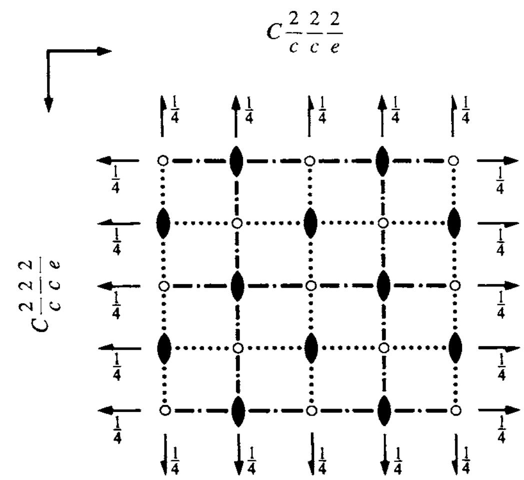
II [2] $Fmmm$ (69); [2] $Pccm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (49); [2] $Cmme$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (67)

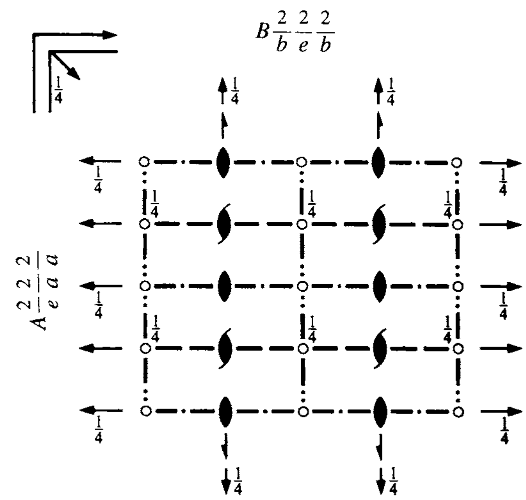
$Ccce$ $\quad D_{2h}^{22}$ $\quad mmm$ $\quad$ Orthorhombic

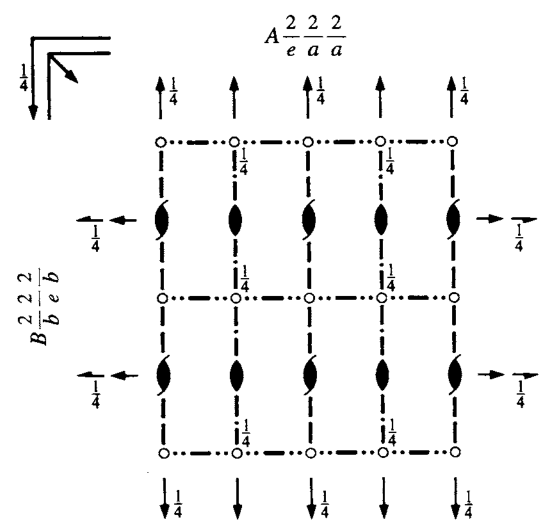
No. 68 $\quad C\,2/c\,2/c\,2/e$ $\quad$ Patterson symmetry $Cmmm$

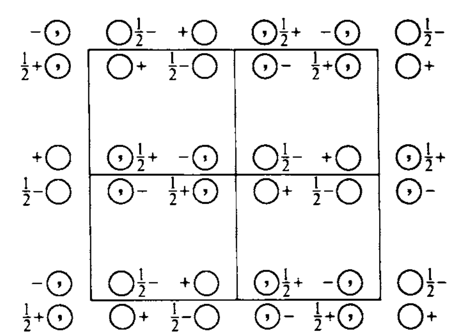
Former space-group symbol $Ccca$; *cf.* Chapter 1.3

ORIGIN CHOICE 2









Origin at $\bar{1}$ at nce, at $0,-\frac{1}{4},-\frac{1}{4}$ from 222

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad \frac{1}{4},0,z$	(3) $2\quad 0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,0,\frac{1}{4}$
(5) $\bar{1}\quad 0,0,0$	(6) $a\quad x,y,0$	(7) $c\quad x,0,z$	(8) $c\quad \frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2\quad x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},0$	(6) $b\quad x,y,0$	(7) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})\quad 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
16	i	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z$ (6) $x+\frac{1}{2},y,\bar{z}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	hkl : $h+k=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	h	..2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}+\frac{1}{2}$	$\frac{3}{4},0,\bar{z}$	$\frac{1}{4},0,z+\frac{1}{2}$	hkl : $l=2n$
8	g	..2	$0,\frac{1}{4},z$	$0,\frac{1}{4},\bar{z}+\frac{1}{2}$	$0,\frac{3}{4},\bar{z}$	$0,\frac{3}{4},z+\frac{1}{2}$	hkl : $k+l=2n$
8	f	.2.	$0,y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$\frac{1}{2},y,\frac{3}{4}$	hkl : $k+l=2n$
8	e	2..	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	hkl : $k+l=2n$
8	d	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl : $k,l=2n$
8	c	$\bar{1}$	$\frac{1}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	hkl : $k,l=2n$
4	b	222	$0,\frac{1}{4},\frac{3}{4}$	$0,\frac{3}{4},\frac{1}{4}$			hkl : $k+l=2n$
4	a	222	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{3}{4}$			hkl : $k+l=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Cc2e$ ($Aea2$, 41)	(1; 3; 6; 8)+
	[2] $C2ce$ ($Aea2$, 41)	(1; 4; 6; 7)+
	[2] $Ccc2$ (37)	(1; 2; 7; 8)+
	[2] $C222$ (21)	(1; 2; 3; 4)+
	[2] $C12/c1$ ($C2/c$, 15)	(1; 3; 5; 7)+
	[2] $C2/c11$ ($C2/c$, 15)	(1; 4; 5; 8)+
	[2] $C112/e$ ($P2/c$, 13)	(1; 2; 5; 6)+
IIa	[2] $Pcnb$ ($Pbcn$, 60)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pnca$ ($Pbcn$, 60)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pcca$ (54)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $Pccb$ ($Pcca$, 54)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pnnb$ ($Pnna$, 52)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pnna$ (52)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pncb$ ($Pban$, 50)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pcna$ ($Pban$, 50)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Ccce$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (68); [3] $Ccce$ ($\mathbf{c}'=3\mathbf{c}$) (68)

Minimal non-isomorphic supergroups

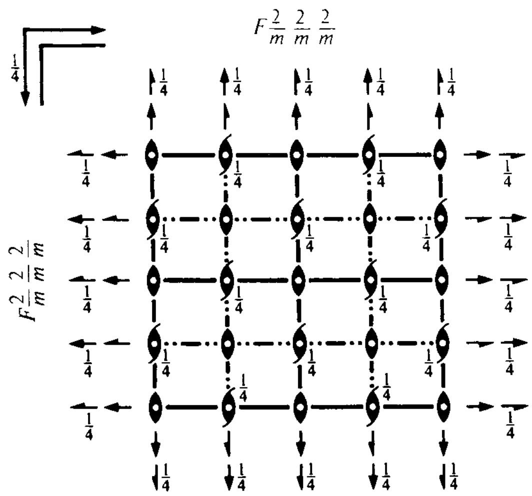
I [2] $P4/nnc$ (126); [2] $P4/ncc$ (130); [2] $P4_2/nbc$ (133); [2] $P4_2/nmc$ (137)

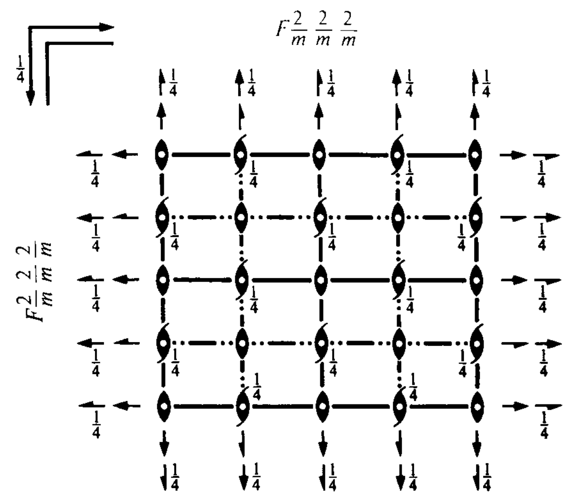
II [2] $Fmmm$ (69); [2] $Pccm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) (49); [2] $Cmme$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (67)

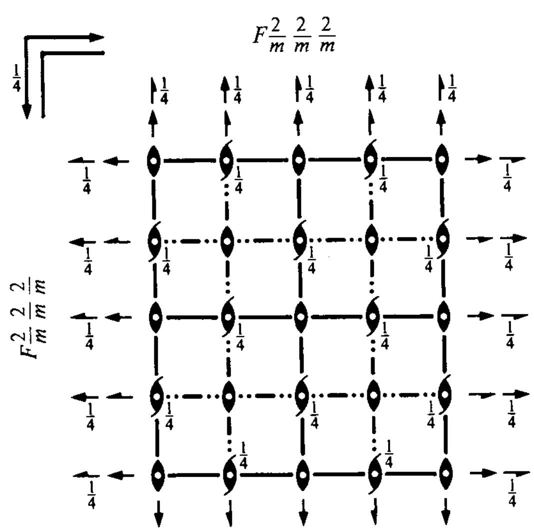
International Tables for Crystallography (2006). Vol. A, Space group 69, pp. 316–318.

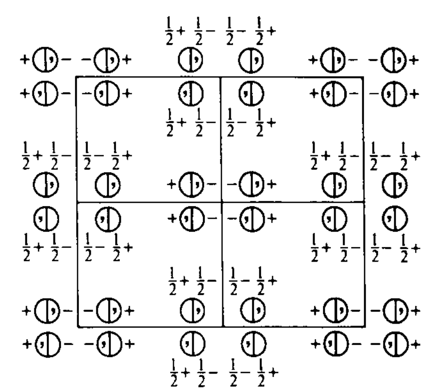
$Fmmm$ $\quad D_{2h}^{23}$ $\quad mmm$ $\quad$ Orthorhombic

No. 69 $\quad F\ 2/m\ 2/m\ 2/m$ $\quad$ Patterson symmetry $Fmmm$









Origin at centre (mmm)

Asymmetric unit $\quad 0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $\bar{1}\quad 0,0,0$	(6) $m\quad x,y,0$	(7) $m\quad x,0,z$	(8) $m\quad 0,y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2\quad x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}\quad 0,\frac{1}{4},\frac{1}{4}$	(6) $b\quad x,y,\frac{1}{4}$	(7) $c\quad x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})\quad 0,y,z$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,0,\frac{1}{4}$
(5) $\bar{1}\quad \frac{1}{4},0,\frac{1}{4}$	(6) $a\quad x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})\quad x,0,z$	(8) $c\quad \frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},0$	(6) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,0$	(7) $a\quad x,\frac{1}{4},z$	(8) $b\quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
32	p	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hkl : $h+k,h+l,k+l=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x,\bar{y},z$	(8) $\bar{x},y,z$	$0kl$: $k,l=2n$
							$h0l$: $h,l=2n$
							$hk0$: $h,k=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
							Special: as above, plus
16	o	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,0$	$x,\bar{y},0$	no extra conditions
16	n	$.m.$	$x,0,z$	$\bar{x},0,z$	$\bar{x},0,\bar{z}$	$x,0,\bar{z}$	no extra conditions
16	m	$m..$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	no extra conditions
16	l	$2..$	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	$x,\frac{1}{4},\frac{3}{4}$	hkl : $h=2n$
16	k	$.2.$	$\frac{1}{4},y,\frac{1}{4}$	$\frac{3}{4},\bar{y},\frac{1}{4}$	$\frac{3}{4},\bar{y},\frac{3}{4}$	$\frac{1}{4},y,\frac{3}{4}$	hkl : $h=2n$
16	j	$..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z$	hkl : $h=2n$
8	i	$mm2$	$0,0,z$	$0,0,\bar{z}$			no extra conditions
8	h	$m2m$	$0,y,0$	$0,\bar{y},0$			no extra conditions
8	g	$2mm$	$x,0,0$	$\bar{x},0,0$			no extra conditions
8	f	222	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$			hkl : $h=2n$
8	e	$..2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$			hkl : $h=2n$
8	d	$.2/m.$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{3}{4},0,\frac{1}{4}$			hkl : $h=2n$
8	c	$2/m..$	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$			hkl : $h=2n$
4	b	mmm	$0,0,\frac{1}{2}$				no extra conditions
4	a	mmm	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Fmm2$ (42)	(1; 2; 7; 8)+
	[2] $Fm2m$ ($Fmm2$, 42)	(1; 3; 6; 8)+
	[2] $F2mm$ ($Fmm2$, 42)	(1; 4; 6; 7)+
	[2] $F222$ (22)	(1; 2; 3; 4)+
	[2] $F112/m$ ($C2/m$, 12)	(1; 2; 5; 6)+
	[2] $F12/m1$ ($C2/m$, 12)	(1; 3; 5; 7)+
	[2] $F2/m11$ ($C2/m$, 12)	(1; 4; 5; 8)+
IIa	[2] $Aeaa$ ($Ccce$, 68)	1; 2; 3; 4; $(1;\ 2;\ 3;\ 4)+(0,\frac{1}{2},\frac{1}{2})$; $(5;\ 6;\ 7;\ 8)+(\frac{1}{2},0,\frac{1}{2})$; $(5;\ 6;\ 7;\ 8)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $Bbeb$ ($Ccce$, 68)	1; 2; 3; 4; $(1;\ 2;\ 3;\ 4)+(\frac{1}{2},0,\frac{1}{2})$; $(5;\ 6;\ 7;\ 8)+(0,\frac{1}{2},\frac{1}{2})$; $(5;\ 6;\ 7;\ 8)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $Ccce$ (68)	1; 2; 3; 4; $(1;\ 2;\ 3;\ 4)+(\frac{1}{2},\frac{1}{2},0)$; $(5;\ 6;\ 7;\ 8)+(0,\frac{1}{2},\frac{1}{2})$; $(5;\ 6;\ 7;\ 8)+(\frac{1}{2},0,\frac{1}{2})$
	[2] $Cmme$ (67)	1; 2; 7; 8; $(1;\ 2;\ 7;\ 8)+(\frac{1}{2},\frac{1}{2},0)$; $(3;\ 4;\ 5;\ 6)+(0,\frac{1}{2},\frac{1}{2})$; $(3;\ 4;\ 5;\ 6)+(\frac{1}{2},0,\frac{1}{2})$
	[2] $Bmem$ ($Cmme$, 67)	1; 3; 6; 8; $(1;\ 3;\ 6;\ 8)+(\frac{1}{2},0,\frac{1}{2})$; $(2;\ 4;\ 5;\ 7)+(0,\frac{1}{2},\frac{1}{2})$; $(2;\ 4;\ 5;\ 7)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $Aemm$ ($Cmme$, 67)	1; 4; 6; 7; $(1;\ 4;\ 6;\ 7)+(0,\frac{1}{2},\frac{1}{2})$; $(2;\ 3;\ 5;\ 8)+(\frac{1}{2},0,\frac{1}{2})$; $(2;\ 3;\ 5;\ 8)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $Cccm$ (66)	1; 2; 5; 6; $(1;\ 2;\ 5;\ 6)+(\frac{1}{2},\frac{1}{2},0)$; $(3;\ 4;\ 7;\ 8)+(0,\frac{1}{2},\frac{1}{2})$; $(3;\ 4;\ 7;\ 8)+(\frac{1}{2},0,\frac{1}{2})$
	[2] $Bbmb$ ($Cccm$, 66)	1; 3; 5; 7; $(1;\ 3;\ 5;\ 7)+(\frac{1}{2},0,\frac{1}{2})$; $(2;\ 4;\ 6;\ 8)+(0,\frac{1}{2},\frac{1}{2})$; $(2;\ 4;\ 6;\ 8)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $Amaa$ ($Cccm$, 66)	1; 4; 5; 8; $(1;\ 4;\ 5;\ 8)+(0,\frac{1}{2},\frac{1}{2})$; $(2;\ 3;\ 6;\ 7)+(\frac{1}{2},0,\frac{1}{2})$; $(2;\ 3;\ 6;\ 7)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $Ammm$ ($Cmmm$, 65)	1; 2; 3; 4; 5; 6; 7; 8; $(1;\ 2;\ 3;\ 4;\ 5;\ 6;\ 7;\ 8)+(0,\frac{1}{2},\frac{1}{2})$
	[2] $Bmmm$ ($Cmmm$, 65)	1; 2; 3; 4; 5; 6; 7; 8; $(1;\ 2;\ 3;\ 4;\ 5;\ 6;\ 7;\ 8)+(\frac{1}{2},0,\frac{1}{2})$
	[2] $Cmmm$ (65)	1; 2; 3; 4; 5; 6; 7; 8; $(1;\ 2;\ 3;\ 4;\ 5;\ 6;\ 7;\ 8)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $Aeam$ ($Cmce$, 64)	1; 2; 5; 6; $(1;\ 2;\ 5;\ 6)+(0,\frac{1}{2},\frac{1}{2})$; $(3;\ 4;\ 7;\ 8)+(\frac{1}{2},0,\frac{1}{2})$; $(3;\ 4;\ 7;\ 8)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $Bbem$ ($Cmce$, 64)	1; 2; 5; 6; $(1;\ 2;\ 5;\ 6)+(\frac{1}{2},0,\frac{1}{2})$; $(3;\ 4;\ 7;\ 8)+(0,\frac{1}{2},\frac{1}{2})$; $(3;\ 4;\ 7;\ 8)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $Aema$ ($Cmce$, 64)	1; 3; 5; 7; $(1;\ 3;\ 5;\ 7)+(0,\frac{1}{2},\frac{1}{2})$; $(2;\ 4;\ 6;\ 8)+(\frac{1}{2},0,\frac{1}{2})$; $(2;\ 4;\ 6;\ 8)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $Ccme$ ($Cmce$, 64)	1; 3; 5; 7; $(1;\ 3;\ 5;\ 7)+(\frac{1}{2},\frac{1}{2},0)$; $(2;\ 4;\ 6;\ 8)+(0,\frac{1}{2},\frac{1}{2})$; $(2;\ 4;\ 6;\ 8)+(\frac{1}{2},0,\frac{1}{2})$
	[2] $Bmeb$ ($Cmce$, 64)	1; 4; 5; 8; $(1;\ 4;\ 5;\ 8)+(\frac{1}{2},0,\frac{1}{2})$; $(2;\ 3;\ 6;\ 7)+(0,\frac{1}{2},\frac{1}{2})$; $(2;\ 3;\ 6;\ 7)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $Cmce$ (64)	1; 4; 5; 8; $(1;\ 4;\ 5;\ 8)+(\frac{1}{2},\frac{1}{2},0)$; $(2;\ 3;\ 6;\ 7)+(0,\frac{1}{2},\frac{1}{2})$; $(2;\ 3;\ 6;\ 7)+(\frac{1}{2},0,\frac{1}{2})$
	[2] $Amam$ ($Cmcm$, 63)	1; 3; 6; 8; $(1;\ 3;\ 6;\ 8)+(0,\frac{1}{2},\frac{1}{2})$; $(2;\ 4;\ 5;\ 7)+(\frac{1}{2},0,\frac{1}{2})$; $(2;\ 4;\ 5;\ 7)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $Amma$ ($Cmcm$, 63)	1; 2; 7; 8; $(1;\ 2;\ 7;\ 8)+(0,\frac{1}{2},\frac{1}{2})$; $(3;\ 4;\ 5;\ 6)+(\frac{1}{2},0,\frac{1}{2})$; $(3;\ 4;\ 5;\ 6)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $Bmmb$ ($Cmcm$, 63)	1; 2; 7; 8; $(1;\ 2;\ 7;\ 8)+(\frac{1}{2},0,\frac{1}{2})$; $(3;\ 4;\ 5;\ 6)+(0,\frac{1}{2},\frac{1}{2})$; $(3;\ 4;\ 5;\ 6)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $Bbmm$ ($Cmcm$, 63)	1; 4; 6; 7; $(1;\ 4;\ 6;\ 7)+(\frac{1}{2},0,\frac{1}{2})$; $(2;\ 3;\ 5;\ 8)+(0,\frac{1}{2},\frac{1}{2})$; $(2;\ 3;\ 5;\ 8)+(\frac{1}{2},\frac{1}{2},0)$
	[2] $Cmcm$ (63)	1; 3; 6; 8; $(1;\ 3;\ 6;\ 8)+(\frac{1}{2},\frac{1}{2},0)$; $(2;\ 4;\ 5;\ 7)+(0,\frac{1}{2},\frac{1}{2})$; $(2;\ 4;\ 5;\ 7)+(\frac{1}{2},0,\frac{1}{2})$
	[2] $Ccmm$ ($Cmcm$, 63)	1; 4; 6; 7; $(1;\ 4;\ 6;\ 7)+(\frac{1}{2},\frac{1}{2},0)$; $(2;\ 3;\ 5;\ 8)+(0,\frac{1}{2},\frac{1}{2})$; $(2;\ 3;\ 5;\ 8)+(\frac{1}{2},0,\frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Fmmm$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (69)

Minimal non-isomorphic supergroups

I [2] $I4/mmm$ (139); [2] $I4/mcm$ (140); [3] $Fm\bar{3}$ (202)

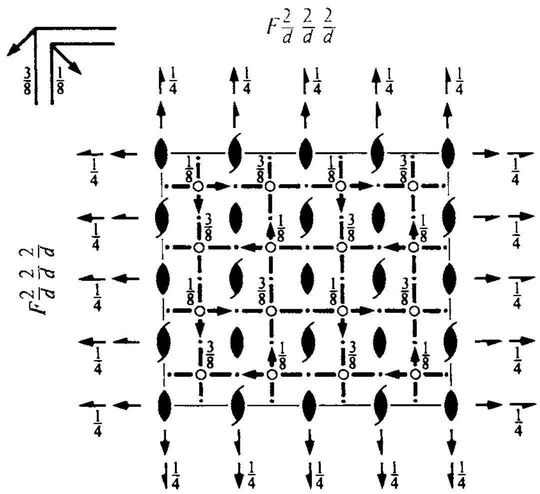
II [2] $Pmmm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (47)

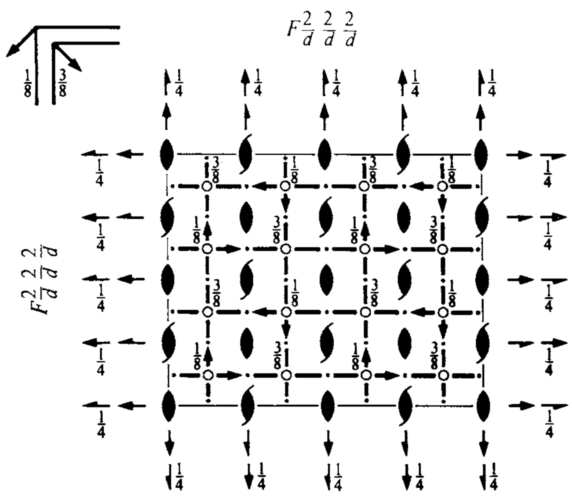
International Tables for Crystallography (2006). Vol. A, Space group 70, pp. 320–323.

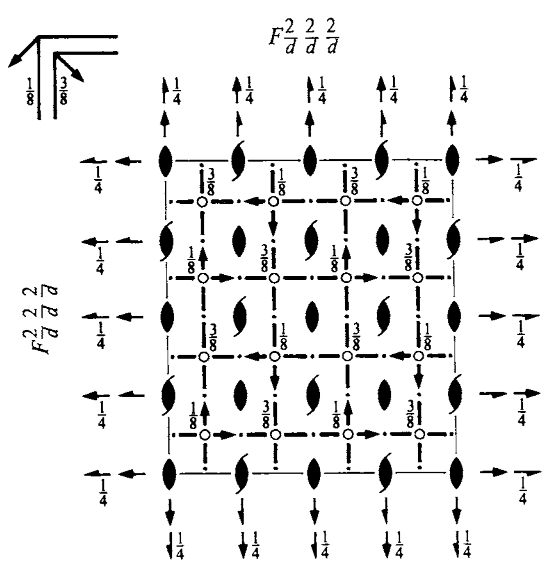
$Fddd$ $\quad D_{2h}^{24}$ $\quad mmm$ $\quad$ Orthorhombic

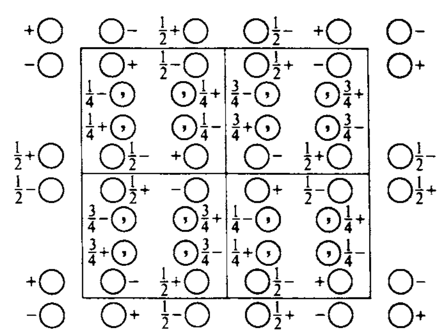
No. 70 $\quad F\ 2/d\ 2/d\ 2/d$ $\quad$ Patterson symmetry $Fmmm$

ORIGIN CHOICE 1









Origin at 222, at $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ from $\bar{1}$

Asymmetric unit $\quad 0 \le x \le \frac{1}{8};\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $\bar{1}\quad \frac{1}{8},\frac{1}{8},\frac{1}{8}$	(6) $d(\frac{1}{4},\frac{1}{4},0)\quad x,y,\frac{1}{8}$	(7) $d(\frac{1}{4},0,\frac{1}{4})\quad x,\frac{1}{8},z$	(8) $d(0,\frac{1}{4},\frac{1}{4})\quad \frac{1}{8},y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2\quad x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}\quad \frac{1}{8},\frac{3}{8},\frac{3}{8}$	(6) $d(\frac{1}{4},\frac{3}{4},0)\quad x,y,\frac{3}{8}$	(7) $d(\frac{1}{4},0,\frac{3}{4})\quad x,\frac{3}{8},z$	(8) $d(0,\frac{3}{4},\frac{3}{4})\quad \frac{1}{8},y,z$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,0,\frac{1}{4}$
(5) $\bar{1}\quad \frac{3}{8},\frac{1}{8},\frac{3}{8}$	(6) $d(\frac{3}{4},\frac{1}{4},0)\quad x,y,\frac{3}{8}$	(7) $d(\frac{3}{4},0,\frac{3}{4})\quad x,\frac{1}{8},z$	(8) $d(0,\frac{1}{4},\frac{3}{4})\quad \frac{3}{8},y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $\bar{1}\quad \frac{3}{8},\frac{3}{8},\frac{1}{8}$	(6) $d(\frac{3}{4},\frac{3}{4},0)\quad x,y,\frac{1}{8}$	(7) $d(\frac{3}{4},0,\frac{1}{4})\quad x,\frac{3}{8},z$	(8) $d(0,\frac{3}{4},\frac{1}{4})\quad \frac{3}{8},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	General:
32	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hkl : $h+k=2n$ and $h+l,k+l=2n$
			(5) $\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(6) $x+\frac{1}{4},y+\frac{1}{4},\bar{z}+\frac{1}{4}$	(7) $x+\frac{1}{4},\bar{y}+\frac{1}{4},z+\frac{1}{4}$	(8) $\bar{x}+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$0kl$: $k+l=4n$ and $k,l=2n$
							$h0l$: $h+l=4n$ and $h,l=2n$
							$hk0$: $h+k=4n$ and $h,k=2n$
							$h00$: $h=4n$
							$0k0$: $k=4n$
							$00l$: $l=4n$
							Special: as above, plus
16	g	. . 2	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{4},\frac{1}{4},\bar{z}+\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{4}$	hkl : $h=2n+1$ or $h+k+l=4n$
16	f	. 2 .	$0,y,0$	$0,\bar{y},0$	$\frac{1}{4},\bar{y}+\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},y+\frac{1}{4},\frac{1}{4}$	
16	e	2 . .	$x,0,0$	$\bar{x},0,0$	$\bar{x}+\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$x+\frac{1}{4},\frac{1}{4},\frac{1}{4}$	
16	d	$\bar{1}$	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{3}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{3}{8}$	$\frac{5}{8},\frac{3}{8},\frac{3}{8}$	hkl : $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16	c	$\bar{1}$	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{7}{8},\frac{1}{8}$	$\frac{7}{8},\frac{1}{8},\frac{7}{8}$	$\frac{1}{8},\frac{7}{8},\frac{7}{8}$	
8	b	2 2 2	$0,0,\frac{1}{2}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$			hkl : $h=2n+1$ or $h+k+l=4n$
8	a	2 2 2	$0,0,0$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$			

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $c2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $F\,d\,d\,2$ (43) (1; 2; 7; 8)+
[2] $F\,d\,2\,d$ ($F\,d\,d\,2$, 43) (1; 3; 6; 8)+
[2] $F\,2\,d\,d$ ($F\,d\,d\,2$, 43) (1; 4; 6; 7)+
[2] $F\,2\,2\,2$ (22) (1; 2; 3; 4)+
[2] $F\,1\,1\,2/d$ ($C\,2/c$, 15) (1; 2; 5; 6)+
[2] $F\,1\,2/d\,1$ ($C\,2/c$, 15) (1; 3; 5; 7)+
[2] $F\,2/d\,1\,1$ ($C\,2/c$, 15) (1; 4; 5; 8)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $F\,d\,d\,d$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$ or $\mathbf{c}'=3\mathbf{c}$) (70)

Minimal non-isomorphic supergroups

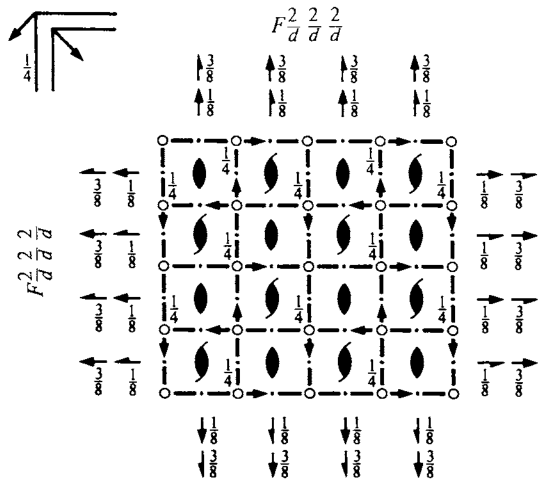
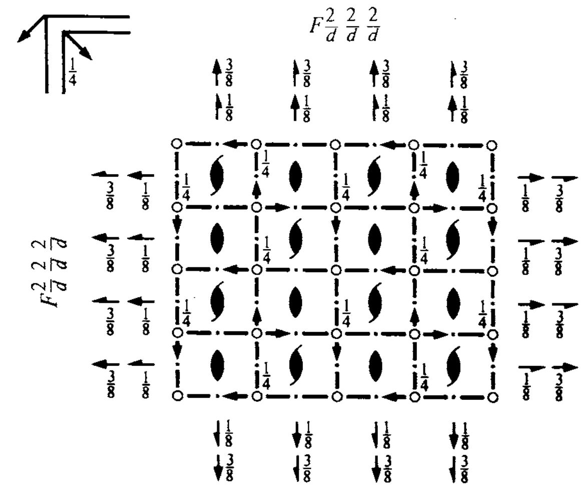
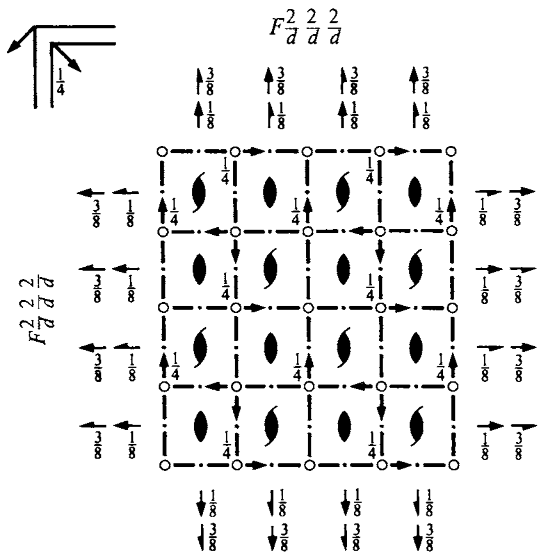
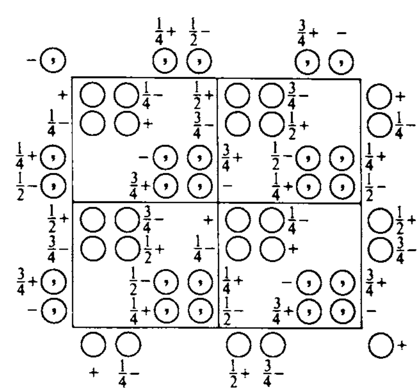
I [2] $I\,4_1/a\,m\,d$ (141); [2] $I\,4_1/a\,c\,d$ (142); [3] $F\,d\,\bar{3}$ (203)

II [2] $P\,n\,n\,n$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (48)

$F\,d\,d\,d$ $\qquad D_{2h}^{24}$ $\qquad mmm$ $\qquad$ Orthorhombic

No. 70 $\qquad F\ 2/d\ 2/d\ 2/d$ $\qquad$ Patterson symmetry $F\,mmm$

ORIGIN CHOICE 2

Origin at $\bar{1}$ at $d\,d\,d$, at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ from 222

Asymmetric unit $\quad 0 \le x \le \frac{1}{8};\quad -\frac{1}{8} \le y \le \frac{1}{8};\quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad \frac{3}{8},\frac{3}{8},z$	(3) $2\quad \frac{3}{8},y,\frac{3}{8}$	(4) $2\quad x,\frac{3}{8},\frac{3}{8}$
(5) $\bar{1}\quad 0,0,0$	(6) $d(\frac{1}{4},\frac{1}{4},0)\quad x,y,0$	(7) $d(\frac{1}{4},0,\frac{1}{4})\quad x,0,z$	(8) $d(0,\frac{1}{4},\frac{1}{4})\quad 0,y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{3}{8},\frac{1}{8},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{3}{8},y,\frac{1}{8}$	(4) $2\quad x,\frac{1}{8},\frac{1}{8}$
(5) $\bar{1}\quad 0,\frac{1}{4},\frac{1}{4}$	(6) $d(\frac{1}{4},\frac{3}{4},0)\quad x,y,\frac{1}{4}$	(7) $d(\frac{1}{4},0,\frac{3}{4})\quad x,\frac{1}{4},z$	(8) $d(0,\frac{3}{4},\frac{3}{4})\quad 0,y,z$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{8},\frac{3}{8},z$	(3) $2\quad \frac{1}{8},y,\frac{1}{8}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{3}{8},\frac{1}{8}$
(5) $\bar{1}\quad \frac{1}{4},0,\frac{1}{4}$	(6) $d(\frac{3}{4},\frac{1}{4},0)\quad x,y,\frac{1}{4}$	(7) $d(\frac{3}{4},0,\frac{3}{4})\quad x,0,z$	(8) $d(0,\frac{1}{4},\frac{3}{4})\quad \frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad \frac{1}{8},\frac{1}{8},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{8},y,\frac{3}{8}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{8},\frac{3}{8}$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},0$	(6) $d(\frac{3}{4},\frac{3}{4},0)\quad x,y,0$	(7) $d(\frac{3}{4},0,\frac{1}{4})\quad x,\frac{1}{4},z$	(8) $d(0,\frac{3}{4},\frac{1}{4})\quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	General:
32	*h*	1	(1) x,y,z	(2) $\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4},z$	(3) $\bar{x}+\frac{3}{4},y,\bar{z}+\frac{3}{4}$	(4) $x,\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4}$	hkl : $h+k,h+l,k+l=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{4},y+\frac{1}{4},\bar{z}$	(7) $x+\frac{1}{4},\bar{y},z+\frac{1}{4}$	(8) $\bar{x},y+\frac{1}{4},z+\frac{1}{4}$	$0kl$: $k+l=4n,\ k,l=2n$
							$h0l$: $h+l=4n,\ h,l=2n$
							$hk0$: $h+k=4n,\ h,k=2n$
							$h00$: $h=4n$
							$0k0$: $k=4n$
							$00l$: $l=4n$
							Special: as above, plus
16	*g*	. . 2	$\frac{1}{8},\frac{1}{8},z$	$\frac{5}{8},\frac{1}{8},\bar{z}+\frac{3}{4}$	$\frac{7}{8},\frac{7}{8},\bar{z}$	$\frac{3}{8},\frac{7}{8},z+\frac{1}{4}$	hkl : $h=2n+1$ or $h+k+l=4n$
16	*f*	. 2 .	$\frac{1}{8},y,\frac{1}{8}$	$\frac{5}{8},\bar{y}+\frac{3}{4},\frac{1}{8}$	$\frac{7}{8},\bar{y},\frac{7}{8}$	$\frac{3}{8},y+\frac{1}{4},\frac{7}{8}$	
16	*e*	2 . .	$x,\frac{1}{8},\frac{1}{8}$	$\bar{x}+\frac{3}{4},\frac{5}{8},\frac{1}{8}$	$\bar{x},\frac{7}{8},\frac{7}{8}$	$x+\frac{1}{4},\frac{3}{8},\frac{7}{8}$	
16	*d*	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	hkl : $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16	*c*	$\bar{1}$	$0,0,0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},0,\frac{3}{4}$	$0,\frac{3}{4},\frac{3}{4}$	
8	*b*	2 2 2	$\frac{1}{8},\frac{1}{8},\frac{5}{8}$	$\frac{7}{8},\frac{7}{8},\frac{3}{8}$			hkl : $h=2n+1$ or $h+k+l=4n$
8	*a*	2 2 2	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$			

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{8},\frac{1}{8},z$

Along [100] $c2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{8},\frac{1}{8}$

Along [010] $c2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $\frac{1}{8},y,\frac{1}{8}$

Maximal non-isomorphic subgroups

I [2] *F d d* 2 (43) (1; 2; 7; 8)+
[2] *F d* 2 *d* (*F d d* 2, 43) (1; 3; 6; 8)+
[2] *F* 2 *d d* (*F d d* 2, 43) (1; 4; 6; 7)+
[2] *F* 2 2 2 (22) (1; 2; 3; 4)+
[2] *F* 1 1 2/*d* (*C* 2/*c*, 15) (1; 2; 5; 6)+
[2] *F* 1 2/*d* 1 (*C* 2/*c*, 15) (1; 3; 5; 7)+
[2] *F* 2/*d* 1 1 (*C* 2/*c*, 15) (1; 4; 5; 8)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] *F d d d* ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$ or $\mathbf{c}'=3\mathbf{c}$) (70)

Minimal non-isomorphic supergroups

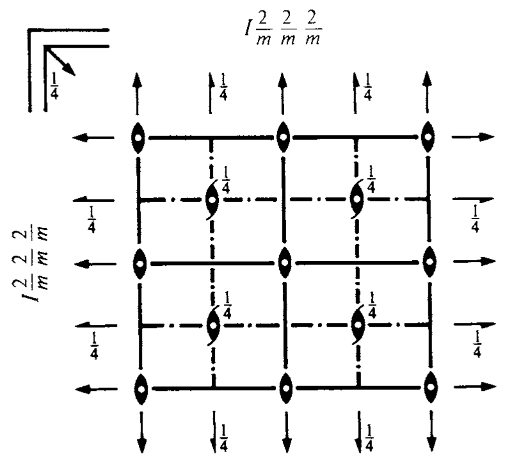
I [2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $Fd\bar{3}$ (203)

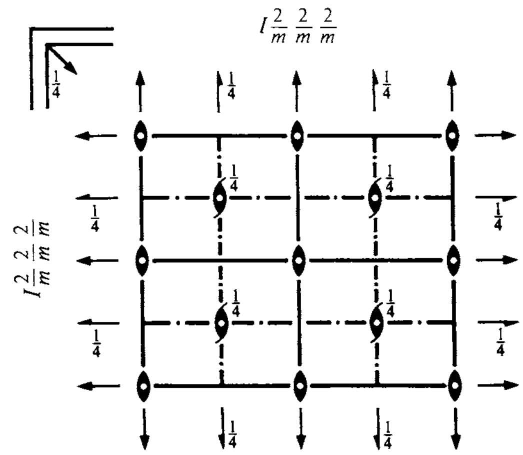
II [2] *P n n n* ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (48)

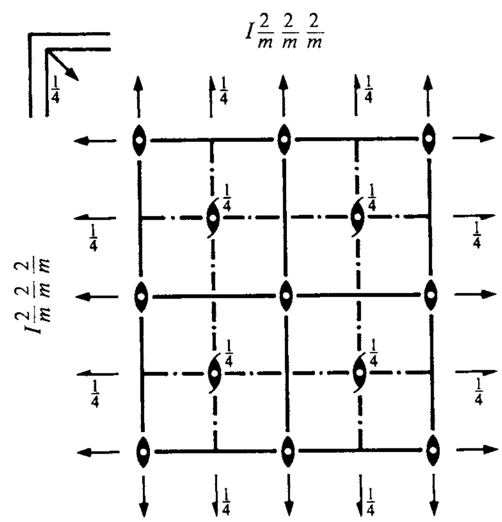
International Tables for Crystallography (2006). Vol. A, Space group 71, pp. 324–325.

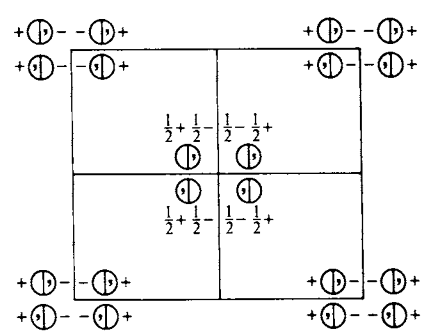
Immm D_{2h}^{25} *mmm* Orthorhombic

No. 71 $I\ 2/m\ 2/m\ 2/m$ Patterson symmetry *Immm*









Origin at centre (mmm)

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $\bar{1}\quad 0,0,0$	(6) $m\quad x,y,0$	(7) $m\quad x,0,z$	(8) $m\quad 0,y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$

Maximal isomorphic subgroups of lowest index

IIc [3] *Immm* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (71)

Minimal non-isomorphic supergroups

I [2] $I4/mmm$ (139); [3] $Im\bar{3}$ (204)

II [2] *Ammm* ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (*Cmmm*, 65); [2] *Bmmm* ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (*Cmmm*, 65); [2] *Cmmm* ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (65)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			General:
16	*o*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}$ (7) $x,\bar{y},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	$hkl: h+k+l=2n$ $0kl: k+l=2n$ $h0l: h+l=2n$ $hk0: h+k=2n$ $h00: h=2n$ $0k0: k=2n$ $00l: l=2n$
							Special: as above, plus
8	*n*	..*m*	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,0$	$x,\bar{y},0$	no extra conditions
8	*m*	.*m*.	$x,0,z$	$\bar{x},0,z$	$\bar{x},0,\bar{z}$	$x,0,\bar{z}$	no extra conditions
8	*l*	*m*..	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	no extra conditions
8	*k*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$hkl: k,l=2n$
4	*j*	*mm*2	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$			no extra conditions
4	*i*	*mm*2	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	*h*	*m*2*m*	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			no extra conditions
4	*g*	*m*2*m*	$0,y,0$	$0,\bar{y},0$			no extra conditions
4	*f*	2*mm*	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$			no extra conditions
4	*e*	2*mm*	$x,0,0$	$\bar{x},0,0$			no extra conditions
2	*d*	*mmm*	$\frac{1}{2},0,\frac{1}{2}$				no extra conditions
2	*c*	*mmm*	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
2	*b*	*mmm*	$0,\frac{1}{2},\frac{1}{2}$				no extra conditions
2	*a*	*mmm*	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] *c*2*mm*
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] *c*2*mm*
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] *c*2*mm*
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

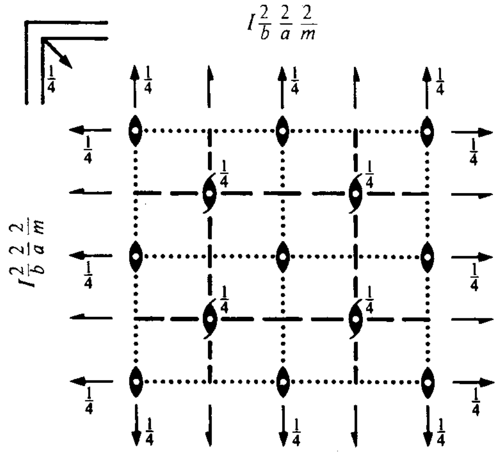
Maximal non-isomorphic subgroups

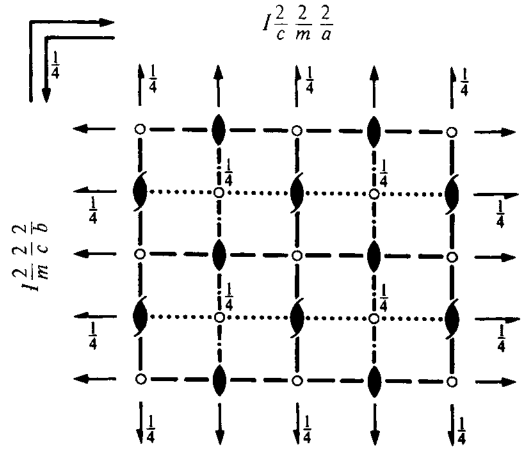
I	[2] *Imm*2 (44)	(1; 2; 7; 8)+
	[2] *Im*2*m* (*Imm*2, 44)	(1; 3; 6; 8)+
	[2] *I*2*mm* (*Imm*2, 44)	(1; 4; 6; 7)+
	[2] *I*222 (23)	(1; 2; 3; 4)+
	[2] *I*112/*m* (*C*2/*m*, 12)	(1; 2; 5; 6)+
	[2] *I*12/*m*1 (*C*2/*m*, 12)	(1; 3; 5; 7)+
	[2] *I*2/*m*11 (*C*2/*m*, 12)	(1; 4; 5; 8)+
IIa	[2] *Pmmn* (59)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] *Pmnm* (*Pmmn*, 59)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] *Pnmm* (*Pmmn*, 59)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] *Pnnm* (58)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] *Pnmn* (*Pnnm*, 58)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] *Pmnn* (*Pnnm*, 58)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] *Pnnn* (48)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] *Pmmm* (47)	1; 2; 3; 4; 5; 6; 7; 8
IIb	none	

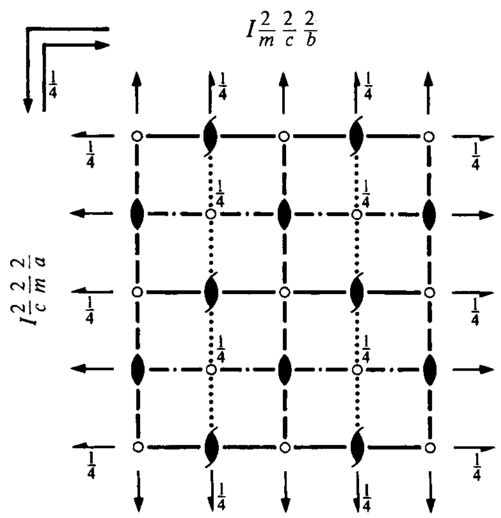
(*Continued on preceding page*)

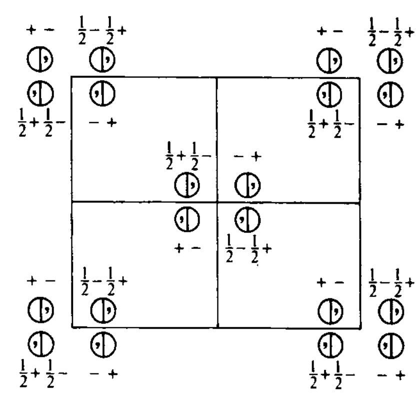
$Ibam$ $\quad D_{2h}^{26}$ $\quad mmm$ $\quad$ Orthorhombic

No. 72 $\quad I\ 2/b\ 2/a\ 2/m$ $\quad$ Patterson symmetry $Immm$









Origin at centre $(2/m)$ at $cc2/m$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $\bar{1}\quad 0,0,0$	(6) $m\quad x,y,0$	(7) $a\quad x,\frac{1}{4},z$	(8) $b\quad \frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},\frac{1}{4},z$	(3) $2\quad 0,y,\frac{1}{4}$	(4) $2\quad x,0,\frac{1}{4}$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,\frac{1}{4}$	(7) $c\quad x,0,z$	(8) $c\quad 0,y,z$

Maximal isomorphic subgroups of lowest index

IIc $\quad$ [3] $Ibam$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (72); [3] $Ibam$ ($\mathbf{c}' = 3\mathbf{c}$) (72)

Minimal non-isomorphic supergroups

I $\quad$ [2] $I4/mcm$ (140)

II $\quad$ [2] $Cmmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (65); [2] $Aemm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Cmme$, 67); [2] $Bmem$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Cmme$, 67)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
16	k	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	hkl : $h+k+l=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	j	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	no extra conditions
8	i	$..2$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$	hkl : $l=2n$
8	h	$..2$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl : $l=2n$
8	g	$.2.$	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	hkl : $l=2n$
8	f	$2..$	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	hkl : $l=2n$
8	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	hkl : $k,l=2n$
4	d	$..2/m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			hkl : $l=2n$
4	c	$..2/m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $l=2n$
4	b	222	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$			hkl : $l=2n$
4	a	222	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

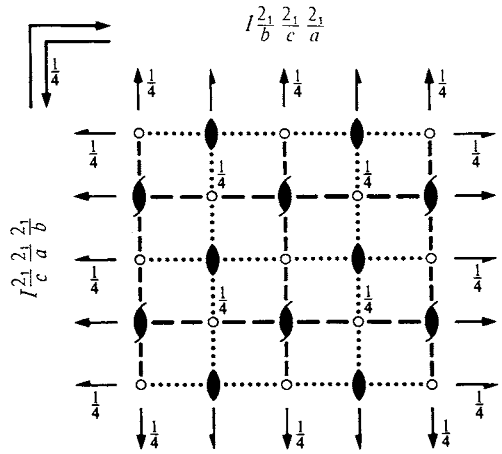
Maximal non-isomorphic subgroups

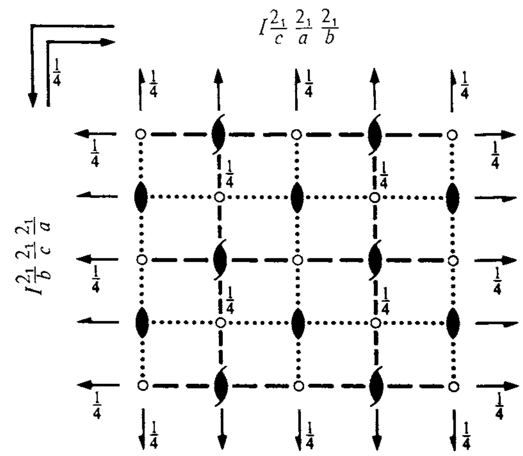
I	[2] $Ib2m$ ($Ima2$, 46)	(1; 3; 6; 8)+
	[2] $I2am$ ($Ima2$, 46)	(1; 4; 6; 7)+
	[2] $Iba2$ (45)	(1; 2; 7; 8)+
	[2] $I222$ (23)	(1; 2; 3; 4)+
	[2] $I12/a1$ ($C2/c$, 15)	(1; 3; 5; 7)+
	[2] $I2/b11$ ($C2/c$, 15)	(1; 4; 5; 8)+
	[2] $I112/m$ ($C2/m$, 12)	(1; 2; 5; 6)+
IIa	[2] $Pcan$ ($Pbcn$, 60)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pbcn$ (60)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pbcm$ (57)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pcam$ ($Pbcm$, 57)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pccn$ (56)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pbam$ (55)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $Pban$ (50)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pccm$ (49)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
IIb	none	

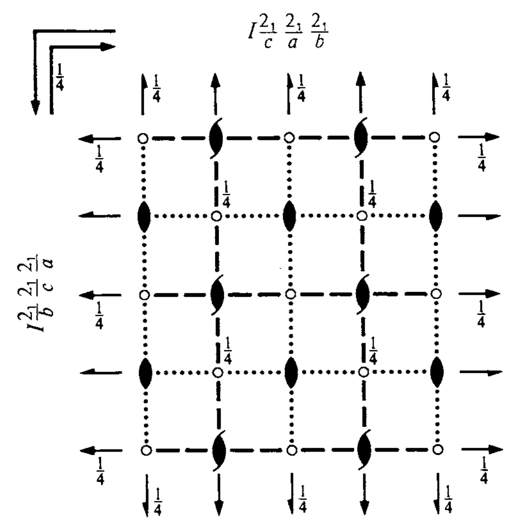
(*Continued on preceding page*)

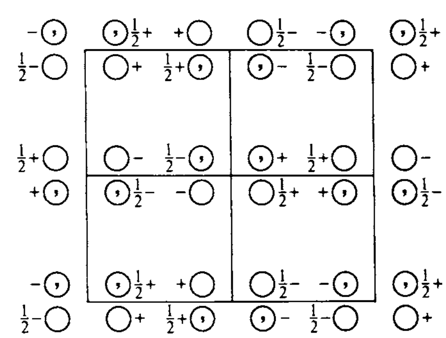
Ibca D_{2h}^{27} *mmm* Orthorhombic

No. 73 $I\ 2_1/b\ 2_1/c\ 2_1/a$ Patterson symmetry *Immm*









Origin at $\bar{1}$ at *cab*

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $\bar{1}\quad 0,0,0$	(6) $a\quad x,y,\frac{1}{4}$	(7) $c\quad x,\frac{1}{4},z$	(8) $b\quad \frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\quad 0,\frac{1}{4},z$	(3) $2\quad \frac{1}{4},y,0$	(4) $2\quad x,0,\frac{1}{4}$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) $b\quad x,y,0$	(7) $a\quad x,0,z$	(8) $c\quad 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates					Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$					General:
16	f	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$		hkl : $h+k+l=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$		$0kl$: $k,l=2n$
								$h0l$: $h,l=2n$
								$hk0$: $h,k=2n$
								$h00$: $h=2n$
								$0k0$: $k=2n$
								$00l$: $l=2n$
								Special: as above, plus
8	e	$..2$	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}+\frac{1}{2}$	$0,\frac{3}{4},\bar{z}$	$0,\frac{1}{4},z+\frac{1}{2}$		hkl : $l=2n$
8	d	$.2.$	$\frac{1}{4},y,0$	$\frac{1}{4},\bar{y},\frac{1}{2}$	$\frac{3}{4},\bar{y},0$	$\frac{3}{4},y,\frac{1}{2}$		hkl : $k=2n$
8	c	$2..$	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\bar{x},0,\frac{3}{4}$	$x+\frac{1}{2},0,\frac{1}{4}$		hkl : $h=2n$
8	b	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$		hkl : $k,l=2n$
8	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$		hkl : $k,l=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $Ibc2$ ($Iba2$, 45)	(1; 2; 7; 8)+
	[2] $Ib2a$ ($Iba2$, 45)	(1; 3; 6; 8)+
	[2] $I2ca$ ($Iba2$, 45)	(1; 4; 6; 7)+
	[2] $I2_12_12_1$ (24)	(1; 2; 3; 4)+
	[2] $I112/a$ ($C2/c$, 15)	(1; 2; 5; 6)+
	[2] $I12/c1$ ($C2/c$, 15)	(1; 3; 5; 7)+
	[2] $I2/b11$ ($C2/c$, 15)	(1; 4; 5; 8)+
IIa	[2] $Pbca$ (61)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $Pcab$ ($Pbca$, 61)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pcaa$ ($Pcca$, 54)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pccb$ ($Pcca$, 54)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pbab$ ($Pcca$, 54)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pbcb$ ($Pcca$, 54)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pbaa$ ($Pcca$, 54)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pcca$ (54)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Ibca$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$ or $\mathbf{c}'=3\mathbf{c}$) (73)

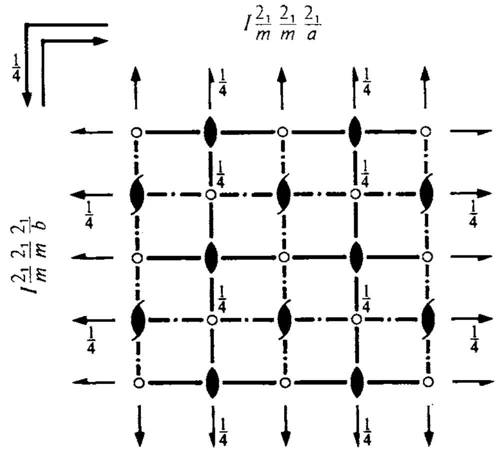
Minimal non-isomorphic supergroups

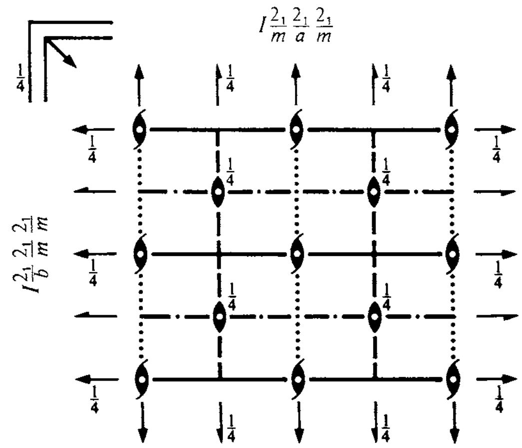
I [2] $I4_1/acd$ (142); [3] $Ia\bar{3}$ (206)

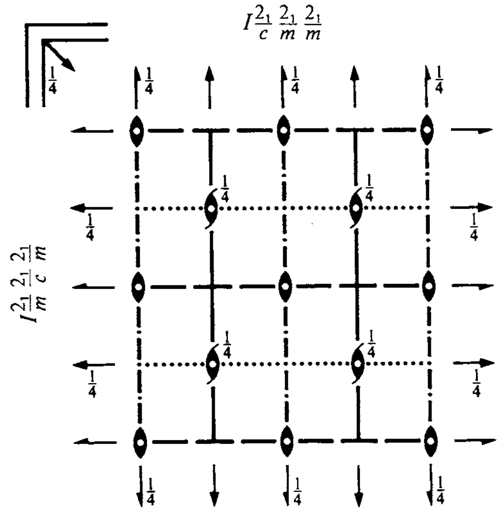
II [2] $Aemm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Cmme$, 67); [2] $Bmem$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Cmme$, 67); [2] $Cmme$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (67)

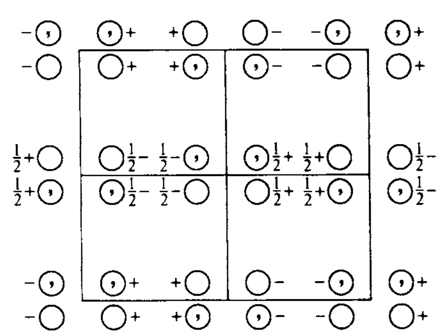
Imma D_{2h}^{28} *mmm* Orthorhombic

No. 74 $I\ 2_1/m\ 2_1/m\ 2_1/a$ Patterson symmetry *Immm*









Origin at centre $(2/m)$ at $2/m2_1/nb$

Asymmetric unit $0 \le x \le \frac{1}{4};\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $\bar{1}\quad 0,0,0$	(6) $b\quad x,y,0$	(7) $m\quad x,\frac{1}{4},z$	(8) $m\quad 0,y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) $a\quad x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})\quad x,0,z$	(8) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$

Maximal isomorphic subgroups of lowest index

IIc [3] *Imma* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (74); [3] *Imma* ($\mathbf{c}' = 3\mathbf{c}$) (74)

Minimal non-isomorphic supergroups

I [2] $I4_1/amd$ (141)

II [2] *Ammm* ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (*Cmmm*, 65); [2] *Bmmm* ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (*Cmmm*, 65); [2] *Cmme* ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (67)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\ \ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
16	j	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y}+\frac{1}{2},z$ (6) $x,y+\frac{1}{2},\bar{z}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	hkl : $h+k+l=2n$ $0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	i	$.\,m\,.$	$x,\frac{1}{4},z$	$\bar{x},\frac{1}{4},z$	$\bar{x},\frac{3}{4},\bar{z}$	$x,\frac{3}{4},\bar{z}$	no extra conditions
8	h	$m\,.\,.$	$0,y,z$	$0,\bar{y}+\frac{1}{2},z$	$0,y+\frac{1}{2},\bar{z}$	$0,\bar{y},\bar{z}$	no extra conditions
8	g	$.\,2\,.$	$\frac{1}{4},y,\frac{1}{4}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},\bar{y},\frac{3}{4}$	$\frac{1}{4},y+\frac{1}{2},\frac{3}{4}$	hkl : $h=2n$
8	f	$2\,.\,.$	$x,0,0$	$\bar{x},\frac{1}{2},0$	$\bar{x},0,0$	$x,\frac{1}{2},0$	hkl : $k=2n$
4	e	$m\,m\,2$	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}$			no extra conditions
4	d	$.\,2/m\,.$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$			hkl : $h=2n$
4	c	$.\,2/m\,.$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$			hkl : $h=2n$
4	b	$2/m\,.\,.$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $h=2n$
4	a	$2/m\,.\,.$	$0,0,0$	$0,\frac{1}{2},0$			hkl : $h=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [010] $c2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

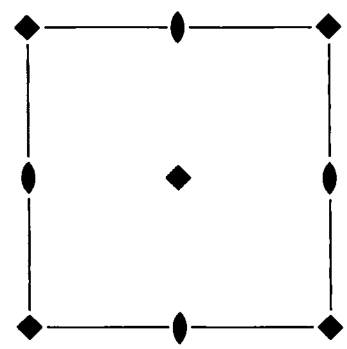
Maximal non-isomorphic subgroups

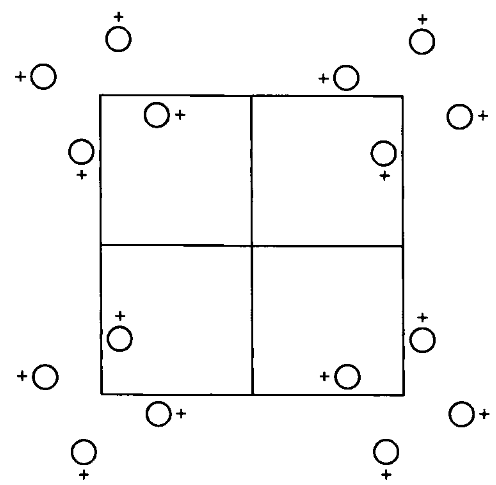
I	[2] $Im2b$ ($Ima2$, 46)	(1; 3; 6; 8)+
	[2] $I2mb$ ($Ima2$, 46)	(1; 4; 6; 7)+
	[2] $Imm2$ (44)	(1; 2; 7; 8)+
	[2] $I2_12_12_1$ (24)	(1; 2; 3; 4)+
	[2] $I112/b$ ($C2/c$, 15)	(1; 2; 5; 6)+
	[2] $I12/m1$ ($C2/m$, 12)	(1; 3; 5; 7)+
	[2] $I2/m11$ ($C2/m$, 12)	(1; 4; 5; 8)+
IIa	[2] $Pnma$ (62)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pmnb$ ($Pnma$, 62)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pnmb$ ($Pmna$, 53)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pmna$ (53)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pnna$ (52)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pnnb$ ($Pnna$, 52)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pmma$ (51)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pmmb$ ($Pmma$, 51)	1; 2; 3; 4; 5; 6; 7; 8
IIb	none	

(*Continued on preceding page*)

$P4$ $\quad C_4^1$ $\quad 4$ $\quad$ Tetragonal

No. 75 $\quad P4$ $\quad$ Patterson symmetry $P4/m$





Origin on 4

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 $\quad$ (2) 2 $0,0,z$ $\quad$ (3) 4^+ $0,0,z$ $\quad$ (4) 4^- $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	*d*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	no conditions
							Special:
2	*c*	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			hkl : $h+k=2n$
1	*b*	4 . .	$\frac{1}{2},\frac{1}{2},z$				no extra conditions
1	*a*	4 . .	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \mathbf{a}$ $\quad$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\quad$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I $\quad$ [2] $P2$ (3) $\quad$ 1; 2
IIa $\quad$ none
IIb $\quad$ [2] $P4_2$ ($\mathbf{c}' = 2\mathbf{c}$) (77); [2] $F4$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4$, 79)

Maximal isomorphic subgroups of lowest index

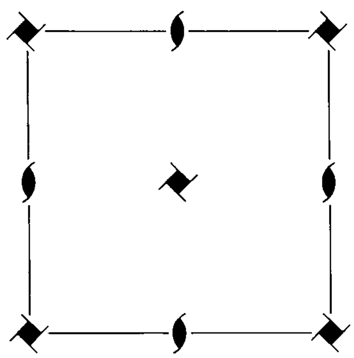
IIc $\quad$ [2] $P4$ ($\mathbf{c}' = 2\mathbf{c}$) (75); [2] $C4$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4$, 75)

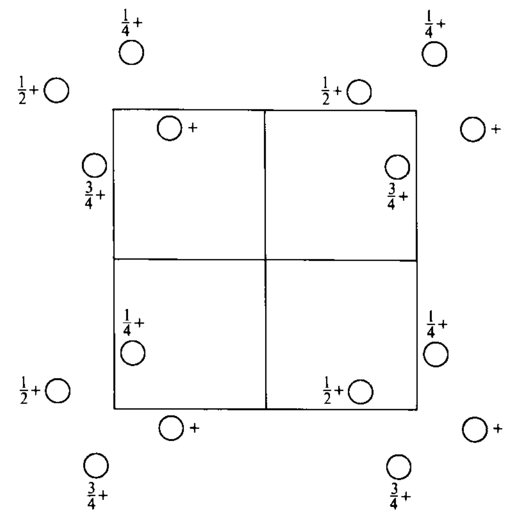
Minimal non-isomorphic supergroups

I $\quad$ [2] $P4/m$ (83); [2] $P4/n$ (85); [2] $P422$ (89); [2] $P42_12$ (90); [2] $P4mm$ (99); [2] $P4bm$ (100); [2] $P4cc$ (103); [2] $P4nc$ (104)
II $\quad$ [2] $I4$ (79)

Tetragonal 4 C_4^2 $P4_1$

Patterson symmetry $P4/m$ $P4_1$ No. 76





Origin on 4_1

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})\quad 0,0,z$ (3) $4^{+}(0,0,\frac{1}{4})\quad 0,0,z$ (4) $4^{-}(0,0,\frac{3}{4})\quad 0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 *a* 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{1}{4}$	(4) $y,\bar{x},z+\frac{3}{4}$	$00l$: $l=4n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1g1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P2_1$ (4) 1; 2
IIa none
IIb none

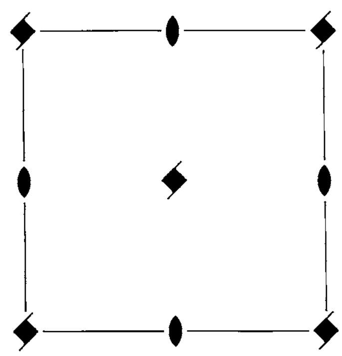
Maximal isomorphic subgroups of lowest index

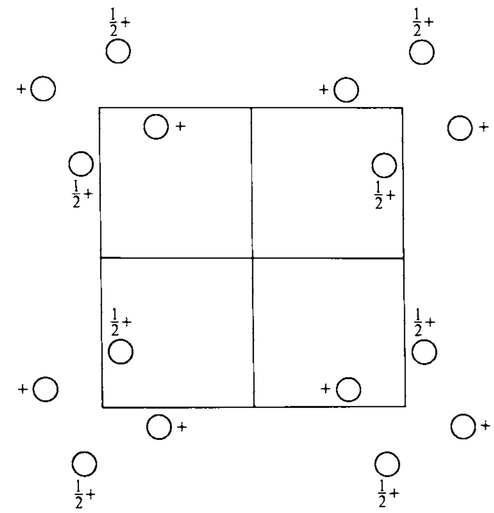
IIc [2] $C4_1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4_1$, 76); [3] $P4_3$ ($\mathbf{c}'=3\mathbf{c}$) (78); [5] $P4_1$ ($\mathbf{c}'=5\mathbf{c}$) (76)

Minimal non-isomorphic supergroups

I [2] $P4_122$ (91); [2] $P4_12_12$ (92)
II [2] $I4_1$ (80); [2] $P4_2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (77)

$P4_2$	C_4^3	4	Tetragonal
No. 77	$P4_2$		Patterson symmetry $P4/m$





Origin on 2 on 4_2

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $4^+(0,0,\frac{1}{2})$ $0,0,z$ (4) $4^-(0,0,\frac{1}{2})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	*d*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	$00l$: $l=2n$
							Special: as above, plus
2	*c*	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$			hkl : $h+k+l=2n$
2	*b*	2 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl : $l=2n$
2	*a*	2 . .	$0,0,z$	$0,0,z+\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P2$ (3) 1; 2

IIa none

IIb [2] $P4_3$ ($\mathbf{c}'=2\mathbf{c}$) (78); [2] $P4_1$ ($\mathbf{c}'=2\mathbf{c}$) (76); [2] $F4_1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4_1$, 80)

Maximal isomorphic subgroups of lowest index

IIc [2] $C4_2$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4_2$, 77); [3] $P4_2$ ($\mathbf{c}'=3\mathbf{c}$) (77)

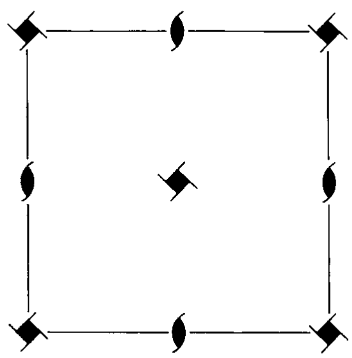
Minimal non-isomorphic supergroups

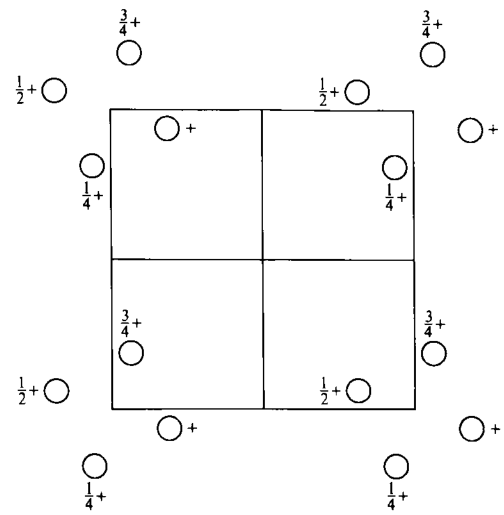
I [2] $P4_2/m$ (84); [2] $P4_2/n$ (86); [2] $P4_222$ (93); [2] $P4_22_12$ (94); [2] $P4_2cm$ (101); [2] $P4_2nm$ (102); [2] $P4_2mc$ (105); [2] $P4_2bc$ (106)

II [2] $I4$ (79); [2] $P4$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (75)

Tetragonal 4 C_4^4 $P4_3$

Patterson symmetry $P4/m$ $P4_3$ No. 78





Origin on 4_3

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) $4^+(0,0,\frac{3}{4})$ $0,0,z$ (4) $4^-(0,0,\frac{1}{4})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 *a* 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{3}{4}$	(4) $y,\bar{x},z+\frac{1}{4}$	$00l$: $l = 4n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1g1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P2_1$ (4) 1; 2
IIa none
IIb none

Maximal isomorphic subgroups of lowest index

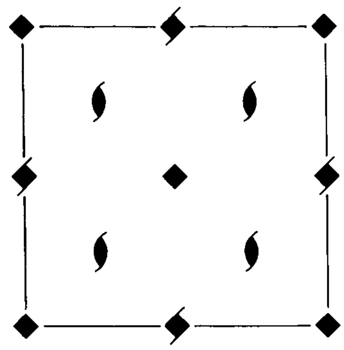
IIc [2] $C4_3$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_3$, 78); [3] $P4_1$ ($\mathbf{c}' = 3\mathbf{c}$) (76); [5] $P4_3$ ($\mathbf{c}' = 5\mathbf{c}$) (78)

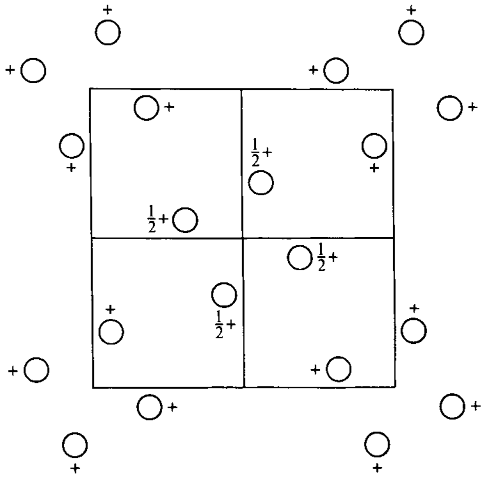
Minimal non-isomorphic supergroups

I [2] $P4_322$ (95); [2] $P4_32_12$ (96)
II [2] $I4_1$ (80); [2] $P4_2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (77)

$I4$ C_4^5 4 Tetragonal

No. 79 $I4$ Patterson symmetry $I4/m$





Origin on 4

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) 4^+ $0,0,z$ (4) 4^- $0,0,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$ (4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
4	b	$2\,.\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			hkl : $l=2n$
2	a	$4\,.\,.$	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $I2$ ($C2$, 5) (1; 2)+

IIa [2] $P4_2$ (77) 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P4$ (75) 1; 2; 3; 4

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4$ ($\mathbf{c}'=3\mathbf{c}$) (79); [5] $I4$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (79)

Minimal non-isomorphic supergroups

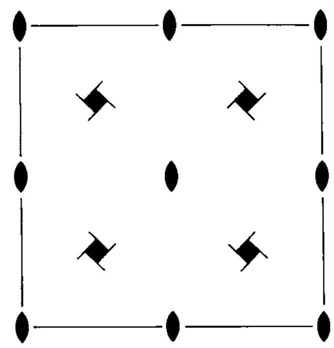
I [2] $I4/m$ (87); [2] $I422$ (97); [2] $I4mm$ (107); [2] $I4cm$ (108)

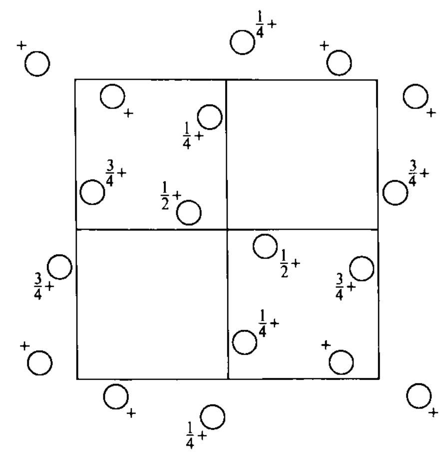
II [2] $C4$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P4$, 75)

International Tables for Crystallography (2006). Vol. A, Space group 80, pp. 338–339.

$I4_1$ C_4^6 4 Tetragonal

No. 80 $I4_1$ Patterson symmetry $I4/m$





Origin on 2

Asymmetric unit $0 \leq x \leq \frac{1}{2};\quad 0 \leq y \leq 1;\quad 0 \leq z \leq \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},\frac{1}{4},z$ (3) $4^+(0,0,\frac{1}{4})\quad -\frac{1}{4},\frac{1}{4},z$ (4) $4^-(0,0,\frac{3}{4})\quad \frac{1}{4},-\frac{1}{4},z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2\quad 0,0,z$ (3) $4^+(0,0,\frac{3}{4})\quad \frac{1}{4},\frac{1}{4},z$ (4) $4^-(0,0,\frac{1}{4})\quad \frac{1}{4},\frac{1}{4},z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
8 b 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $00l$: $l=4n$ $h00$: $h=2n$
					Special: as above, plus
4 a 2 . .	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$			hkl : $l=2n+1$ or $2h+l=4n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $I2$ ($C2$, 5) (1; 2)+

IIa [2] $P4_3$ (78) 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P4_1$ (76) 1; 2; 3; 4

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1$ ($\mathbf{c}'=3\mathbf{c}$) (80); [5] $I4_1$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (80)

Minimal non-isomorphic supergroups

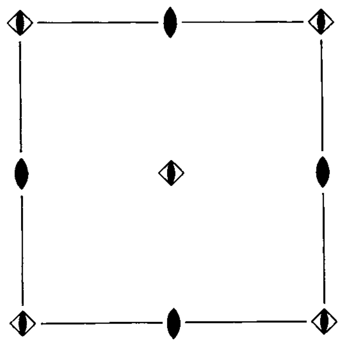
I [2] $I4_1/a$ (88); [2] $I4_122$ (98); [2] $I4_1md$ (109); [2] $I4_1cd$ (110)

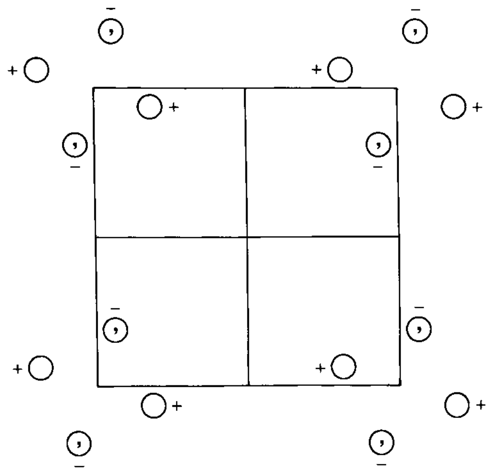
II [2] $C4_2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P4_2$, 77)

International Tables for Crystallography (2006). Vol. A, Space group 81, pp. 340–341.

$P\bar{4}$ S_4^1 $\bar{4}$ Tetragonal

No. 81 $P\bar{4}$ Patterson symmetry $P4/m$





Origin at $\bar{4}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $\bar{4}^{+}$ $0,0,z$; $0,0,0$ (4) $\bar{4}^{-}$ $0,0,z$; $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	no conditions
							Special:
2	g	$2\,.\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			$hk0$: $h+k=2n$
2	f	$2\,.\,.$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	e	$2\,.\,.$	$0,0,z$	$0,0,\bar{z}$			no extra conditions
1	d	$\bar{4}\,.\,.$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				no extra conditions
1	c	$\bar{4}\,.\,.$	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	b	$\bar{4}\,.\,.$	$0,0,\frac{1}{2}$				no extra conditions
1	a	$\bar{4}\,.\,.$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P2$ (3) 1; 2

IIa none

IIb [2] $F\bar{4}$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I\bar{4}$, 82)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{4}$ ($\mathbf{c}'=2\mathbf{c}$) (81); [2] $C\bar{4}$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P\bar{4}$, 81)

Minimal non-isomorphic supergroups

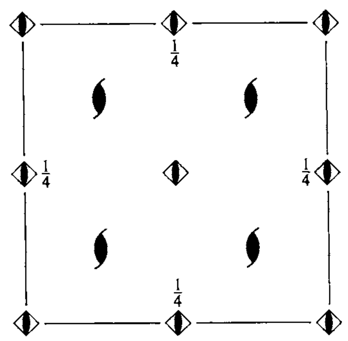
I [2] $P4/m$ (83); [2] $P4_2/m$ (84); [2] $P4/n$ (85); [2] $P4_2/n$ (86); [2] $P\bar{4}2m$ (111); [2] $P\bar{4}2c$ (112); [2] $P\bar{4}2_1m$ (113); [2] $P\bar{4}2_1c$ (114); [2] $P\bar{4}m2$ (115); [2] $P\bar{4}c2$ (116); [2] $P\bar{4}b2$ (117); [2] $P\bar{4}n2$ (118)

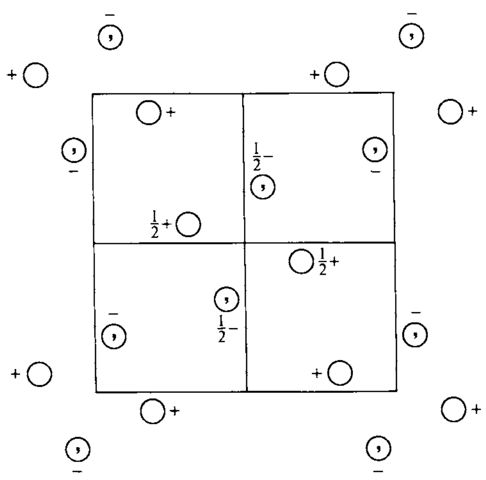
II [2] $I\bar{4}$ (82)

International Tables for Crystallography (2006). Vol. A, Space group 82, pp. 342–343.

$I\bar{4}$ S_4^2 $\bar{4}$ Tetragonal

No. 82 $I\bar{4}$ Patterson symmetry $I4/m$





Origin at $\bar{4}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) $2 \quad 0,0,z$ (3) $\bar{4}^{+} \quad 0,0,z;\ \ 0,0,0$ (4) $\bar{4}^{-} \quad 0,0,z;\ \ 0,0,0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4},\frac{1}{4},z$ (3) $\bar{4}^{+} \quad \frac{1}{2},0,z;\ \ \frac{1}{2},0,\frac{1}{4}$ (4) $\bar{4}^{-} \quad 0,\frac{1}{2},z;\ \ 0,\frac{1}{2},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: no extra conditions
4	f	$2\,.\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			
4	e	$2\,.\,.$	$0,0,z$	$0,0,\bar{z}$			
2	d	$\bar{4}\,.\,.$	$0,\frac{1}{2},\frac{3}{4}$				
2	c	$\bar{4}\,.\,.$	$0,\frac{1}{2},\frac{1}{4}$				
2	b	$\bar{4}\,.\,.$	$0,0,\frac{1}{2}$				
2	a	$\bar{4}\,.\,.$	$0,0,0$				

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $I2$ ($C2$, 5) (1; 2)+

IIa [2] $P\bar{4}$ (81) 1; 2; 3; 4
[2] $P\bar{4}$ (81) 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I\bar{4}$ ($\mathbf{c}'=3\mathbf{c}$) (82); [5] $I\bar{4}$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (82)

Minimal non-isomorphic supergroups

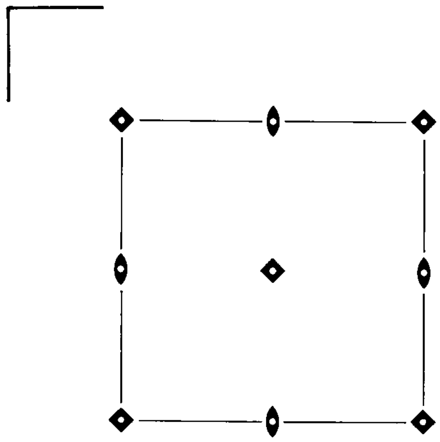
I [2] $I4/m$ (87); [2] $I4_1/a$ (88); [2] $I\bar{4}m2$ (119); [2] $I\bar{4}c2$ (120); [2] $I\bar{4}2m$ (121); [2] $I\bar{4}2d$ (122)

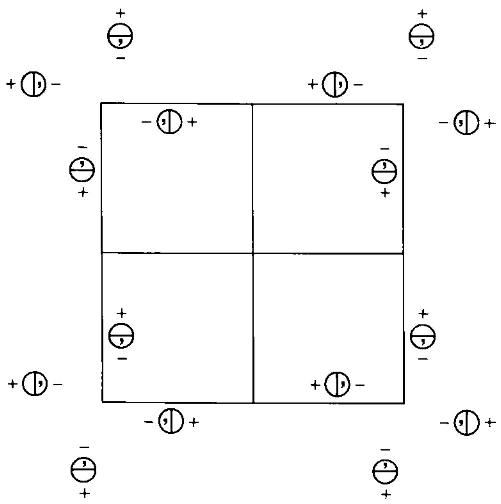
II [2] $C\bar{4}$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P\bar{4}$, 81)

International Tables for Crystallography (2006). Vol. A, Space group 83, pp. 344–345.

$P4/m$ C_{4h}^1 $4/m$ Tetragonal

No. 83 $P4/m$ Patterson symmetry $P4/m$





Origin at centre $(4/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) $\bar{1}$ $0,0,0$	(6) m $x,y,0$	(7) $\bar{4}^+$ $0,0,z$; $0,0,0$	(8) $\bar{4}^-$ $0,0,z$; $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	l	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{y},x,z$ (7) $y,\bar{x},\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y},x,\bar{z}$	no conditions
							Special:
4	k	$m\,.\,.$	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
4	j	$m\,.\,.$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
4	i	$2\,.\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hkl : $h+k=2n$
2	h	$4\,.\,.$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	g	$4\,.\,.$	$0,0,z$	$0,0,\bar{z}$			no extra conditions
2	f	$2/m\,.\,.$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k=2n$
2	e	$2/m\,.\,.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $h+k=2n$
1	d	$4/m\,.\,.$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				no extra conditions
1	c	$4/m\,.\,.$	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	b	$4/m\,.\,.$	$0,0,\frac{1}{2}$				no extra conditions
1	a	$4/m\,.\,.$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}$ (81) 1; 2; 7; 8
[2] $P4$ (75) 1; 2; 3; 4
[2] $P2/m$ (10) 1; 2; 5; 6

IIa none

IIb [2] $P4_2/m$ ($\mathbf{c}'=2\mathbf{c}$) (84); [2] $C4/e$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4/n$, 85); [2] $F4/m$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4/m$, 87)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/m$ ($\mathbf{c}'=2\mathbf{c}$) (83); [2] $C4/m$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4/m$, 83)

Minimal non-isomorphic supergroups

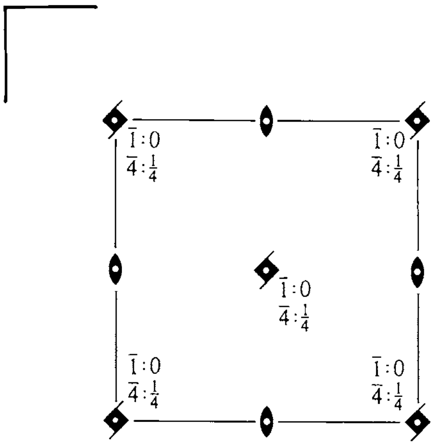
I [2] $P4/mmm$ (123); [2] $P4/mcc$ (124); [2] $P4/mbm$ (127); [2] $P4/mnc$ (128)

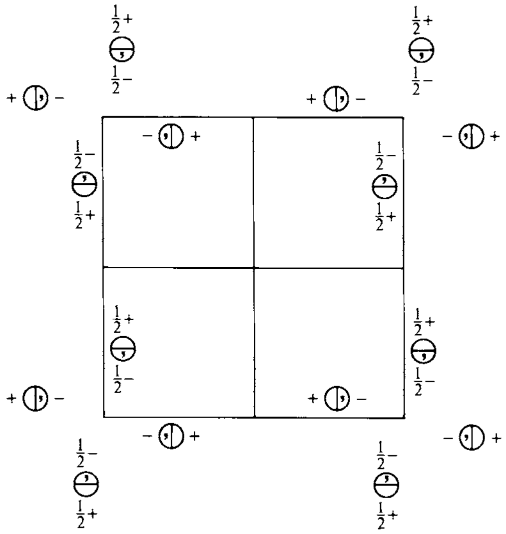
II [2] $I4/m$ (87)

International Tables for Crystallography (2006). Vol. A, Space group 84, pp. 346–347.

$P4_2/m$ $\quad C_{4h}^2$ $\quad 4/m$ $\quad$ Tetragonal

No. 84 $\quad P4_2/m$ $\quad$ Patterson symmetry $P4/m$





Origin at centre $(2/m)$ on 4_2

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^{+}(0,0,\frac{1}{2})\quad 0,0,z$	(4) $4^{-}(0,0,\frac{1}{2})\quad 0,0,z$
(5) $\bar{1}\quad 0,0,0$	(6) $m\quad x,y,0$	(7) $\bar{4}^{+}\quad 0,0,z;\ 0,0,\frac{1}{4}$	(8) $\bar{4}^{-}\quad 0,0,z;\ 0,0,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	$00l$: $l=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $y,\bar{x},\bar{z}+\frac{1}{2}$	(8) $\bar{y},x,\bar{z}+\frac{1}{2}$	
							Special: as above, plus
4	j	$m\,.\,.$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
4	i	$2\,.\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	hkl : $h+k+l=2n$
4	h	$2\,.\,.$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl : $l=2n$
4	g	$2\,.\,.$	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	hkl : $l=2n$
2	f	$\bar{4}\,.\,.$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl : $l=2n$
2	e	$\bar{4}\,.\,.$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl : $l=2n$
2	d	$2/m\,.\,.$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$			hkl : $h+k+l=2n$
2	c	$2/m\,.\,.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k+l=2n$
2	b	$2/m\,.\,.$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
2	a	$2/m\,.\,.$	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}$ (81) 1; 2; 7; 8
[2] $P4_2$ (77) 1; 2; 3; 4
[2] $P2/m$ (10) 1; 2; 5; 6

IIa none

IIb [2] $C4_2/e$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4_2/n$, 86)

Maximal isomorphic subgroups of lowest index

IIc [2] $C4_2/m$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4_2/m$, 84); [3] $P4_2/m$ ($\mathbf{c}'=3\mathbf{c}$) (84)

Minimal non-isomorphic supergroups

I [2] $P4_2/mmc$ (131); [2] $P4_2/mcm$ (132); [2] $P4_2/mbc$ (135); [2] $P4_2/mnm$ (136)

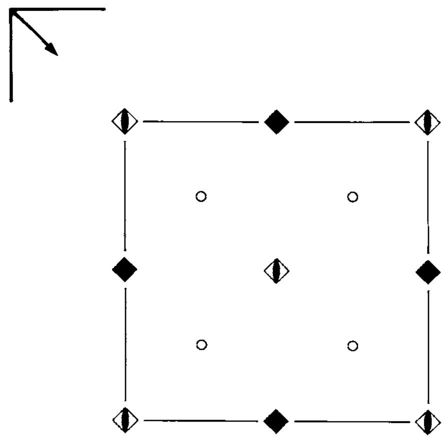
II [2] $I4/m$ (87); [2] $P4/m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (83)

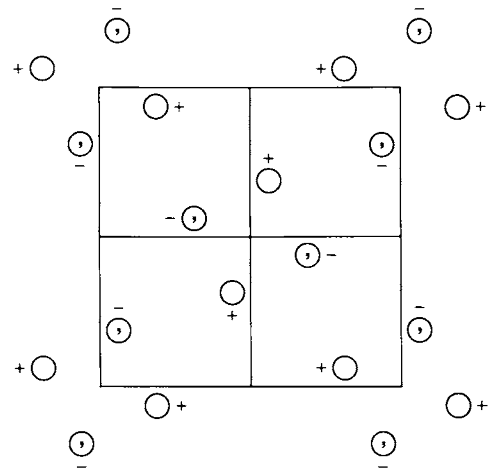
International Tables for Crystallography (2006). Vol. A, Space group 85, pp. 348–351.

$P4/n$ $\quad C_{4h}^3$ $\quad 4/m$ $\quad$ Tetragonal

No. 85 $\quad P4/n$ $\quad$ Patterson symmetry $P4/m$

ORIGIN CHOICE 1





Origin at $\bar{4}$ on n, at $-\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2 \quad 0,0,z$	(3) $4^+ \quad 0,\frac{1}{2},z$	(4) $4^- \quad \frac{1}{2},0,z$
(5) $\bar{1} \quad \frac{1}{4},\frac{1}{4},0$	(6) $n(\frac{1}{2},\frac{1}{2},0) \quad x,y,0$	(7) $\bar{4}^+ \quad 0,0,z; \quad 0,0,0$	(8) $\bar{4}^- \quad 0,0,z; \quad 0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*g*	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z$ (7) $y,\bar{x},\bar{z}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z$ (8) $\bar{y},x,\bar{z}$	$hk0$: $h+k=2n$ $h00$: $h=2n$
							Special: as above, plus
4	*f*	$2\,.\,.$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	hkl : $h+k=2n$
4	*e*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	hkl : $h,k=2n$
4	*d*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl : $h,k=2n$
2	*c*	$4\,.\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			no extra conditions
2	*b*	$\bar{4}\,.\,.$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	*a*	$\bar{4}\,.\,.$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}$ (81) 1; 2; 7; 8
[2] $P4$ (75) 1; 2; 3; 4
[2] $P2/n$ ($P2/c$, 13) 1; 2; 5; 6

IIa none

IIb [2] $P4_2/n$ ($\mathbf{c}'=2\mathbf{c}$) (86)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/n$ ($\mathbf{c}'=2\mathbf{c}$) (85); [5] $P4/n$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (85)

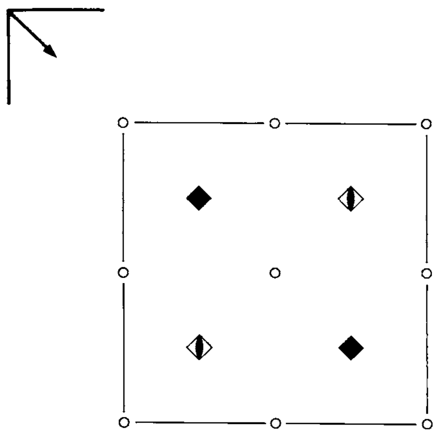
Minimal non-isomorphic supergroups

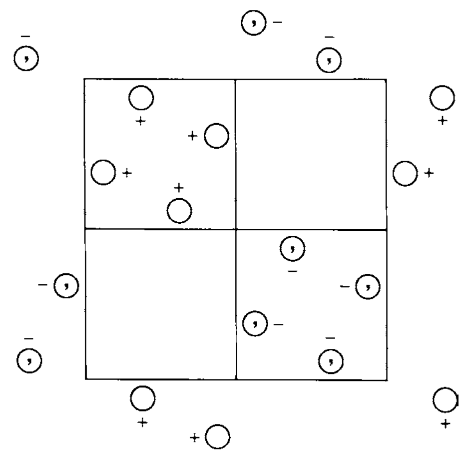
I [2] $P4/nbm$ (125); [2] $P4/nnc$ (126); [2] $P4/nmm$ (129); [2] $P4/ncc$ (130)

II [2] $C4/m$ ($P4/m$, 83); [2] $I4/m$ (87)

$P4/n$	C_{4h}^3	$4/m$	Tetragonal
No. 85	$P4/n$		Patterson symmetry $P4/m$

ORIGIN CHOICE 2





Origin at $\bar{1}$ on n, at $\frac{1}{4},-\frac{1}{4},0$ from $\bar{4}$

Asymmetric unit $\quad -\frac{1}{4} \le x \le \frac{1}{4}; \quad -\frac{1}{4} \le y \le \frac{1}{4}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2\ \ \frac{1}{4},\frac{1}{4},z$	(3) $4^+\ \ \frac{1}{4},\frac{1}{4},z$	(4) $4^-\ \ \frac{1}{4},\frac{1}{4},z$
(5) $\bar{1}\ \ 0,0,0$	(6) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$	(7) $\bar{4}^+\ \ \frac{1}{4},-\frac{1}{4},z;\ \ \frac{1}{4},-\frac{1}{4},0$	(8) $\bar{4}^-\ \ -\frac{1}{4},\frac{1}{4},z;\ \ -\frac{1}{4},\frac{1}{4},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{y}+\frac{1}{2},x,z$ (7) $y+\frac{1}{2},\bar{x},\bar{z}$	(4) $y,\bar{x}+\frac{1}{2},z$ (8) $\bar{y},x+\frac{1}{2},\bar{z}$	$hk0$: $h+k=2n$ $h00$: $h=2n$
							Special: as above, plus
4	f	$2\,.\,.$	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	hkl : $h+k=2n$
4	e	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl : $h,k=2n$
4	d	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hkl : $h,k=2n$
2	c	$4\,.\,.$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}$			no extra conditions
2	b	$\bar{4}\,.\,.$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl : $h+k=2n$
2	a	$\bar{4}\,.\,.$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}$ (81) 1; 2; 7; 8
[2] $P4$ (75) 1; 2; 3; 4
[2] $P2/n$ ($P2/c$, 13) 1; 2; 5; 6

IIa none

IIb [2] $P4_2/n$ ($\mathbf{c}'=2\mathbf{c}$) (86)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/n$ ($\mathbf{c}'=2\mathbf{c}$) (85); [5] $P4/n$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (85)

Minimal non-isomorphic supergroups

I [2] $P4/nbm$ (125); [2] $P4/nnc$ (126); [2] $P4/nmm$ (129); [2] $P4/ncc$ (130)

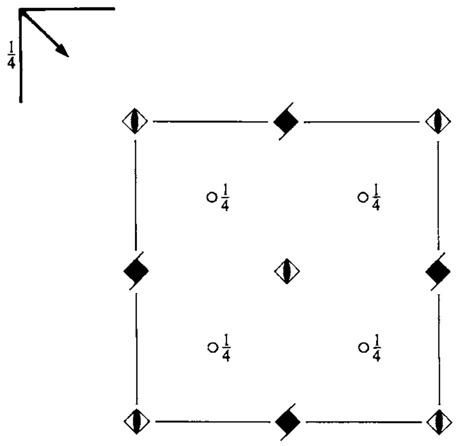
II [2] $C4/m$ ($P4/m$, 83); [2] $I4/m$ (87)

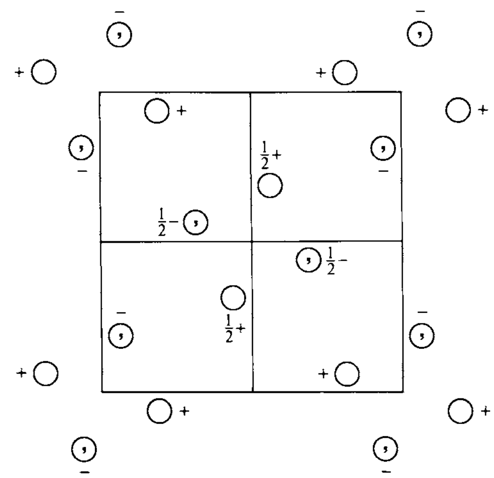
International Tables for Crystallography (2006). Vol. A, Space group 86, pp. 352–355.

$P4_2/n$ $\quad C_{4h}^4$ $\quad 4/m$ $\quad$ Tetragonal

No. 86 $\quad P4_2/n$ $\quad$ Patterson symmetry $P4/m$

ORIGIN CHOICE 1





Origin at $\bar{4}$, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\ \ 0,0,z$	(3) $4^+(0,0,\frac{1}{2})\ \ 0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})\ \ \frac{1}{2},0,z$
(5) $\bar{1}\ \ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,\frac{1}{4}$	(7) $\bar{4}^+\ 0,0,z;\ \ 0,0,0$	(8) $\bar{4}^-\ 0,0,z;\ \ 0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ (7) $y,\bar{x},\bar{z}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (8) $\bar{y},x,\bar{z}$	$hk0$: $h+k=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
4	f	$2\,.\,.$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	hkl: $h+k+l=2n$
4	e	$2\,.\,.$	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	hkl: $l=2n$
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	hkl: $h+k,h+l,k+l=2n$
4	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	hkl: $h+k,h+l,k+l=2n$
2	b	$\bar{4}\,.\,.$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	a	$\bar{4}\,.\,.$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{1}{4}$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}$ (81) 1; 2; 7; 8
[2] $P4_2$ (77) 1; 2; 3; 4
[2] $P2/n$ ($P2/c$, 13) 1; 2; 5; 6

IIa none

IIb [2] $F4_1/d$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4_1/a$, 88)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/n$ ($\mathbf{c}'=3\mathbf{c}$) (86); [5] $P4_2/n$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (86)

Minimal non-isomorphic supergroups

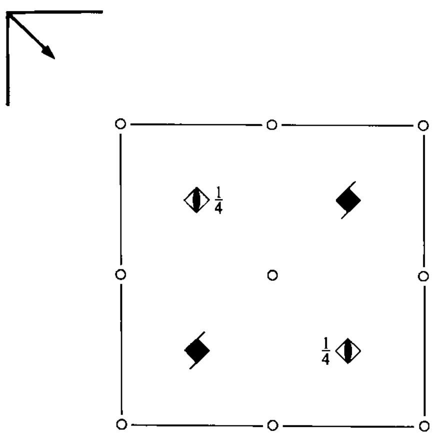
I [2] $P4_2/nbc$ (133); [2] $P4_2/nnm$ (134); [2] $P4_2/nmc$ (137); [2] $P4_2/ncm$ (138)

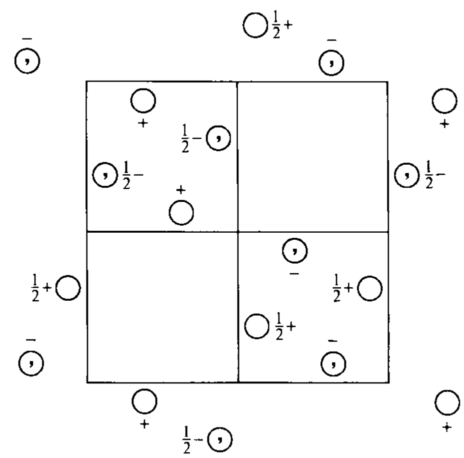
II [2] $C4_2/m$ ($P4_2/m$, 84); [2] $I4/m$ (87); [2] $P4/n$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (85)

$P4_2/n$ $\quad C_{4h}^4$ $\quad 4/m$ $\quad$ Tetragonal

No. 86 $\quad P4_2/n$ $\quad$ Patterson symmetry $P4/m$

ORIGIN CHOICE 2





Origin at $\bar{1}$ on n, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{4}$

Asymmetric unit $\quad -\frac{1}{4} \le x \le \frac{1}{4}; \quad -\frac{1}{4} \le y \le \frac{1}{4}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2 \quad \frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2}) \quad -\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{2}) \quad \frac{1}{4},-\frac{1}{4},z$
(5) $\bar{1} \quad 0,0,0$	(6) $n(\frac{1}{2},\frac{1}{2},0) \quad x,y,0$	(7) $\bar{4}^+ \quad \frac{1}{4},\frac{1}{4},z; \quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(8) $\bar{4}^- \quad \frac{1}{4},\frac{1}{4},z; \quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{2}$ (7) $y,\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{1}{2}$ (8) $\bar{y}+\frac{1}{2},x,\bar{z}+\frac{1}{2}$	$hk0$: $h+k=2n$; $00l$: $l=2n$; $h00$: $h=2n$
							Special: as above, plus
4	f	$2\,.\,.$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},z+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	hkl : $h+k+l=2n$
4	e	$2\,.\,.$	$\frac{3}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},z+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	hkl : $l=2n$
4	d	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	hkl : $h+k,h+l,k+l=2n$
4	c	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl : $h+k,h+l,k+l=2n$
2	b	$\bar{4}\,.\,.$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$			hkl : $h+k+l=2n$
2	a	$\bar{4}\,.\,.$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}$ (81) 1; 2; 7; 8
[2] $P4_2$ (77) 1; 2; 3; 4
[2] $P2/n$ ($P2/c$, 13) 1; 2; 5; 6

IIa none

IIb [2] $F4_1/d$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4_1/a$, 88)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/n$ ($\mathbf{c}'=3\mathbf{c}$) (86); [5] $P4_2/n$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (86)

Minimal non-isomorphic supergroups

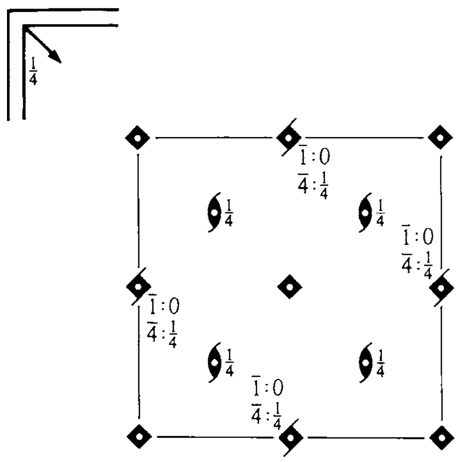
I [2] $P4_2/nbc$ (133); [2] $P4_2/nnm$ (134); [2] $P4_2/nmc$ (137); [2] $P4_2/ncm$ (138)

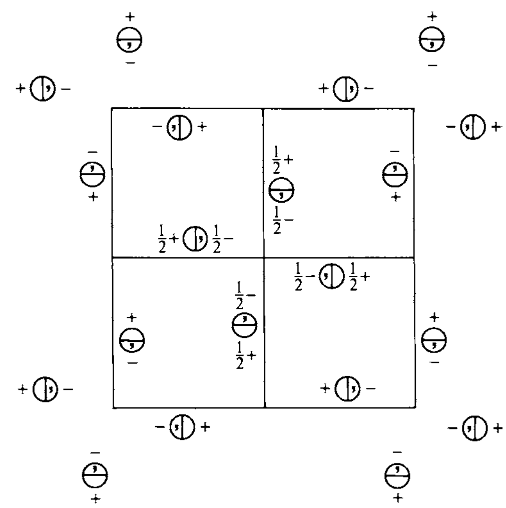
II [2] $C4_2/m$ ($P4_2/m$, 84); [2] $I4/m$ (87); [2] $P4/n$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (85)

International Tables for Crystallography (2006). Vol. A, Space group 87, pp. 356–357.

$I4/m$ $\quad C_{4h}^5$ $\quad 4/m$ $\quad$ Tetragonal

No. 87 $\quad I4/m$ $\quad$ Patterson symmetry $I4/m$





Origin at centre $(4/m)$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2 \quad 0,0,z$	(3) $4^+ \quad 0,0,z$	(4) $4^- \quad 0,0,z$
(5) $\bar{1} \quad 0,0,0$	(6) $m \quad x,y,0$	(7) $\bar{4}^+ \quad 0,0,z; \quad 0,0,0$	(8) $\bar{4}^- \quad 0,0,z; \quad 0,0,0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2}) \quad 0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2}) \quad \frac{1}{2},0,z$
(5) $\bar{1} \quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) $n(\frac{1}{2},\frac{1}{2},0) \quad x,y,\frac{1}{4}$	(7) $\bar{4}^+ \quad \frac{1}{2},0,z; \quad \frac{1}{2},0,\frac{1}{4}$	(8) $\bar{4}^- \quad 0,\frac{1}{2},z; \quad 0,\frac{1}{2},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			General:
16	i	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{y},x,z$ (7) $y,\bar{x},\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y},x,\bar{z}$	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
8	h	$m\,.\,.$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
8	g	$2\,.\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hkl : $l=2n$
8	f	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	hkl : $k,l=2n$
4	e	$4\,.\,.$	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	d	$\bar{4}\,.\,.$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$			hkl : $l=2n$
4	c	$2/m\,.\,.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $l=2n$
2	b	$4/m\,.\,.$	$0,0,\frac{1}{2}$				no extra conditions
2	a	$4/m\,.\,.$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}$ (82)	(1; 2; 7; 8)+
	[2] $I4$ (79)	(1; 2; 3; 4)+
	[2] $I2/m$ ($C2/m$, 12)	(1; 2; 5; 6)+
IIa	[2] $P4_2/n$ (86)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4/n$ (85)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4_2/m$ (84)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4/m$ (83)	1; 2; 3; 4; 5; 6; 7; 8
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I4/m$ ($\mathbf{c}'=3\mathbf{c}$) (87); [5] $I4/m$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (87)

Minimal non-isomorphic supergroups

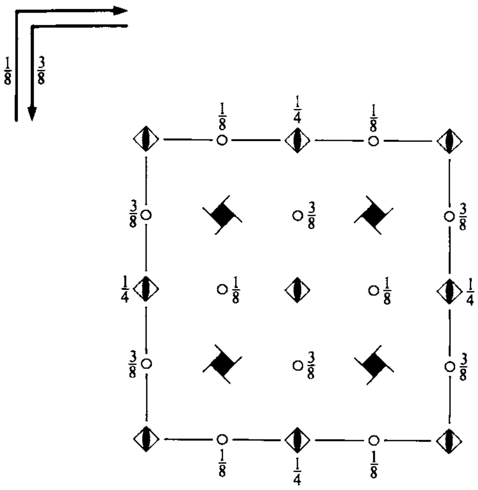
I [2] $I4/mmm$ (139); [2] $I4/mcm$ (140)

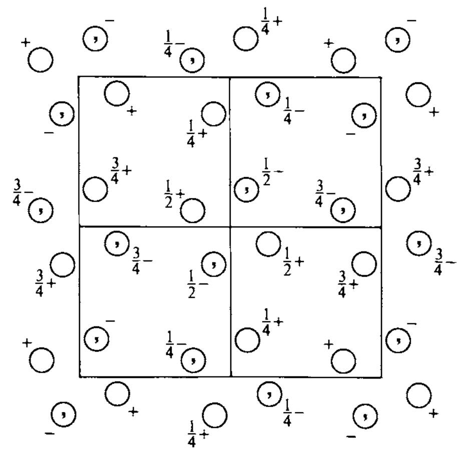
II [2] $C4/m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P4/m$, 83)

$I4_1/a$ $\quad C_{4h}^6$ $\quad 4/m$ $\quad$ Tetragonal

No. 88 $\quad I4_1/a$ $\quad$ Patterson symmetry $I4/m$

ORIGIN CHOICE 1





Origin at $\bar{4}$, at $0,-\frac{1}{4},-\frac{1}{8}$ from $\bar{1}$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{4})\quad -\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{3}{4})\quad \frac{1}{4},-\frac{1}{4},z$
(5) $\bar{1}\quad 0,\frac{1}{4},\frac{1}{8}$	(6) $a\quad x,y,\frac{3}{8}$	(7) $\bar{4}^+\ 0,0,z;\ 0,0,0$	(8) $\bar{4}^-\ 0,\frac{1}{2},z;\ 0,\frac{1}{2},\frac{1}{4}$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\quad 0,0,z$	(3) $4^+(0,0,\frac{3}{4})\quad \frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{4})\quad \frac{1}{4},\frac{1}{4},z$
(5) $\bar{1}\quad \frac{1}{4},0,\frac{3}{8}$	(6) $b\quad x,y,\frac{1}{8}$	(7) $\bar{4}^+\ \frac{1}{2},0,z;\ \frac{1}{2},0,\frac{1}{4}$	(8) $\bar{4}^-\ 0,0,z;\ 0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
16	f	1	(1) x,y,z (5) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$ (7) $y,\bar{x},\bar{z}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$ (8) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl : $h+k+l=2n$ $hk0$: $h,k=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $00l$: $l=4n$ $h00$: $h=2n$ $h\bar{h}0$: $h=2n$
							Special: as above, plus
8	e	$2\,.\,.$	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$	$0,\frac{1}{2},\bar{z}+\frac{1}{4}$	$0,0,\bar{z}$	hkl : $l=2n+1$ or $2h+l=4n$
8	d	$\bar{1}$	$0,\frac{1}{4},\frac{5}{8}$	$\frac{1}{2},\frac{1}{4},\frac{1}{8}$	$\frac{3}{4},\frac{1}{2},\frac{7}{8}$	$\frac{3}{4},0,\frac{3}{8}$	hkl : $l=2n+1$ or $h,k=2n,\quad h+k+l=4n$
8	c	$\bar{1}$	$0,\frac{1}{4},\frac{1}{8}$	$\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},\frac{1}{2},\frac{3}{8}$	$\frac{3}{4},0,\frac{7}{8}$	
4	b	$\bar{4}\,.\,.$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{3}{4}$			hkl : $l=2n+1$ or $2h+l=4n$
4	a	$\bar{4}\,.\,.$	$0,0,0$	$0,\frac{1}{2},\frac{1}{4}$			

Symmetry of special projections

Along [001] $p4$	Along [100] $c2mm$	Along [110] $p2mg$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}\quad \mathbf{b}'=\frac{1}{2}\mathbf{b}$	$\mathbf{a}'=\mathbf{b}\quad \mathbf{b}'=\mathbf{c}$	$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})\quad \mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,\frac{3}{8}$	Origin at $x,x+\frac{1}{4},\frac{1}{8}$

Maximal non-isomorphic subgroups

I [2] $I\bar{4}$ (82) (1; 2; 7; 8)+
[2] $I4_1$ (80) (1; 2; 3; 4)+
[2] $I2/a$ ($C2/c$, 15) (1; 2; 5; 6)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1/a$ ($\mathbf{c}'=3\mathbf{c}$) (88); [5] $I4_1/a$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (88)

Minimal non-isomorphic supergroups

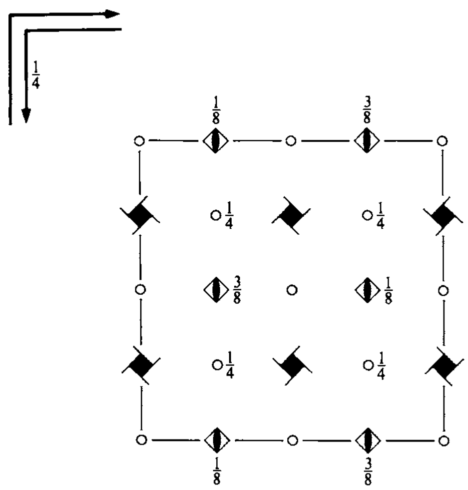
I [2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142)

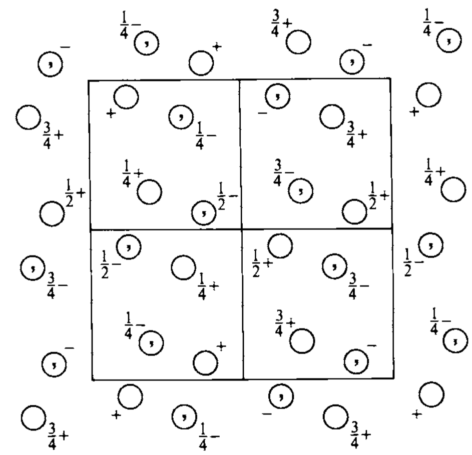
II [2] $C4_2/a$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P4_2/n$, 86)

$I4_1/a$ $\quad C_{4h}^6$ $\quad 4/m$ $\quad$ Tetragonal

No. 88 $\quad I4_1/a$ $\quad$ Patterson symmetry $I4/m$

ORIGIN CHOICE 2





Origin at $\bar{1}$ on glide plane b, at $0,\frac{1}{4},\frac{1}{8}$ from $\bar{4}$

Asymmetric unit $\quad 0 \le x \le \frac{1}{4};\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $4^+(0,0,\frac{1}{4})\quad \frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{3}{4})\quad \frac{3}{4},0,z$
(5) $\bar{1}\quad 0,0,0$	(6) $a\quad x,y,\frac{1}{4}$	(7) $\bar{4}^+\quad \frac{1}{2},\frac{1}{4},z;\quad \frac{1}{2},\frac{1}{4},\frac{3}{8}$	(8) $\bar{4}^-\quad 0,\frac{1}{4},z;\quad 0,\frac{1}{4},\frac{1}{8}$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\quad 0,\frac{1}{4},z$	(3) $4^+(0,0,\frac{3}{4})\quad -\frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{4})\quad \frac{1}{4},0,z$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) $b\quad x,y,0$	(7) $\bar{4}^+\quad \frac{1}{2},-\frac{1}{4},z;\quad \frac{1}{2},-\frac{1}{4},\frac{1}{8}$	(8) $\bar{4}^-\quad 0,\frac{3}{4},z;\quad 0,\frac{3}{4},\frac{3}{8}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
16	f	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{y}+\frac{3}{4},x+\frac{1}{4},z+\frac{1}{4}$ (7) $y+\frac{1}{4},\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4}$	(4) $y+\frac{3}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$ (8) $\bar{y}+\frac{1}{4},x+\frac{1}{4},\bar{z}+\frac{1}{4}$	hkl : $h+k+l=2n$ $hk0$: $h,k=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $00l$: $l=4n$ $h00$: $h=2n$ $h\bar{h}0$: $h=2n$
							Special: as above, plus
8	e	$2\,.\,.$	$0,\frac{1}{4},z$	$\frac{1}{2},\frac{1}{4},z+\frac{1}{4}$	$0,\frac{3}{4},\bar{z}$	$\frac{1}{2},\frac{3}{4},\bar{z}+\frac{3}{4}$	hkl : $l=2n+1$ or $2h+l=4n$
8	d	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	hkl : $l=2n+1$ or $h,k=2n,\quad h+k+l=4n$
8	c	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	
4	b	$\bar{4}\,.\,.$	$0,\frac{1}{4},\frac{5}{8}$	$\frac{1}{2},\frac{1}{4},\frac{7}{8}$			hkl : $l=2n+1$ or $2h+l=4n$
4	a	$\bar{4}\,.\,.$	$0,\frac{1}{4},\frac{1}{8}$	$\frac{1}{2},\frac{1}{4},\frac{3}{8}$			

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}\qquad\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{4},0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}\qquad\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [110] $p2mg$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})\qquad\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $I\bar{4}$ (82) (1; 2; 7; 8)+
[2] $I4_1$ (80) (1; 2; 3; 4)+
[2] $I2/a$ ($C2/c$, 15) (1; 2; 5; 6)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1/a$ ($\mathbf{c}'=3\mathbf{c}$) (88); [5] $I4_1/a$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (88)

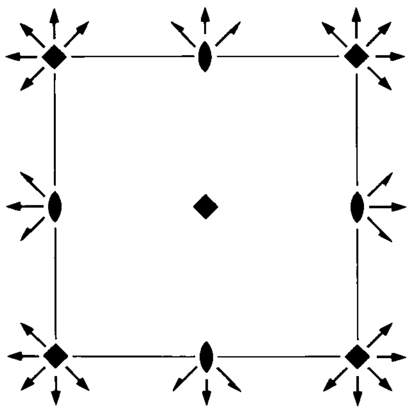
Minimal non-isomorphic supergroups

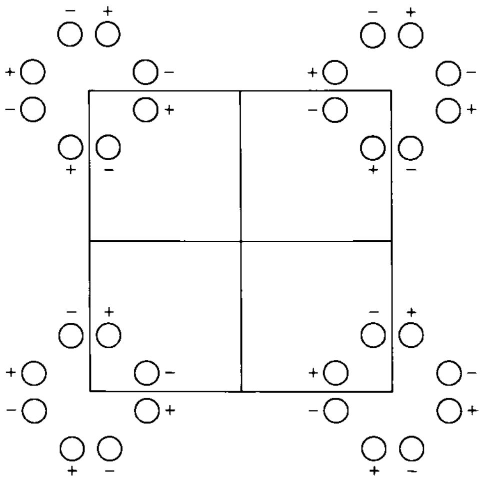
I [2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142)

II [2] $C4_2/a$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P4_2/n$, 86)

$P422$ D_4^1 422 Tetragonal

No. 89 $P422$ Patterson symmetry $P4/mmm$





Origin at 422

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) 2 $0,y,0$	(6) 2 $x,0,0$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	p	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$	(3) $\bar{y},x,z$ (7) $y,x,\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y},\bar{x},\bar{z}$	no conditions
							Special:
4	o	. 2 .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	no extra conditions
4	n	. 2 .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	no extra conditions
4	m	. 2 .	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	no extra conditions
4	l	. 2 .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	no extra conditions
4	k	. . 2	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	no extra conditions
4	j	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	no extra conditions
4	i	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hkl : $h+k=2n$
2	h	4 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	g	4 . .	$0,0,z$	$0,0,\bar{z}$			no extra conditions
2	f	2 2 2 .	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	e	2 2 2 .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			hkl : $h+k=2n$
1	d	4 2 2	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				no extra conditions
1	c	4 2 2	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	b	4 2 2	$0,0,\frac{1}{2}$				no extra conditions
1	a	4 2 2	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P411$ ($P4$, 75) 1; 2; 3; 4
[2] $P212$ ($C222$, 21) 1; 2; 7; 8
[2] $P221$ ($P222$, 16) 1; 2; 5; 6

IIa none

IIb [2] $P4_222$ ($\mathbf{c}'=2\mathbf{c}$) (93); [2] $C422_1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P42_12$, 90); [2] $F422$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I422$, 97)

Maximal isomorphic subgroups of lowest index

IIc [2] $P422$ ($\mathbf{c}'=2\mathbf{c}$) (89); [2] $C422$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P422$, 89)

Minimal non-isomorphic supergroups

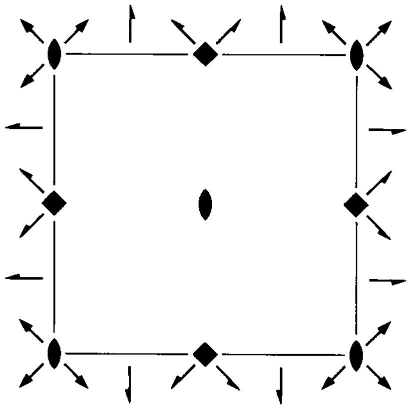
I [2] $P4/mmm$ (123); [2] $P4/mcc$ (124); [2] $P4/nbm$ (125); [2] $P4/nnc$ (126); [3] $P432$ (207)

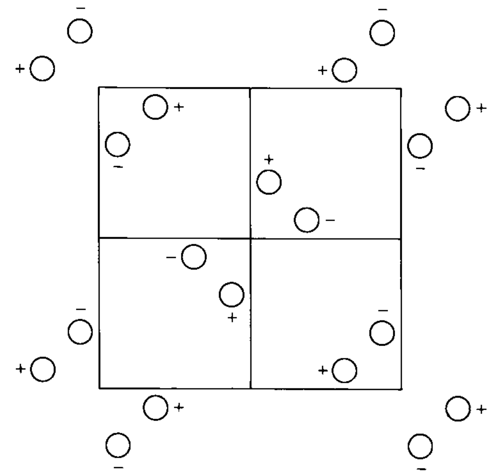
II [2] $I422$ (97)

International Tables for Crystallography (2006). Vol. A, Space group 90, pp. 364–365.

$P42_12$ D_4^2 422 Tetragonal

No. 90 $P42_12$ Patterson symmetry $P4/mmm$





Origin at 222 at 212

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) 4^+ $0,\frac{1}{2},z$ (4) 4^- $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ (6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ (7) 2 $x,x,0$ (8) 2 $x,\bar{x},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z$ (7) $y,x,\bar{z}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z$ (8) $\bar{y},\bar{x},\bar{z}$	$h00$: $h=2n$
							Special: as above, plus
4	f	. . 2	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$0kl$: $k=2n$
4	e	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$0kl$: $k=2n$
4	d	2 . .	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	hkl : $h+k=2n$
2	c	4 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			$hk0$: $h+k=2n$
2	b	2 . 22	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	a	2 . 22	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,\frac{1}{2},z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P411$ ($P4$, 75) 1; 2; 3; 4
[2] $P212$ ($C222$, 21) 1; 2; 7; 8
[2] $P22_11$ ($P2_12_12$, 18) 1; 2; 5; 6

IIa none

IIb [2] $P4_22_12$ ($\mathbf{c}'=2\mathbf{c}$) (94)

Maximal isomorphic subgroups of lowest index

IIc [2] $P42_12$ ($\mathbf{c}'=2\mathbf{c}$) (90); [9] $P42_12$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (90)

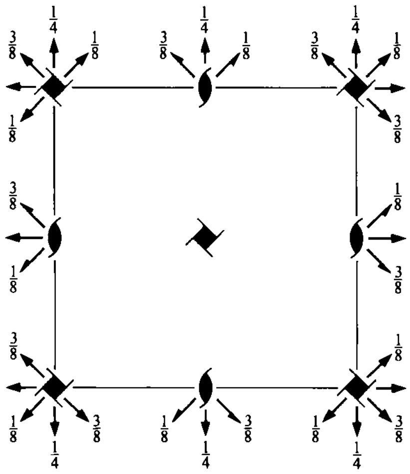
Minimal non-isomorphic supergroups

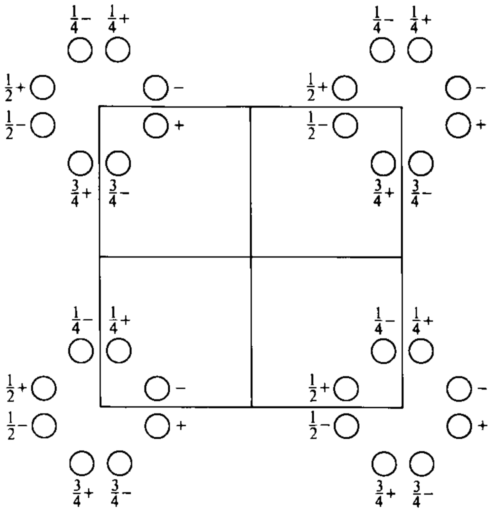
I [2] $P4/mbm$ (127); [2] $P4/mnc$ (128); [2] $P4/nmm$ (129); [2] $P4/ncc$ (130)

II [2] $C422$ ($P422$, 89); [2] $I422$ (97)

$P4_122$ D_4^3 422 Tetragonal

No. 91 $P4_122$ Patterson symmetry $P4/mmm$





Origin on $2[010]$ at $4_1(1,2)1$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{8}$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})\quad 0,0,z$	(3) $4^+(0,0,\frac{1}{4})\quad 0,0,z$	(4) $4^-(0,0,\frac{3}{4})\quad 0,0,z$
(5) $2\quad 0,y,0$	(6) $2\quad x,0,\frac{1}{4}$	(7) $2\quad x,x,\frac{3}{8}$	(8) $2\quad x,\bar{x},\frac{1}{8}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z+\frac{1}{2}$ (6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{1}{4}$ (7) $y,x,\bar{z}+\frac{3}{4}$	(4) $y,\bar{x},z+\frac{3}{4}$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{4}$	$00l$: $l=4n$
							Special: as above, plus
4	c	. . 2	$x,x,\frac{3}{8}$	$\bar{x},\bar{x},\frac{7}{8}$	$\bar{x},x,\frac{5}{8}$	$x,\bar{x},\frac{1}{8}$	$0kl$: $l=2n+1$ or $l=4n$
4	b	. 2 .	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},\frac{1}{2}$	$\bar{y},\frac{1}{2},\frac{1}{4}$	$y,\frac{1}{2},\frac{3}{4}$	hhl : $l=2n+1$ or $l=4n$
4	a	. 2 .	$0,y,0$	$0,\bar{y},\frac{1}{2}$	$\bar{y},0,\frac{1}{4}$	$y,0,\frac{3}{4}$	hhl : $l=2n+1$ or $l=4n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,\frac{1}{4}$

Along [110] $p2gm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{3}{8}$

Maximal non-isomorphic subgroups

I [2] $P4_111$ ($P4_1$, 76) 1; 2; 3; 4
[2] $P2_121$ ($P222_1$, 17) 1; 2; 5; 6
[2] $P2_112$ ($C222_1$, 20) 1; 2; 7; 8

IIa none

IIb [2] $C4_122_1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4_12_12$, 92)

Maximal isomorphic subgroups of lowest index

IIc [2] $C4_122$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4_122$, 91); [3] $P4_322$ ($\mathbf{c}'=3\mathbf{c}$) (95); [5] $P4_122$ ($\mathbf{c}'=5\mathbf{c}$) (91)

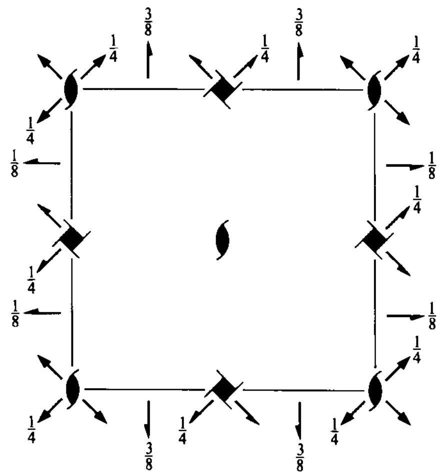
Minimal non-isomorphic supergroups

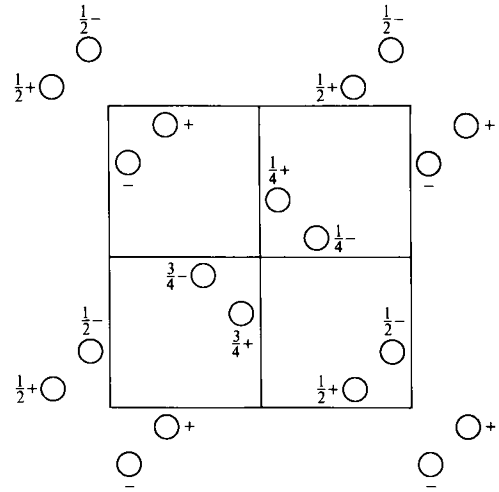
I none

II [2] $I4_122$ (98); [2] $P4_222$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (93)

$P4_12_12$ D_4^4 422 Tetragonal

No. 92 $P4_12_12$ Patterson symmetry $P4/mmm$





Origin on $2[110]$ at $2_11(1,2)$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{8}$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})\quad 0,0,z$	(3) $4^+(0,0,\frac{1}{4})\quad 0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{3}{4})\quad \frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,\frac{1}{8}$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{3}{8}$	(7) $2\quad x,x,0$	(8) $2\quad x,\bar{x},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	b	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{3}{4}$	$00l$: $l=4n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{4}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{3}{4}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$h00$: $h=2n$
							Special: as above, plus
4	a	. . 2	$x,x,0$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$	$0kl$: $l=2n+1$ or $2k+l=4n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,\frac{1}{2},z$

Along [100] $p2gg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{3}{8}$

Along [110] $p2gm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P4_111$ ($P4_1$, 76) 1; 2; 3; 4
[2] $P2_112$ ($C222_1$, 20) 1; 2; 7; 8
[2] $P2_12_11$ ($P2_12_12_1$, 19) 1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_32_12$ ($\mathbf{c}'=3\mathbf{c}$) (96); [5] $P4_12_12$ ($\mathbf{c}'=5\mathbf{c}$) (92); [9] $P4_12_12$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (92)

Minimal non-isomorphic supergroups

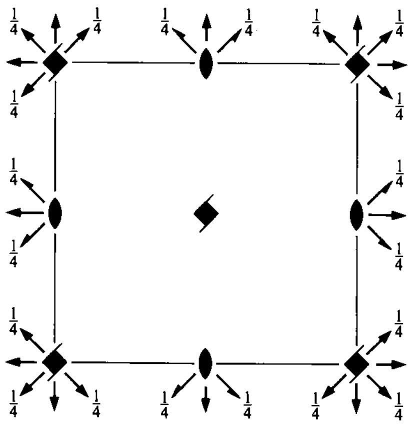
I [3] $P4_132$ (213)

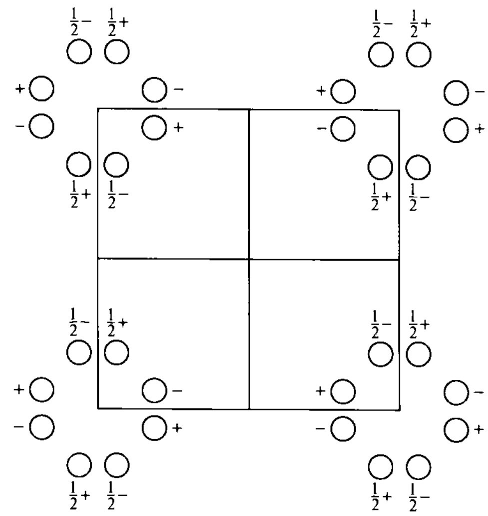
II [2] $C4_122$ ($P4_122$, 91); [2] $I4_122$ (98); [2] $P4_22_12$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (94)

International Tables for Crystallography (2006). Vol. A, Space group 93, pp. 370–371.

$P4_222$ D_4^5 422 Tetragonal

No. 93 $P4_222$ Patterson symmetry $P4/mmm$





Origin at 222 at 4_221

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) $4^+(0,0,\frac{1}{2})$ $0,0,z$	(4) $4^-(0,0,\frac{1}{2})$ $0,0,z$
(5) 2 $0,y,0$	(6) 2 $x,0,0$	(7) 2 $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	p	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	$00l$: $l=2n$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	
							Special: as above, plus
4	o	$..2$	$x,x,\frac{3}{4}$	$\bar{x},\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{1}{4}$	$x,\bar{x},\frac{1}{4}$	$0kl$: $l=2n$
4	n	$..2$	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{3}{4}$	$x,\bar{x},\frac{3}{4}$	$0kl$: $l=2n$
4	m	$.2.$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	hhl : $l=2n$
4	l	$.2.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,0$	$0,\bar{x},0$	hhl : $l=2n$
4	k	$.2.$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	hhl : $l=2n$
4	j	$.2.$	$x,0,0$	$\bar{x},0,0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	hhl : $l=2n$
4	i	$2..$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	hkl : $h+k+l=2n$
4	h	$2..$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl : $l=2n$
4	g	$2..$	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	hkl : $l=2n$
2	f	2.22	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl : $l=2n$
2	e	2.22	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl : $l=2n$
2	d	$222.$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$			hkl : $h+k+l=2n$
2	c	$222.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k+l=2n$
2	b	$222.$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
2	a	$222.$	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{1}{4}$

Maximal non-isomorphic subgroups

I [2] $P4_211$ ($P4_2$, 77) 1; 2; 3; 4
[2] $P212$ ($C222$, 21) 1; 2; 7; 8
[2] $P221$ ($P222$, 16) 1; 2; 5; 6

IIa none

IIb [2] $P4_322$ ($\mathbf{c}'=2\mathbf{c}$) (95); [2] $P4_122$ ($\mathbf{c}'=2\mathbf{c}$) (91); [2] $C4_222_1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4_22_12$, 94);
[2] $F4_122$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4_122$, 98)

Maximal isomorphic subgroups of lowest index

IIc [2] $C4_222$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4_222$, 93); [3] $P4_222$ ($\mathbf{c}'=3\mathbf{c}$) (93)

Minimal non-isomorphic supergroups

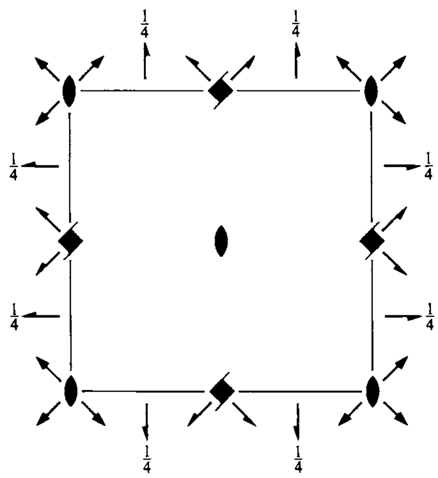
I [2] $P4_2/mmc$ (131); [2] $P4_2/mcm$ (132); [2] $P4_2/nbc$ (133); [2] $P4_2/nnm$ (134); [3] $P4_232$ (208)

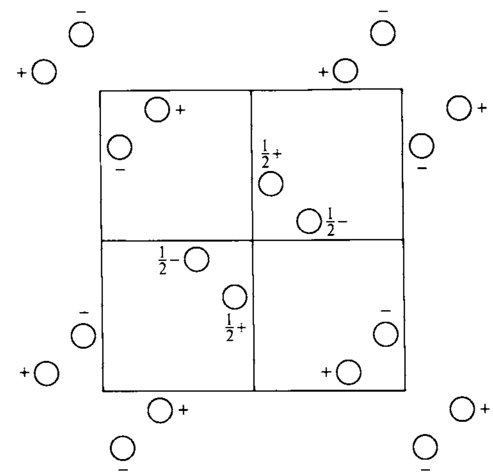
II [2] $I422$ (97); [2] $P422$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (89)

International Tables for Crystallography (2006). Vol. A, Space group 94, pp. 372–373.

$P4_22_12$ D_4^6 422 Tetragonal

No. 94 $P4_22_12$ Patterson symmetry $P4/mmm$





Origin at 222 at 212

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ (7) $y,x,\bar{z}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (8) $\bar{y},\bar{x},\bar{z}$	$00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
4	f	. . 2	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$0kl$: $k+l=2n$
4	e	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$0kl$: $k+l=2n$
4	d	2 . .	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	hkl : $l=2n$ $hk0$: $h+k=2n$
4	c	2 . .	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	hkl : $h+k+l=2n$
2	b	2 . 2 2	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k+l=2n$
2	a	2 . 2 2	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,\frac{1}{2},z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P4_2 1 1$ ($P4_2$, 77) 1; 2; 3; 4
[2] $P2 1 2$ ($C222$, 21) 1; 2; 7; 8
[2] $P2 2_1 1$ ($P2_1 2_1 2$, 18) 1; 2; 5; 6

IIa none

IIb [2] $P4_3 2_1 2$ ($\mathbf{c}'=2\mathbf{c}$) (96); [2] $P4_1 2_1 2$ ($\mathbf{c}'=2\mathbf{c}$) (92)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2 2_1 2$ ($\mathbf{c}'=3\mathbf{c}$) (94); [9] $P4_2 2_1 2$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (94)

Minimal non-isomorphic supergroups

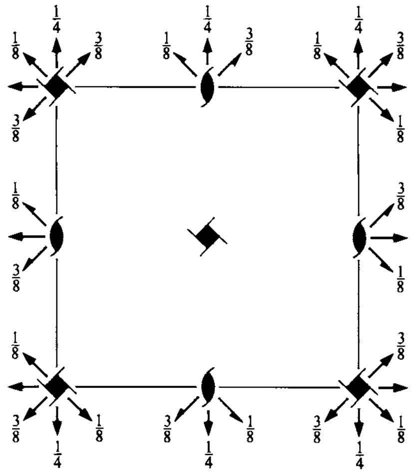
I [2] $P4_2/mbc$ (135); [2] $P4_2/mnm$ (136); [2] $P4_2/nmc$ (137); [2] $P4_2/ncm$ (138)

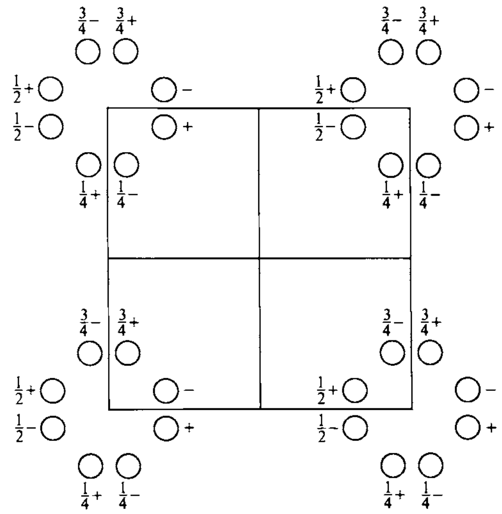
II [2] $C4_2 2 2$ ($P4_2 2 2$, 93); [2] $I422$ (97); [2] $P42_1 2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (90)

International Tables for Crystallography (2006). Vol. A, Space group 95, pp. 374–375.

$P4_3 22$ D_4^7 422 Tetragonal

No. 95 $P4_3 22$ Patterson symmetry $P4/mmm$





Origin on $2[010]$ at $4_3(1,2)1$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{8}$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})\quad 0,0,z$	(3) $4^+(0,0,\frac{3}{4})\quad 0,0,z$	(4) $4^-(0,0,\frac{1}{4})\quad 0,0,z$
(5) $2\quad 0,y,0$	(6) $2\quad x,0,\frac{1}{4}$	(7) $2\quad x,x,\frac{1}{8}$	(8) $2\quad x,\bar{x},\frac{3}{8}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z+\frac{1}{2}$ (6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{3}{4}$ (7) $y,x,\bar{z}+\frac{1}{4}$	(4) $y,\bar{x},z+\frac{1}{4}$ (8) $\bar{y},\bar{x},\bar{z}+\frac{3}{4}$	$00l$: $l=4n$
							Special: as above, plus
4	c	. . 2	$x,x,\frac{5}{8}$	$\bar{x},\bar{x},\frac{1}{8}$	$\bar{x},x,\frac{3}{8}$	$x,\bar{x},\frac{7}{8}$	$0kl$: $l=2n+1$ or $l=4n$
4	b	. 2 .	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},\frac{1}{2}$	$\bar{y},\frac{1}{2},\frac{3}{4}$	$y,\frac{1}{2},\frac{1}{4}$	hhl : $l=2n+1$ or $l=4n$
4	a	. 2 .	$0,y,0$	$0,\bar{y},\frac{1}{2}$	$\bar{y},0,\frac{3}{4}$	$y,0,\frac{1}{4}$	hhl : $l=2n+1$ or $l=4n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,\frac{1}{4}$

Along [110] $p2gm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{1}{8}$

Maximal non-isomorphic subgroups

I [2] $P4_311$ ($P4_3$, 78) 1; 2; 3; 4
[2] $P2_112$ ($C222_1$, 20) 1; 2; 7; 8
[2] $P2_121$ ($P222_1$, 17) 1; 2; 5; 6

IIa none

IIb [2] $C4_322_1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4_32_12$, 96)

Maximal isomorphic subgroups of lowest index

IIc [2] $C4_322$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4_322$, 95); [3] $P4_122$ ($\mathbf{c}'=3\mathbf{c}$) (91); [5] $P4_322$ ($\mathbf{c}'=5\mathbf{c}$) (95)

Minimal non-isomorphic supergroups

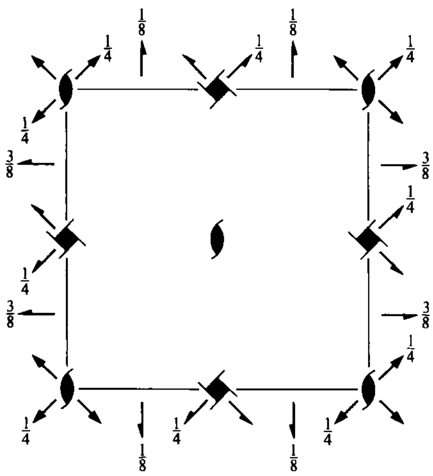
I none

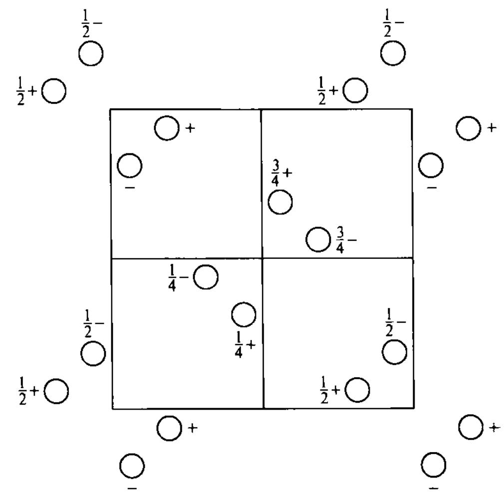
II [2] $I4_122$ (98); [2] $P4_222$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (93)

International Tables for Crystallography (2006). Vol. A, Space group 96, pp. 376–377.

$P4_32_12$ D_4^8 422 Tetragonal

No. 96 $P4_32_12$ Patterson symmetry $P4/mmm$





Origin on $2[110]$ at $2_11(1,2)$

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le \frac{1}{8}$

Symmetry operations

(1) 1
(2) $2(0,0,\frac{1}{2})$ $0,0,z$
(3) $4^+(0,0,\frac{3}{4})$ $0,\frac{1}{2},z$
(4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{3}{8}$
(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{8}$
(7) 2 $x,x,0$
(8) 2 $x,\bar{x},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	b	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{3}{4}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{4}$	$00l$: $l=4n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{3}{4}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$h00$: $h=2n$
							Special: as above, plus
4	a	$..2$	$x,x,0$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{4}$	$0kl$: $l=2n+1$ or $2k+l=4n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,\frac{1}{2},z$

Along [100] $p2gg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{8}$

Along [110] $p2gm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P4_311$ ($P4_3$, 78) 1; 2; 3; 4
[2] $P2_112$ ($C222_1$, 20) 1; 2; 7; 8
[2] $P2_12_11$ ($P2_12_12_1$, 19) 1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_12_12$ ($\mathbf{c}'=3\mathbf{c}$) (92); [5] $P4_32_12$ ($\mathbf{c}'=5\mathbf{c}$) (96); [9] $P4_32_12$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (96)

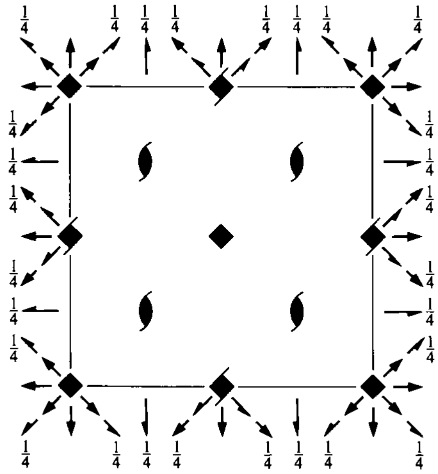
Minimal non-isomorphic supergroups

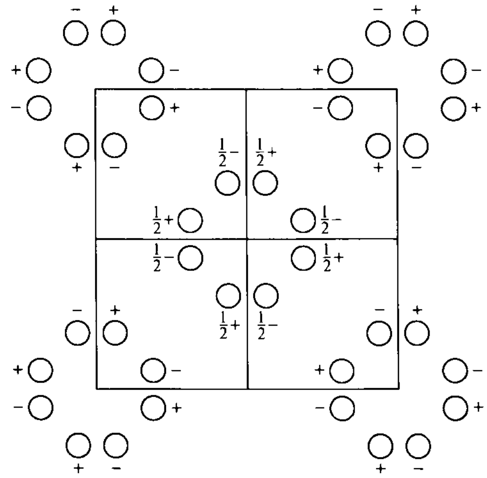
I [3] $P4_332$ (212)

II [2] $C4_322$ ($P4_322$, 95); [2] $I4_122$ (98); [2] $P4_22_12$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (94)

$I422$ D_4^9 422 Tetragonal

No. 97 $I422$ Patterson symmetry $I4/mmm$





Origin at 422

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\ \ 0,0,z$	(3) $4^{+}\ \ 0,0,z$	(4) $4^{-}\ \ 0,0,z$
(5) $2\ \ 0,y,0$	(6) $2\ \ x,0,0$	(7) $2\ \ x,x,0$	(8) $2\ \ x,\bar{x},0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$	(3) $4^{+}(0,0,\frac{1}{2})\ \ 0,\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{1}{2})\ \ \frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)\ \ \frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x,\frac{1}{4}$	(8) $2\ \ x,\bar{x}+\frac{1}{2},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
16	k	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$	(3) $\bar{y},x,z$ (7) $y,x,\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y},\bar{x},\bar{z}$	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
8	j	. . 2	$x,x+\frac{1}{2},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x,\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{1}{4}$	$0kl$: $k=2n$
8	i	. 2 .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	no extra conditions
8	h	. 2 .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	no extra conditions
8	g	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	no extra conditions
8	f	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hkl : $l=2n$
4	e	4 . .	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	d	2 . 22	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$			hkl : $l=2n$
4	c	2 2 2 .	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $l=2n$
2	b	4 2 2	$0,0,\frac{1}{2}$				no extra conditions
2	a	4 2 2	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $I411$ ($I4$, 79) (1; 2; 3; 4)+
[2] $I221$ ($I222$, 23) (1; 2; 5; 6)+
[2] $I212$ ($F222$, 22) (1; 2; 7; 8)+

IIa [2] $P4_22_12$ (94) 1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P4_222$ (93) 1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P42_12$ (90) 1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P422$ (89) 1; 2; 3; 4; 5; 6; 7; 8

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I422$ ($\mathbf{c}'=3\mathbf{c}$) (97); [9] $I422$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (97)

Minimal non-isomorphic supergroups

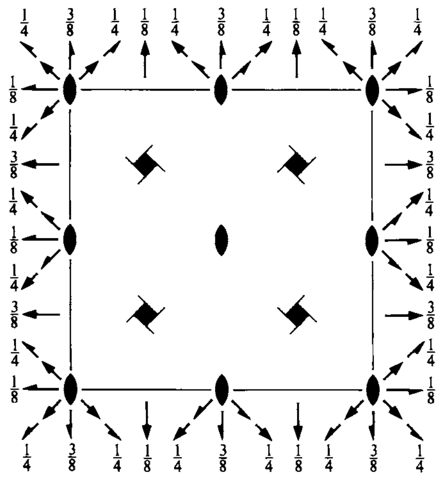
I [2] $I4/mmm$ (139); [2] $I4/mcm$ (140); [3] $F432$ (209); [3] $I432$ (211)

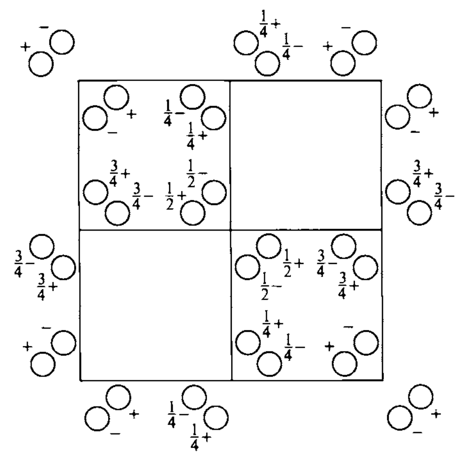
II [2] $C422$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P422$, 89)

International Tables for Crystallography (2006). Vol. A, Space group 98, pp. 380–381.

$I4_122$ D_4^{10} 422 Tetragonal

No. 98 $I4_122$ Patterson symmetry $I4/mmm$





Origin at 222 at 212

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{4},z$ (4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},-\frac{1}{4},z$

(5) 2 $\frac{1}{4},y,\frac{3}{8}$ (6) 2 $x,\frac{1}{4},\frac{1}{8}$ (7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$ (8) 2 $x,\bar{x},0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) 2 $0,0,z$ (3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{4},z$ (4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},\frac{1}{4},z$

(5) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{8}$ (6) $2(\frac{1}{2},0,0)$ $x,0,\frac{3}{8}$ (7) 2 $x,x,0$ (8) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
16	g	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$ (8) $\bar{y},\bar{x},\bar{z}$	$hkl: h+k+l=2n$ $hk0: h+k=2n$ $0kl: k+l=2n$ $hhl: l=2n$ $00l: l=4n$ $h00: h=2n$
							Special: as above, plus
8	f	. 2 .	$x,\frac{1}{4},\frac{1}{8}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},x+\frac{1}{2},\frac{3}{8}$	$\frac{3}{4},\bar{x},\frac{7}{8}$	$hhl: l=4n$
8	e	. . 2	$\bar{x},x,0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},x,\frac{3}{4}$	$0kl: k=2n+1$ or $l=4n$
8	d	. . 2	$x,x,0$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	$0kl: k=2n+1$ or $l=4n$
8	c	2 . .	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$	$\frac{1}{2},0,\bar{z}+\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$hkl: l=2n+1$ or $2h+l=4n$
4	b	2 . 22	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{3}{4}$			$hkl: l=2n+1$ or $2h+l=4n$
4	a	2 . 22	$0,0,0$	$0,\frac{1}{2},\frac{1}{4}$			$hkl: l=2n+1$ or $2h+l=4n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,\frac{3}{8}$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $I4_111$ ($I4_1$, 80) (1; 2; 3; 4)+
[2] $I2_121$ ($I2_12_12_1$, 24) (1; 2; 5; 6)+
[2] $I2_112$ ($F222$, 22) (1; 2; 7; 8)+

IIa [2] $P4_32_12$ (96) 1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P4_322$ (95) 1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P4_12_12$ (92) 1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P4_122$ (91) 1; 2; 3; 4; 5; 6; 7; 8

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_122$ ($\mathbf{c}'=3\mathbf{c}$) (98); [9] $I4_122$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (98)

Minimal non-isomorphic supergroups

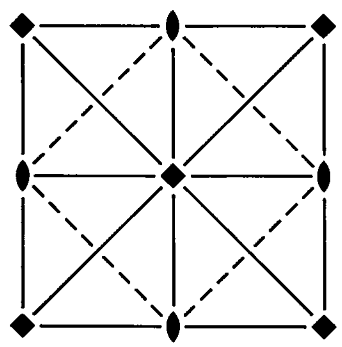
I [2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $F4_132$ (210); [3] $I4_132$ (214)

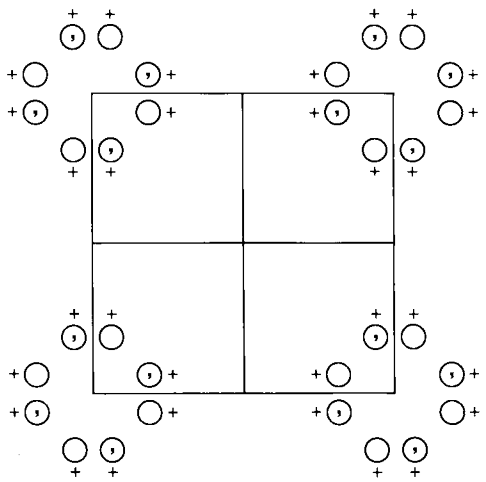
II [2] $C4_222$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P4_222$, 93)

International Tables for Crystallography (2006). Vol. A, Space group 99, pp. 382–383.

$P4mm$ C_{4v}^{1} $4mm$ Tetragonal

No. 99 $P4mm$ Patterson symmetry $P4/mmm$





Origin on $4mm$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $x \le y$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^{+} $0,0,z$	(4) 4^{-} $0,0,z$
(5) m $x,0,z$	(6) m $0,y,z$	(7) m $x,\bar{x},z$	(8) m x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z (5) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z$	(3) $\bar{y},x,z$ (7) $\bar{y},\bar{x},z$	(4) $y,\bar{x},z$ (8) y,x,z	no conditions
							Special:
4	f	$.\,m\,.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z$	$\frac{1}{2},\bar{x},z$	no extra conditions
4	e	$.\,m\,.$	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$	no extra conditions
4	d	$.\,.\,m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
2	c	$2\,m\,m\,.$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$			$hkl: h+k=2n$
1	b	$4\,m\,m$	$\frac{1}{2},\frac{1}{2},z$				no extra conditions
1	a	$4\,m\,m$	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P411$ ($P4$, 75) 1; 2; 3; 4
[2] $P21m$ ($Cmm2$, 35) 1; 2; 7; 8
[2] $P2m1$ ($Pmm2$, 25) 1; 2; 5; 6

IIa none

IIb [2] $P4_2mc$ ($\mathbf{c}'=2\mathbf{c}$) (105); [2] $P4cc$ ($\mathbf{c}'=2\mathbf{c}$) (103); [2] $P4_2cm$ ($\mathbf{c}'=2\mathbf{c}$) (101); [2] $C4md$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4bm$, 100); [2] $F4mc$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4cm$, 108); [2] $F4mm$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4mm$, 107)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4mm$ ($\mathbf{c}'=2\mathbf{c}$) (99); [2] $C4mm$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4mm$, 99)

Minimal non-isomorphic supergroups

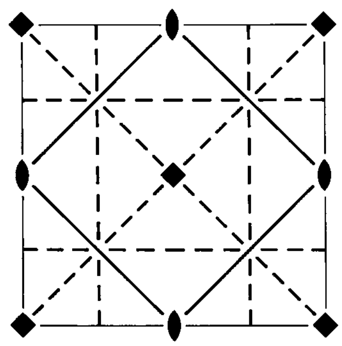
I [2] $P4/mmm$ (123); [2] $P4/nmm$ (129)

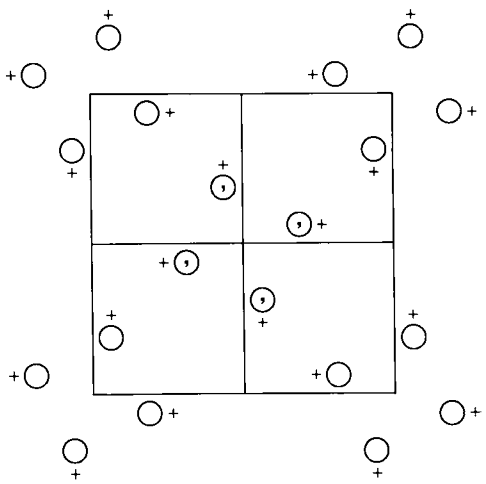
II [2] $I4mm$ (107)

International Tables for Crystallography (2006). Vol. A, Space group 100, pp. 384–385.

$P4bm$ C_{4v}^{2} $4mm$ Tetragonal

No. 100 $P4bm$ Patterson symmetry $P4/mmm$





Origin on $41g$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $y \le \frac{1}{2} - x$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^{+} $0,0,z$	(4) 4^{-} $0,0,z$
(5) a $x,\frac{1}{4},z$	(6) b $\frac{1}{4},y,z$	(7) m $x+\frac{1}{2},\bar{x},z$	(8) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z (5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(3) $\bar{y},x,z$ (7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(4) $y,\bar{x},z$ (8) $y+\frac{1}{2},x+\frac{1}{2},z$	$0kl$: $k=2n$ $h00$: $h=2n$
							Special: as above, plus
4	c	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	no extra conditions
2	b	$2.mm$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$			hkl : $h+k=2n$
2	a	$4..$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P411$ ($P4$, 75) 1; 2; 3; 4
[2] $P21m$ ($Cmm2$, 35) 1; 2; 7; 8
[2] $P2b1$ ($Pba2$, 32) 1; 2; 5; 6

IIa none

IIb [2] $P4_2bc$ ($\mathbf{c}'=2\mathbf{c}$) (106); [2] $P4nc$ ($\mathbf{c}'=2\mathbf{c}$) (104); [2] $P4_2nm$ ($\mathbf{c}'=2\mathbf{c}$) (102)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4bm$ ($\mathbf{c}'=2\mathbf{c}$) (100); [9] $P4bm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (100)

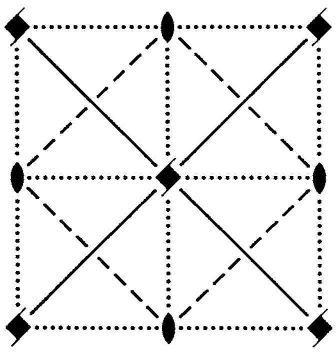
Minimal non-isomorphic supergroups

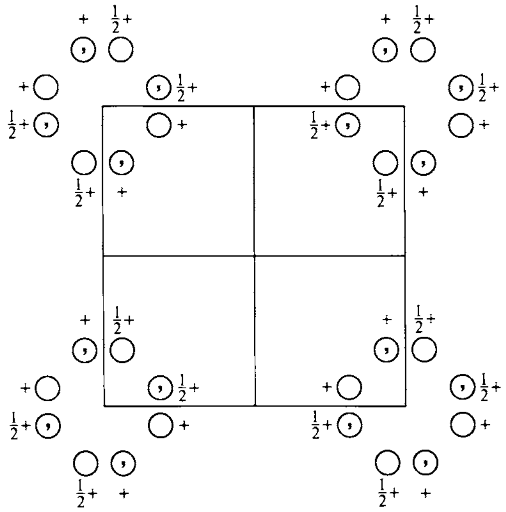
I [2] $P4/nbm$ (125); [2] $P4/mbm$ (127)

II [2] $C4mm$ ($P4mm$, 99); [2] $I4cm$ (108)

$P4_2cm$ C_{4v}^3 $4mm$ Tetragonal

No. 101 $P4_2cm$ Patterson symmetry $P4/mmm$





Origin on $2mm$ on 4_2cm

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le 1;\quad x \le y$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^+(0,0,\frac{1}{2})\quad 0,0,z$	(4) $4^-(0,0,\frac{1}{2})\quad 0,0,z$
(5) $c\quad x,0,z$	(6) $c\quad 0,y,z$	(7) $m\quad x,\bar{x},z$	(8) $m\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*e*	1	(1) x,y,z (5) $x,\bar{y},z+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{1}{2}$ (7) $\bar{y},\bar{x},z$	(4) $y,\bar{x},z+\frac{1}{2}$ (8) y,x,z	$0kl$: $l=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*d*	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z+\frac{1}{2}$	$x,\bar{x},z+\frac{1}{2}$	no extra conditions
4	*c*	$2..$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,z$	hkl : $h+k,l=2n$
2	*b*	$2.mm$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl : $l=2n$
2	*a*	$2.mm$	$0,0,z$	$0,0,z+\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P4_211$ ($P4_2$, 77) 1; 2; 3; 4
[2] $P21m$ ($Cmm2$, 35) 1; 2; 7; 8
[2] $P2c1$ ($Pcc2$, 27) 1; 2; 5; 6

IIa none

IIb [2] $C4_2cd$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4_2bc$, 106); [2] $C4_2cm$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4_2mc$, 105)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2cm$ ($\mathbf{c}'=3\mathbf{c}$) (101); [9] $P4_2cm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (101)

Minimal non-isomorphic supergroups

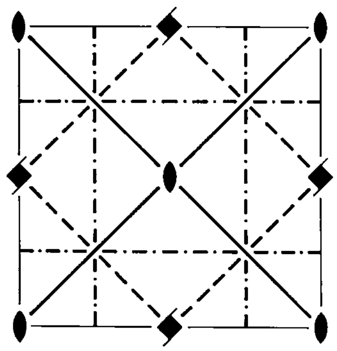
I [2] $P4_2/mcm$ (132); [2] $P4_2/ncm$ (138)

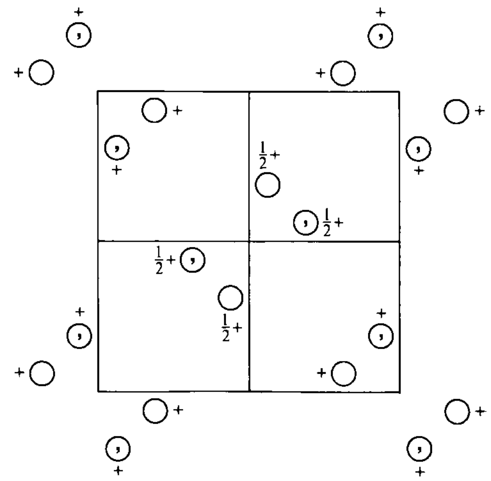
II [2] $C4_2cm$ ($P4_2mc$, 105); [2] $I4cm$ (108); [2] $P4mm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (99)

International Tables for Crystallography (2006). Vol. A, Space group 102, pp. 388–389.

$P4_2nm$ C_{4v}^4 $4mm$ Tetragonal

No. 102 $P4_2nm$ Patterson symmetry $P4/mmm$





Origin on $2mm$ on $21m$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $x \le y$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$ (4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (6) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$ (7) m $x,\bar{x},z$ (8) m x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*d*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(7) $\bar{y},\bar{x},z$	(8) y,x,z	$00l$: $l=2n$
							$h00$: $h=2n$
							Special: as above, plus
4	*c*	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	no extra conditions
4	*b*	$2..$	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	$\frac{1}{2},0,z$	hkl : $h+k,l=2n$
2	*a*	$2.mm$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4gm$	Along [100] $c1m1$	Along [110] $p1m1$
$\mathbf{a}'=\mathbf{a}$ $\quad \mathbf{b}'=\mathbf{b}$	$\mathbf{a}'=\mathbf{b}$ $\quad \mathbf{b}'=\mathbf{c}$	$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad \mathbf{b}'=\mathbf{c}$
Origin at $0,\frac{1}{2},z$	Origin at $x,0,0$	Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P4_211$ ($P4_2$, 77) 1; 2; 3; 4
[2] $P21m$ ($Cmm2$, 35) 1; 2; 7; 8
[2] $P2n1$ ($Pnn2$, 34) 1; 2; 5; 6

IIa none

IIb [2] $F4_1dc$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4_1cd$, 110); [2] $F4_1dm$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4_1md$, 109)

Maximal isomorphic subgroups of lowest index

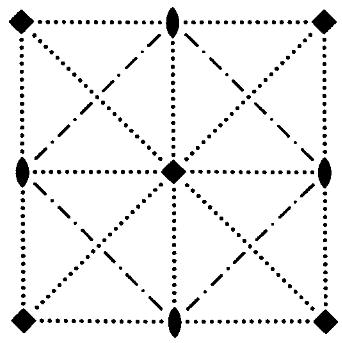
IIc [3] $P4_2nm$ ($\mathbf{c}'=3\mathbf{c}$) (102); [9] $P4_2nm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (102)

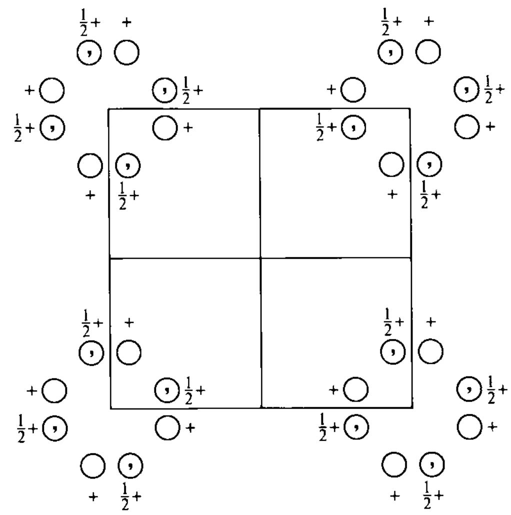
Minimal non-isomorphic supergroups

I [2] $P4_2/nnm$ (134); [2] $P4_2/mnm$ (136)

II [2] $C4_2cm$ ($P4_2mc$, 105); [2] $I4mm$ (107); [2] $P4bm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (100)

$P4cc$	C_{4v}^{5}	$4mm$	Tetragonal
No. 103	$P4cc$		Patterson symmetry $P4/mmm$





Origin on $4cc$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^{+} $0,0,z$	(4) 4^{-} $0,0,z$
(5) c $x,0,z$	(6) c $0,y,z$	(7) c $x,\bar{x},z$	(8) c x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*d*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$0kl$: $l=2n$
			(5) $x,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},y,z+\frac{1}{2}$	(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $y,x,z+\frac{1}{2}$	hhl : $l=2n$
							$00l$: $l=2n$
							Special: as above, plus
4	*c*	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	hkl : $h+k,l=2n$
2	*b*	4 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl : $l=2n$
2	*a*	4 . .	$0,0,z$	$0,0,z+\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P411$ ($P4$, 75) 1; 2; 3; 4
[2] $P21c$ ($Ccc2$, 37) 1; 2; 7; 8
[2] $P2c1$ ($Pcc2$, 27) 1; 2; 5; 6

IIa none

IIb [2] $C4cd$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4nc$, 104)

Maximal isomorphic subgroups of lowest index

IIc [2] $C4cc$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4cc$, 103); [3] $P4cc$ ($\mathbf{c}'=3\mathbf{c}$) (103)

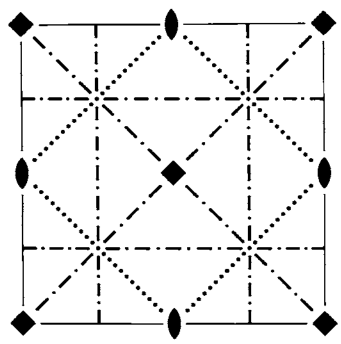
Minimal non-isomorphic supergroups

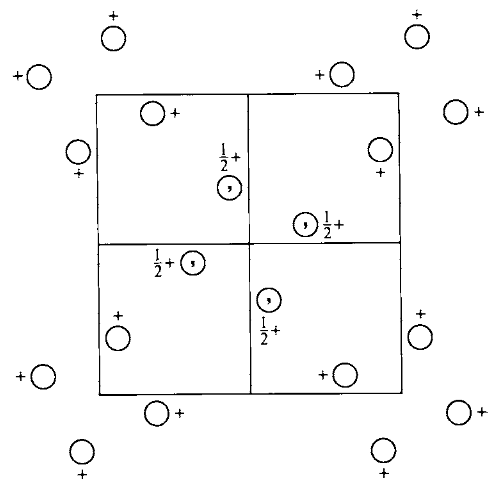
I [2] $P4/mcc$ (124); [2] $P4/ncc$ (130)

II [2] $I4cm$ (108); [2] $P4mm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (99)

$P4nc$ $\quad C_{4v}^{6}$ $\quad 4mm$ $\quad$ Tetragonal

No. 104 $\quad P4nc$ $\quad$ Patterson symmetry $P4/mmm$





Origin on $41n$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2 \quad 0,0,z$	(3) $4^{+} \quad 0,0,z$	(4) $4^{-} \quad 0,0,z$
(5) $n(\frac{1}{2},0,\frac{1}{2}) \quad x,\frac{1}{4},z$	(6) $n(0,\frac{1}{2},\frac{1}{2}) \quad \frac{1}{4},y,z$	(7) $c \quad x+\frac{1}{2},\bar{x},z$	(8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2}) \quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$0kl$: $k+l=2n$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(8) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	hhl : $l=2n$
							$00l$: $l=2n$
							$h00$: $h=2n$
							Special: as above, plus
4	b	$2\,.\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl : $h+k,l=2n$
2	a	$4\,.\,.$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P411$ ($P4$, 75) 1; 2; 3; 4
[2] $P21c$ ($Ccc2$, 37) 1; 2; 7; 8
[2] $P2n1$ ($Pnn2$, 34) 1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4nc$ ($\mathbf{c}'=3\mathbf{c}$) (104); [9] $P4nc$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (104)

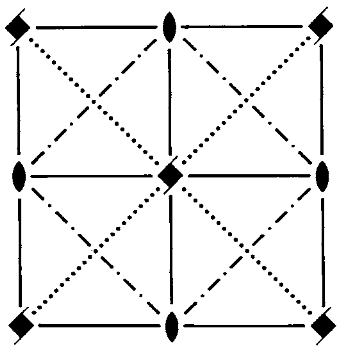
Minimal non-isomorphic supergroups

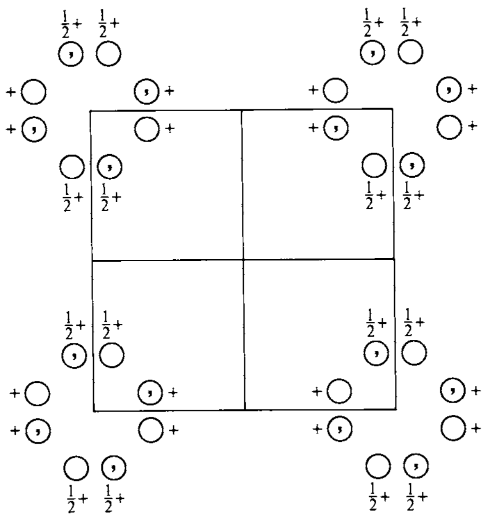
I [2] $P4/nnc$ (126); [2] $P4/mnc$ (128)

II [2] $C4cc$ ($P4cc$, 103); [2] $I4mm$ (107); [2] $P4bm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (100)

$P4_2mc$ $\quad C_{4v}^7$ $\quad 4mm$ $\quad$ Tetragonal

No. 105 $\quad P4_2mc$ $\quad$ Patterson symmetry $P4/mmm$





Origin on $2mm$ on 4_2mc

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $\;0,0,z$	(3) $4^+(0,0,\frac{1}{2})\;\; 0,0,z$	(4) $4^-(0,0,\frac{1}{2})\;\; 0,0,z$
(5) $m\;\; x,0,z$	(6) $m\;\; 0,y,z$	(7) $c\;\; x,\bar{x},z$	(8) $c\;\; x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	hhl : $l=2n$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $y,x,z+\frac{1}{2}$	$00l$: $l=2n$
							Special: as above, plus
4	e	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z+\frac{1}{2}$	$\frac{1}{2},\bar{x},z+\frac{1}{2}$	no extra conditions
4	d	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z+\frac{1}{2}$	$0,\bar{x},z+\frac{1}{2}$	no extra conditions
2	c	$2mm.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$			hkl : $h+k+l=2n$
2	b	$2mm.$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl : $l=2n$
2	a	$2mm.$	$0,0,z$	$0,0,z+\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P4_211$ ($P4_2$, 77) 1; 2; 3; 4
[2] $P21c$ ($Ccc2$, 37) 1; 2; 7; 8
[2] $P2m1$ ($Pmm2$, 25) 1; 2; 5; 6

IIa none

IIb [2] $C4_2md$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4_2nm$, 102); [2] $C4_2mc$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4_2cm$, 101)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2mc$ ($\mathbf{c}'=3\mathbf{c}$) (105); [9] $P4_2mc$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (105)

Minimal non-isomorphic supergroups

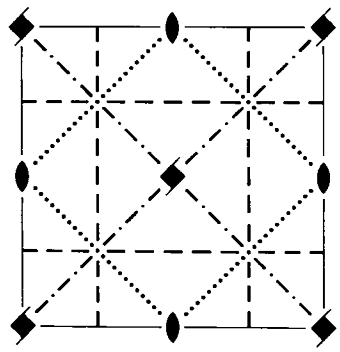
I [2] $P4_2/mmc$ (131); [2] $P4_2/nmc$ (137)

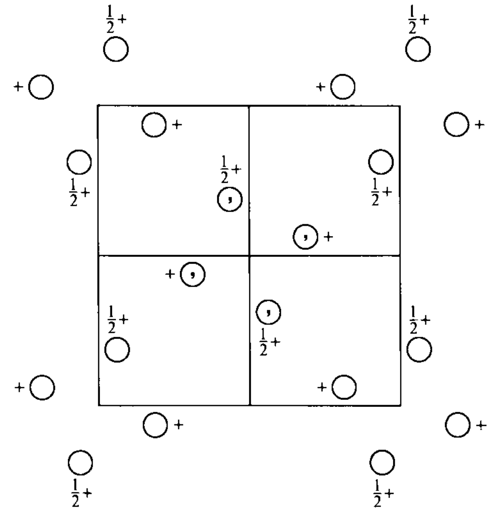
II [2] $C4_2mc$ ($P4_2cm$, 101); [2] $I4mm$ (107); [2] $P4mm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (99)

International Tables for Crystallography (2006). Vol. A, Space group 106, pp. 396–397.

$P4_2bc$ $\quad C_{4v}^8$ $\quad 4mm$ $\quad$ Tetragonal

No. 106 $\quad P4_2bc$ $\quad$ Patterson symmetry $P4/mmm$





Origin on 2 on 4_21n

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $\quad 0,0,z$	(3) $4^+(0,0,\frac{1}{2}) \quad 0,0,z$	(4) $4^-(0,0,\frac{1}{2}) \quad 0,0,z$
(5) $a \quad x,\frac{1}{4},z$	(6) $b \quad \frac{1}{4},y,z$	(7) $c \quad x+\frac{1}{2},\bar{x},z$	(8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2}) \quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	c	1	(1) x,y,z (5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(3) $\bar{y},x,z+\frac{1}{2}$ (7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$ (8) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k=2n$ hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
4	b	$2\,.\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl : $h+k,l=2n$
4	a	$2\,.\,.$	$0,0,z$	$0,0,z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl : $h+k,l=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P4_211$ ($P4_2$, 77) 1; 2; 3; 4
[2] $P21c$ ($Ccc2$, 37) 1; 2; 7; 8
[2] $P2b1$ ($Pba2$, 32) 1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2bc$ ($\mathbf{c}'=3\mathbf{c}$) (106); [9] $P4_2bc$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (106)

Minimal non-isomorphic supergroups

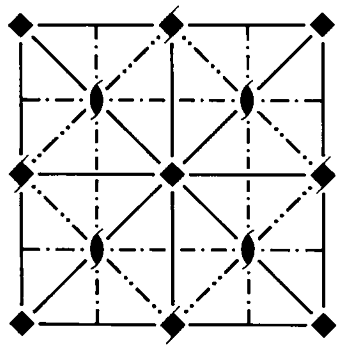
I [2] $P4_2/nbc$ (133); [2] $P4_2/mbc$ (135)

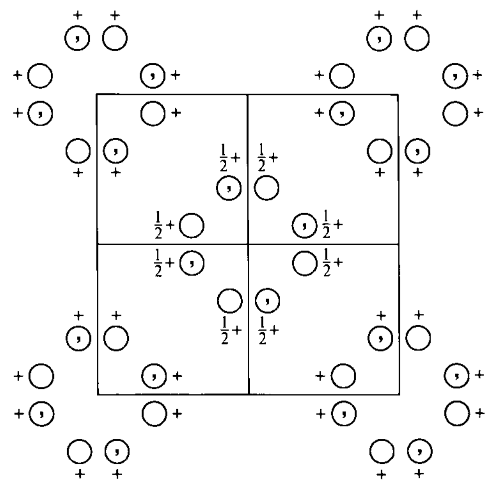
II [2] $C4_2mc$ ($P4_2cm$, 101); [2] $I4cm$ (108); [2] $P4bm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (100)

International Tables for Crystallography (2006). Vol. A, Space group 107, pp. 398–399.

$I4mm$ $\quad C_{4v}^{9}$ $\quad 4mm$ $\quad$ Tetragonal

No. 107 $\quad I4mm$ $\quad$ Patterson symmetry $I4/mmm$





Origin on $4mm$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}; \quad x \le y$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2 \quad 0,0,z$	(3) $4^{+} \quad 0,0,z$	(4) $4^{-} \quad 0,0,z$
(5) $m \quad x,0,z$	(6) $m \quad 0,y,z$	(7) $m \quad x,\bar{x},z$	(8) $m \quad x,x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4},\frac{1}{4},z$	(3) $4^{+}(0,0,\frac{1}{2}) \quad 0,\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{1}{2}) \quad \frac{1}{2},0,z$
(5) $n(\frac{1}{2},0,\frac{1}{2}) \quad x,\frac{1}{4},z$	(6) $n(0,\frac{1}{2},\frac{1}{2}) \quad \frac{1}{4},y,z$	(7) $c \quad x+\frac{1}{2},\bar{x},z$	(8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2}) \quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
16	e	1	(1) x,y,z (5) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z$	(3) $\bar{y},x,z$ (7) $\bar{y},\bar{x},z$	(4) $y,\bar{x},z$ (8) y,x,z	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
8	d	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$	no extra conditions
8	c	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
4	b	$2mm.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			hkl : $l=2n$
2	a	$4mm$	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I411$ ($I4$, 79)	(1; 2; 3; 4)+
	[2] $I2m1$ ($Imm2$, 44)	(1; 2; 5; 6)+
	[2] $I21m$ ($Fmm2$, 42)	(1; 2; 7; 8)+
IIa	[2] $P4_2mc$ (105)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4nc$ (104)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4_2nm$ (102)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4mm$ (99)	1; 2; 3; 4; 5; 6; 7; 8
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I4mm$ ($\mathbf{c}'=3\mathbf{c}$) (107); [9] $I4mm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (107)

Minimal non-isomorphic supergroups

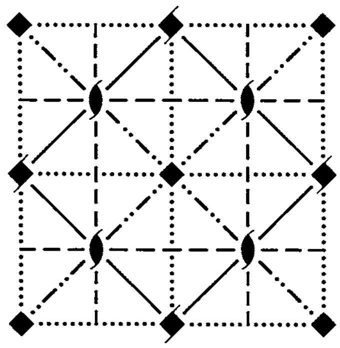
I [2] $I4/mmm$ (139)

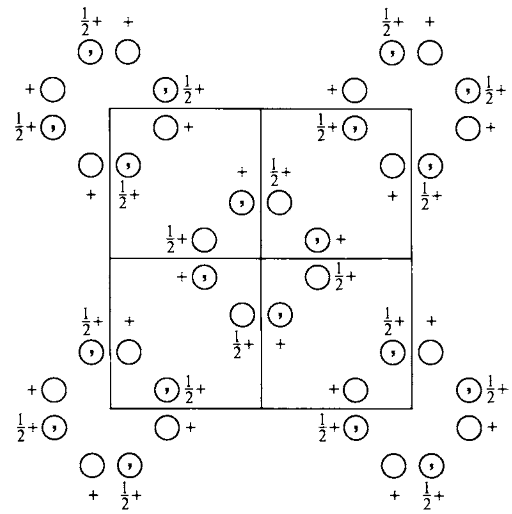
II [2] $C4mm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P4mm$, 99)

International Tables for Crystallography (2006). Vol. A, Space group 108, pp. 400–401.

$I4cm$ $\quad C_{4v}^{10}$ $\quad 4mm$ $\quad$ Tetragonal

No. 108 $\quad I4cm$ $\quad$ Patterson symmetry $I4/mmm$





Origin on $4ce$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}; \quad y \le \frac{1}{2} - x$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2 \quad 0,0,z$	(3) $4^{+} \quad 0,0,z$	(4) $4^{-} \quad 0,0,z$
(5) $c \quad x,0,z$	(6) $c \quad 0,y,z$	(7) $c \quad x,\bar{x},z$	(8) $c \quad x,x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4},\frac{1}{4},z$	(3) $4^{+}(0,0,\frac{1}{2}) \quad 0,\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{1}{2}) \quad \frac{1}{2},0,z$
(5) $a \quad x,\frac{1}{4},z$	(6) $b \quad \frac{1}{4},y,z$	(7) $m \quad x+\frac{1}{2},\bar{x},z$	(8) $g(\frac{1}{2},\frac{1}{2},0) \quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
16	d	1	(1) x,y,z (5) $x,\bar{y},z+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z+\frac{1}{2}$	(3) $\bar{y},x,z$ (7) $\bar{y},\bar{x},z+\frac{1}{2}$	(4) $y,\bar{x},z$ (8) $y,x,z+\frac{1}{2}$	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k,l=2n$ hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
8	c	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	no extra conditions
4	b	$2.mm$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$			hkl : $l=2n$
4	a	$4..$	$0,0,z$	$0,0,z+\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I411$ ($I4$, 79)	(1; 2; 3; 4)+
	[2] $I2c1$ ($Iba2$, 45)	(1; 2; 5; 6)+
	[2] $I21m$ ($Fmm2$, 42)	(1; 2; 7; 8)+
IIa	[2] $P4_2bc$ (106)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4cc$ (103)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2cm$ (101)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4bm$ (100)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I4cm$ ($\mathbf{c}'=3\mathbf{c}$) (108); [9] $I4cm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (108)

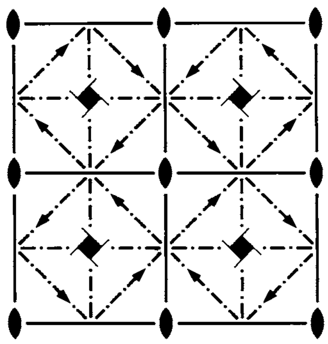
Minimal non-isomorphic supergroups

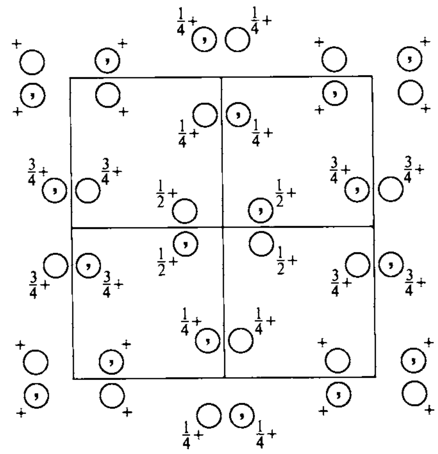
I [2] $I4/mcm$ (140)

II [2] $C4mm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P4mm$, 99)

$I4_1md$ $\quad C_{4v}^{11}$ $\quad 4mm$ $\quad$ Tetragonal

No. 109 $\quad I4_1md$ $\quad$ Patterson symmetry $I4/mmm$





Origin on $2mm$ on $2m1$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},\frac{1}{4},z$	(3) $4^{+}(0,0,\frac{1}{4})\quad -\frac{1}{4},\frac{1}{4},z$	(4) $4^{-}(0,0,\frac{3}{4})\quad \frac{1}{4},-\frac{1}{4},z$
(5) $m\quad x,0,z$	(6) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$	(7) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})\quad x+\frac{1}{4},\bar{x},z$	(8) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})\quad x+\frac{1}{4},x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\quad 0,0,z$	(3) $4^{+}(0,0,\frac{3}{4})\quad \frac{1}{4},\frac{1}{4},z$	(4) $4^{-}(0,0,\frac{1}{4})\quad \frac{1}{4},\frac{1}{4},z$
(5) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(6) $m\quad 0,y,z$	(7) $d(\frac{1}{4},-\frac{1}{4},\frac{3}{4})\quad x+\frac{1}{4},\bar{x},z$	(8) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\quad x-\frac{1}{4},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
16	c	1	(1) x,y,z (5) $x,\bar{y},z$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$ (7) $\bar{y},\bar{x}+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$ (8) $y+\frac{1}{2},x,z+\frac{3}{4}$	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl : $2h+l=4n$ $00l$: $l=4n$ $h00$: $h=2n$ $h\bar{h}0$: $h=2n$
							Special: as above, plus
8	b	$.\,m\,.$	$0,y,z$	$\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$\bar{y},\frac{1}{2},z+\frac{1}{4}$	$y+\frac{1}{2},0,z+\frac{3}{4}$	no extra conditions
4	a	$2\,m\,m\,.$	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$			hkl : $l=2n+1$ or $2h+l=4n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $c1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $I4_111$ ($I4_1$, 80) (1; 2; 3; 4)+
[2] $I2m1$ ($Imm2$, 44) (1; 2; 5; 6)+
[2] $I21d$ ($Fdd2$, 43) (1; 2; 7; 8)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1md$ ($\mathbf{c}'=3\mathbf{c}$) (109); [9] $I4_1md$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (109)

Minimal non-isomorphic supergroups

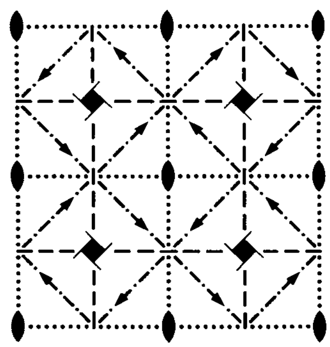
I [2] $I4_1/amd$ (141)

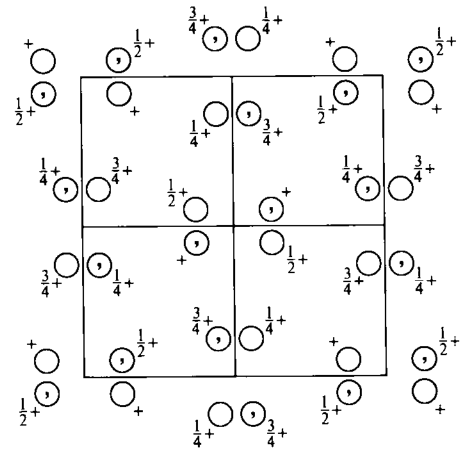
II [2] $C4_2md$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P4_2nm$, 102)

International Tables for Crystallography (2006). Vol. A, Space group 110, pp. 404–405.

$I4_1cd$ C_{4v}^{12} $4mm$ Tetragonal

No. 110 $I4_1cd$ Patterson symmetry $I4/mmm$





Origin on $2c1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},-\frac{1}{4},z$
(5) c $x,0,z$	(6) b $\frac{1}{4},y,z$	(7) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},\bar{x},z$	(8) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,0,z$	(3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},\frac{1}{4},z$
(5) a $x,\frac{1}{4},z$	(6) c $0,y,z$	(7) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},\bar{x},z$	(8) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x-\frac{1}{4},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
16	b	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$	hkl : $h+k+l=2n$
			(5) $x,\bar{y},z+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $\bar{y},\bar{x}+\frac{1}{2},z+\frac{3}{4}$	(8) $y+\frac{1}{2},x,z+\frac{1}{4}$	$hk0$: $h+k=2n$
							$0kl$: $k,l=2n$
							hhl : $2h+l=4n$
							$00l$: $l=4n$
							$h00$: $h=2n$
							$h\bar{h}0$: $h=2n$
							Special: as above, plus
8	a	$2\,.\,.$	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$	$0,0,z+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{3}{4}$	hkl : $2h+l=4n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $c1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $I4_1 1 1$ ($I4_1$, 80) (1; 2; 3; 4)+
[2] $I2c1$ ($Iba2$, 45) (1; 2; 5; 6)+
[2] $I21d$ ($Fdd2$, 43) (1; 2; 7; 8)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1cd$ ($\mathbf{c}'=3\mathbf{c}$) (110); [9] $I4_1cd$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (110)

Minimal non-isomorphic supergroups

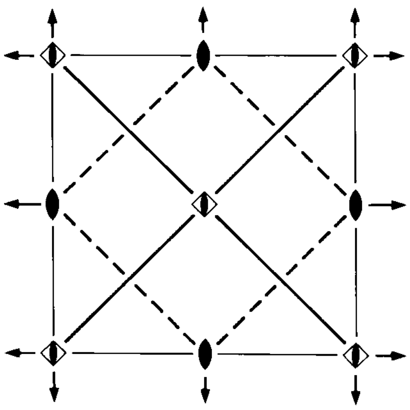
I [2] $I4_1/acd$ (142)

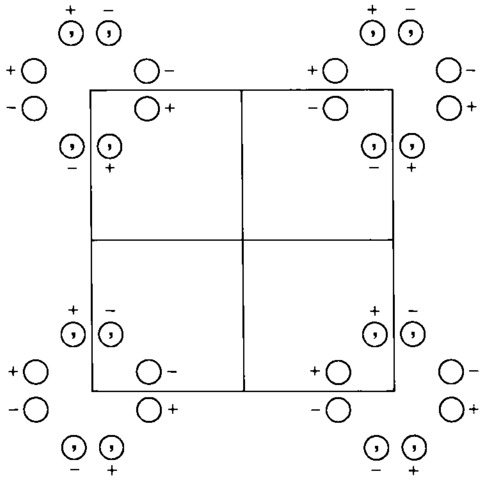
II [2] $C4_2md$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P4_2nm$, 102)

International Tables for Crystallography (2006). Vol. A, Space group 111, pp. 406–407.

$P\bar{4}2m$ $\quad D_{2d}^{1}$ $\quad \bar{4}2m$ $\quad$ Tetragonal

No. 111 $\quad P\bar{4}2m$ $\quad$ Patterson symmetry $P4/mmm$





Origin at $\bar{4}2m$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1; \quad x \le y$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $\bar{4}^{+}\ 0,0,z;\ \ 0,0,0$	(4) $\bar{4}^{-}\ 0,0,z;\ \ 0,0,0$
(5) $2\quad 0,y,0$	(6) $2\quad x,0,0$	(7) $m\quad x,\bar{x},z$	(8) $m\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	o	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$	(3) $y,\bar{x},\bar{z}$ (7) $\bar{y},\bar{x},z$	(4) $\bar{y},x,\bar{z}$ (8) y,x,z	no conditions
							Special:
4	n	$..m$	x,x,z	$\bar{x},\bar{x},z$	$x,\bar{x},\bar{z}$	$\bar{x},x,\bar{z}$	no extra conditions
4	m	$2..$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$	hkl : $h+k=2n$
4	l	$.2.$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},\bar{x},0$	$\frac{1}{2},x,0$	no extra conditions
4	k	$.2.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$0,x,\frac{1}{2}$	no extra conditions
4	j	$.2.$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	no extra conditions
4	i	$.2.$	$x,0,0$	$\bar{x},0,0$	$0,\bar{x},0$	$0,x,0$	no extra conditions
2	h	$2.mm$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	g	$2.mm$	$0,0,z$	$0,0,\bar{z}$			no extra conditions
2	f	$222.$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	e	$222.$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			hkl : $h+k=2n$
1	d	$\bar{4}2m$	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	c	$\bar{4}2m$	$0,0,\frac{1}{2}$				no extra conditions
1	b	$\bar{4}2m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				no extra conditions
1	a	$\bar{4}2m$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
[2] $P21m$ ($Cmm2$, 35) 1; 2; 7; 8
[2] $P221$ ($P222$, 16) 1; 2; 5; 6

IIa none

IIb [2] $P\bar{4}2c$ ($\mathbf{c}'=2\mathbf{c}$) (112); [2] $C\bar{4}2d$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P\bar{4}b2$, 117); [2] $C\bar{4}2m$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P\bar{4}m2$, 115); [2] $F\bar{4}2c$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I\bar{4}c2$, 120); [2] $F\bar{4}2m$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I\bar{4}m2$, 119)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{4}2m$ ($\mathbf{c}'=2\mathbf{c}$) (111); [9] $P\bar{4}2m$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (111)

Minimal non-isomorphic supergroups

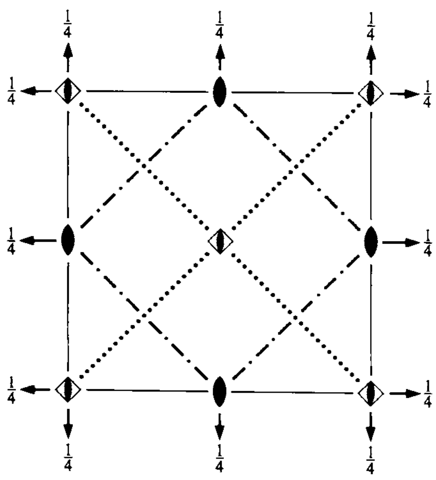
I [2] $P4/mmm$ (123); [2] $P4/nbm$ (125); [2] $P4_2/mcm$ (132); [2] $P4_2/nnm$ (134); [3] $P\bar{4}3m$ (215)

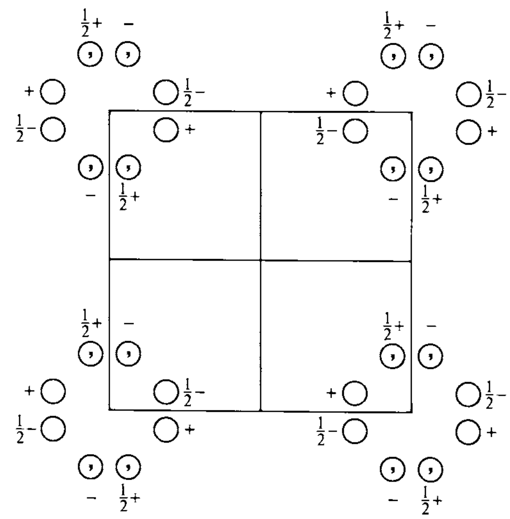
II [2] $C\bar{4}2m$ ($P\bar{4}m2$, 115); [2] $I\bar{4}2m$ (121)

International Tables for Crystallography (2006). Vol. A, Space group 112, pp. 408–409.

$P\bar{4}2c$ $\quad D_{2d}^{2}$ $\quad \bar{4}2m$ $\quad$ Tetragonal

No. 112 $\quad P\bar{4}2c$ $\quad$ Patterson symmetry $P4/mmm$





Origin at $\bar{4}1c$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $\bar{4}^{+}\quad 0,0,z;\ \ 0,0,0$	(4) $\bar{4}^{-}\quad 0,0,z;\ \ 0,0,0$
(5) $2\quad 0,y,\frac{1}{4}$	(6) $2\quad x,0,\frac{1}{4}$	(7) $c\quad x,\bar{x},z$	(8) $c\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	n	1	(1) x,y,z (5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(3) $y,\bar{x},\bar{z}$ (7) $\bar{y},\bar{x},z+\frac{1}{2}$	(4) $\bar{y},x,\bar{z}$ (8) $y,x,z+\frac{1}{2}$	hhl : $l=2n$ $00l$: $l=2n$
							Special: as above, plus
4	m	$2\,.\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	hkl : $h+k+l=2n$
4	l	$2\,.\,.$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl : $l=2n$
4	k	$2\,.\,.$	$0,0,z$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,z+\frac{1}{2}$	hkl : $l=2n$
4	j	$.\,2\,.$	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$y,0,\frac{3}{4}$	$\bar{y},0,\frac{3}{4}$	no extra conditions
4	i	$.\,2\,.$	$x,\frac{1}{2},\frac{1}{4}$	$\bar{x},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\bar{x},\frac{3}{4}$	$\frac{1}{2},x,\frac{3}{4}$	no extra conditions
4	h	$.\,2\,.$	$\frac{1}{2},y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{1}{4}$	$y,\frac{1}{2},\frac{3}{4}$	$\bar{y},\frac{1}{2},\frac{3}{4}$	no extra conditions
4	g	$.\,2\,.$	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$0,\bar{x},\frac{3}{4}$	$0,x,\frac{3}{4}$	no extra conditions
2	f	$\bar{4}\,.\,.$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
2	e	$\bar{4}\,.\,.$	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$
2	d	$2\,2\,2\,.$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$			hkl : $h+k+l=2n$
2	c	$2\,2\,2\,.$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl : $l=2n$
2	b	$2\,2\,2\,.$	$\frac{1}{2},0,\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl : $h+k+l=2n$
2	a	$2\,2\,2\,.$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,\frac{1}{4}$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
[2] $P21c$ ($Ccc2$, 37) 1; 2; 7; 8
[2] $P221$ ($P222$, 16) 1; 2; 5; 6

IIa none

IIb [2] $C\bar{4}2d$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P\bar{4}n2$, 118); [2] $C\bar{4}2c$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P\bar{4}c2$, 116)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{4}2c$ ($\mathbf{c}'=3\mathbf{c}$) (112); [9] $P\bar{4}2c$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (112)

Minimal non-isomorphic supergroups

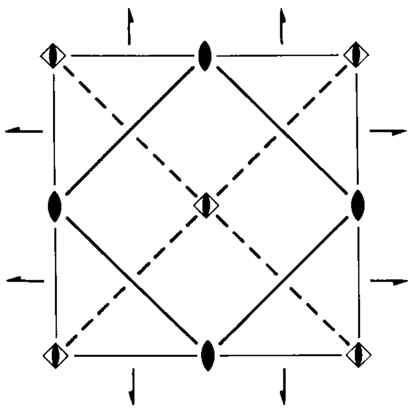
I [2] $P4/mcc$ (124); [2] $P4/nnc$ (126); [2] $P4_2/mmc$ (131); [2] $P4_2/nbc$ (133); [3] $P\bar{4}3n$ (218)

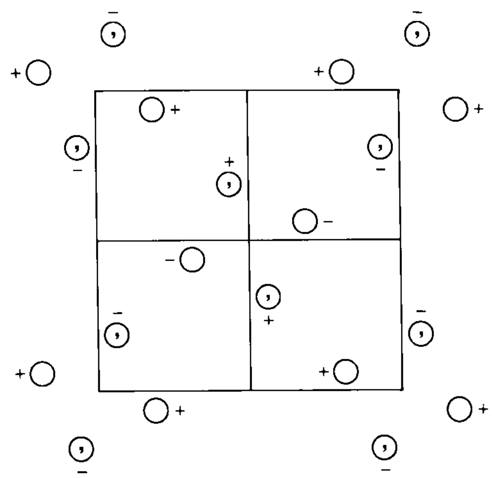
II [2] $C\bar{4}2c$ ($P\bar{4}c2$, 116); [2] $I\bar{4}2m$ (121); [2] $P\bar{4}2m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (111)

International Tables for Crystallography (2006). Vol. A, Space group 113, pp. 410–411.

$P\bar{4}2_1m$ | D_{2d}^3 | $\bar{4}2m$ | Tetragonal

No. 113 | $P\bar{4}2_1m$ | Patterson symmetry $P4/mmm$





Origin at $\bar{4}1g$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $y \le \frac{1}{2} - x$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) $\bar{4}^+$ $0,0,z$; $0,0,0$	(4) $\bar{4}^-$ $0,0,z$; $0,0,0$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$	(7) m $x+\frac{1}{2},\bar{x},z$	(8) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	f	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(3) $y,\bar{x},\bar{z}$ (7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(4) $\bar{y},x,\bar{z}$ (8) $y+\frac{1}{2},x+\frac{1}{2},z$	$h00$: $h=2n$
							Special: as above, plus
4	e	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$x+\frac{1}{2},\bar{x},\bar{z}$	$\bar{x}+\frac{1}{2},x,\bar{z}$	no extra conditions
4	d	$2..$	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl : $h+k=2n$
2	c	$2.mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			$hk0$: $h+k=2n$
2	b	$\bar{4}..$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	a	$\bar{4}..$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
[2] $P21m$ ($Cmm2$, 35) 1; 2; 7; 8
[2] $P22_11$ ($P2_12_12$, 18) 1; 2; 5; 6

IIa none

IIb [2] $P\bar{4}2_1c$ ($\mathbf{c}'=2\mathbf{c}$) (114)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{4}2_1m$ ($\mathbf{c}'=2\mathbf{c}$) (113); [9] $P\bar{4}2_1m$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (113)

Minimal non-isomorphic supergroups

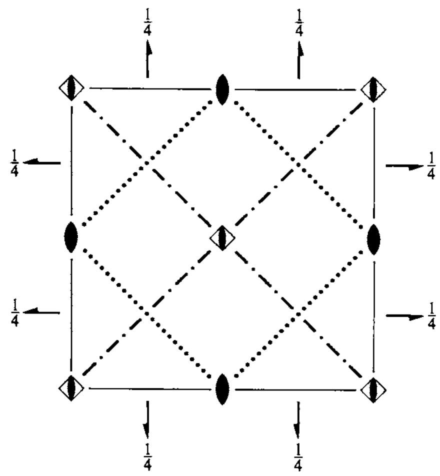
I [2] $P4/mbm$ (127); [2] $P4/nmm$ (129); [2] $P4_2/mnm$ (136); [2] $P4_2/ncm$ (138)

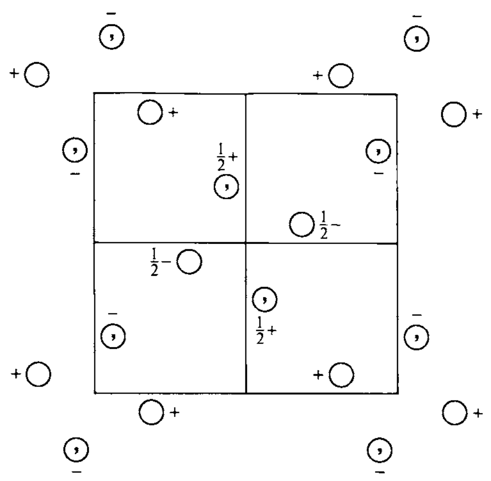
II [2] $C\bar{4}2m$ ($P\bar{4}m2$, 115); [2] $I\bar{4}2m$ (121)

International Tables for Crystallography (2006). Vol. A, Space group 114, pp. 412–413.

$P\bar{4}2_1c$ D_{2d}^4 $\bar{4}2m$ Tetragonal

No. 114 $P\bar{4}2_1c$ Patterson symmetry $P4/mmm$





Origin at $\bar{4}1n$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) $\bar{4}^{+}$ $0,0,z$; $0,0,0$	(4) $\bar{4}^{-}$ $0,0,z$; $0,0,0$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$	(7) c $x+\frac{1}{2},\bar{x},z$	(8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	e	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $y,\bar{x},\bar{z}$ (7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(4) $\bar{y},x,\bar{z}$ (8) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
4	d	$2\,.\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl : $l=2n$ $hk0$: $h+k=2n$
4	c	$2\,.\,.$	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl : $h+k+l=2n$
2	b	$\bar{4}\,.\,.$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k+l=2n$
2	a	$\bar{4}\,.\,.$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
[2] $P21c$ ($Ccc2$, 37) 1; 2; 7; 8
[2] $P22_11$ ($P2_12_12$, 18) 1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{4}2_1c$ ($\mathbf{c}'=3\mathbf{c}$) (114); [9] $P\bar{4}2_1c$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (114)

Minimal non-isomorphic supergroups

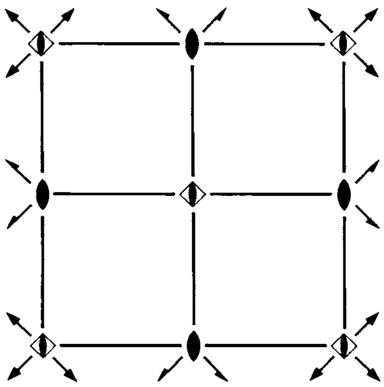
I [2] $P4/mnc$ (128); [2] $P4/ncc$ (130); [2] $P4_2/mbc$ (135); [2] $P4_2/nmc$ (137)

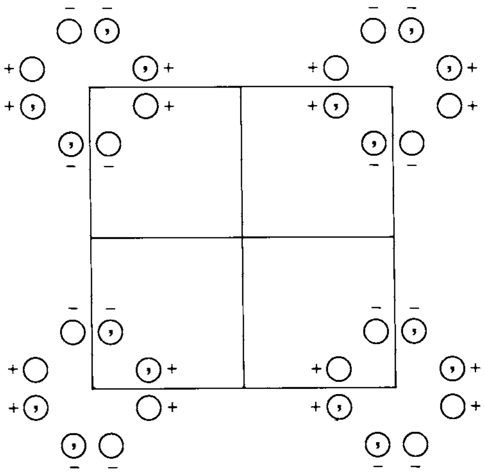
II [2] $C\bar{4}2c$ ($P\bar{4}c2$, 116); [2] $I\bar{4}2m$ (121); [2] $P\bar{4}2_1m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (113)

International Tables for Crystallography (2006). Vol. A, Space group 115, pp. 414–415.

$P\bar{4}m2$ D_{2d}^{5} $\bar{4}m2$ Tetragonal

No. 115 $P\bar{4}m2$ Patterson symmetry $P4/mmm$





Origin at $\bar{4}m2$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) $\bar{4}^{+}$ $0,0,z$; $0,0,0$	(4) $\bar{4}^{-}$ $0,0,z$; $0,0,0$
(5) m $x,0,z$	(6) m $0,y,z$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	l	1	(1) x,y,z (5) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z$	(3) $y,\bar{x},\bar{z}$ (7) $y,x,\bar{z}$	(4) $\bar{y},x,\bar{z}$ (8) $\bar{y},\bar{x},\bar{z}$	no conditions
							Special:
4	k	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},\bar{x},\bar{z}$	$\frac{1}{2},x,\bar{z}$	no extra conditions
4	j	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,\bar{x},\bar{z}$	$0,x,\bar{z}$	no extra conditions
4	i	$..2$	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	no extra conditions
4	h	$..2$	$x,x,0$	$\bar{x},\bar{x},0$	$x,\bar{x},0$	$\bar{x},x,0$	no extra conditions
2	g	$2mm.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			$hk0$: $h+k=2n$
2	f	$2mm.$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	e	$2mm.$	$0,0,z$	$0,0,\bar{z}$			no extra conditions
1	d	$\bar{4}m2$	$0,0,\frac{1}{2}$				no extra conditions
1	c	$\bar{4}m2$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				no extra conditions
1	b	$\bar{4}m2$	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	a	$\bar{4}m2$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
[2] $P2m1$ ($Pmm2$, 25) 1; 2; 5; 6
[2] $P212$ ($C222$, 21) 1; 2; 7; 8

IIa none

IIb [2] $P\bar{4}c2$ ($\mathbf{c}'=2\mathbf{c}$) (116); [2] $C\bar{4}m2_1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P\bar{4}2_1m$, 113); [2] $C\bar{4}m2$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P\bar{4}2m$, 111); [2] $F\bar{4}m2$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I\bar{4}2m$, 121)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{4}m2$ ($\mathbf{c}'=2\mathbf{c}$) (115); [9] $P\bar{4}m2$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (115)

Minimal non-isomorphic supergroups

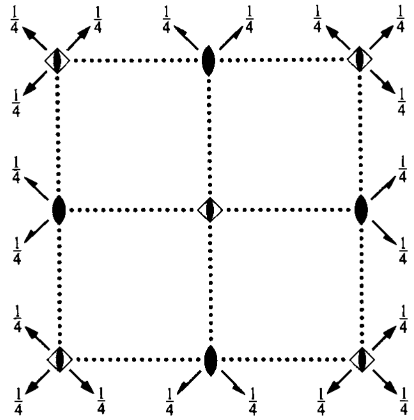
I [2] $P4/mmm$ (123); [2] $P4/nmm$ (129); [2] $P4_2/mmc$ (131); [2] $P4_2/nmc$ (137)

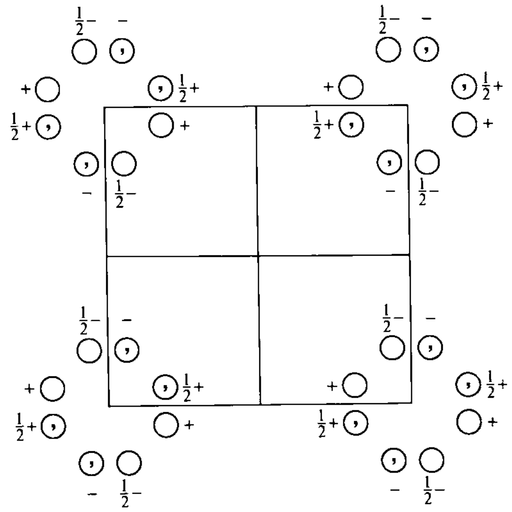
II [2] $C\bar{4}m2$ ($P\bar{4}2m$, 111); [2] $I\bar{4}m2$ (119)

International Tables for Crystallography (2006). Vol. A, Space group 116, pp. 416–417.

$P\bar{4}c2$ D_{2d}^{6} $\bar{4}m2$ Tetragonal

No. 116 $P\bar{4}c2$ Patterson symmetry $P4/mmm$





Origin at $\bar{4}c1$

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $\bar{4}^{+}\quad 0,0,z;\ \ 0,0,0$	(4) $\bar{4}^{-}\quad 0,0,z;\ \ 0,0,0$
(5) $c\quad x,0,z$	(6) $c\quad 0,y,z$	(7) $2\quad x,x,\frac{1}{4}$	(8) $2\quad x,\bar{x},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	j	1	(1) x,y,z (5) $x,\bar{y},z+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z+\frac{1}{2}$	(3) $y,\bar{x},\bar{z}$ (7) $y,x,\bar{z}+\frac{1}{2}$	(4) $\bar{y},x,\bar{z}$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$0kl$: $l=2n$ $00l$: $l=2n$
							Special: as above, plus
4	i	$2\,.\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	hkl : $l=2n$ $hk0$: $h+k=2n$
4	h	$2\,.\,.$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl : $l=2n$
4	g	$2\,.\,.$	$0,0,z$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$	hkl : $l=2n$
4	f	$.\,.\,2$	$x,x,\frac{3}{4}$	$\bar{x},\bar{x},\frac{3}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{1}{4}$	no extra conditions
4	e	$.\,.\,2$	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	no extra conditions
2	d	$\bar{4}\,.\,.$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
2	c	$\bar{4}\,.\,.$	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$
2	b	$2\,.\,22$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl : $l=2n$
2	a	$2\,.\,22$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{1}{4}$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
[2] $P2c1$ ($Pcc2$, 27) 1; 2; 5; 6
[2] $P212$ ($C222$, 21) 1; 2; 7; 8

IIa none

IIb [2] $C\bar{4}c2_1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P\bar{4}2_1c$, 114); [2] $C\bar{4}c2$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P\bar{4}2c$, 112)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{4}c2$ ($\mathbf{c}'=3\mathbf{c}$) (116); [9] $P\bar{4}c2$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (116)

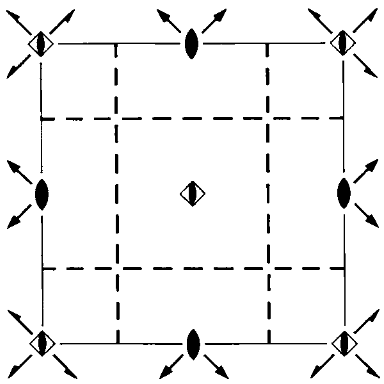
Minimal non-isomorphic supergroups

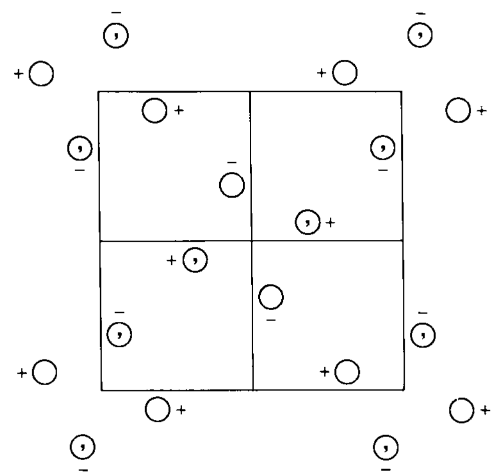
I [2] $P4/mcc$ (124); [2] $P4/ncc$ (130); [2] $P4_2/mcm$ (132); [2] $P4_2/ncm$ (138)

II [2] $C\bar{4}c2$ ($P\bar{4}2c$, 112); [2] $I\bar{4}c2$ (120); [2] $P\bar{4}m2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (115)

$P\bar{4}b2$ D_{2d}^{7} $\bar{4}m2$ Tetragonal

No. 117 $P\bar{4}b2$ Patterson symmetry $P4/mmm$





Origin at $\bar{4}12_1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) $\bar{4}^{+}$ $0,0,z$; $0,0,0$	(4) $\bar{4}^{-}$ $0,0,z$; $0,0,0$
(5) a $x,\frac{1}{4},z$	(6) b $\frac{1}{4},y,z$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$	(8) 2 $x,\bar{x}+\frac{1}{2},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	i	1	(1) x,y,z (5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(3) $y,\bar{x},\bar{z}$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(4) $\bar{y},x,\bar{z}$ (8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$0kl$: $k=2n$ $h00$: $h=2n$
							Special: as above, plus
4	h	. . 2	$x,x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,\frac{1}{2}$	no extra conditions
4	g	. . 2	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x},0$	$\bar{x}+\frac{1}{2},x,0$	no extra conditions
4	f	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	hkl : $h+k=2n$
4	e	2 . .	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	hkl : $h+k=2n$
2	d	2 . 22	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k=2n$
2	c	2 . 22	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $h+k=2n$
2	b	$\bar{4}$ . .	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	a	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
[2] $P2b1$ ($Pba2$, 32) 1; 2; 5; 6
[2] $P212$ ($C222$, 21) 1; 2; 7; 8

IIa none

IIb [2] $P\bar{4}n2$ ($\mathbf{c}'=2\mathbf{c}$) (118)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{4}b2$ ($\mathbf{c}'=2\mathbf{c}$) (117); [9] $P\bar{4}b2$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (117)

Minimal non-isomorphic supergroups

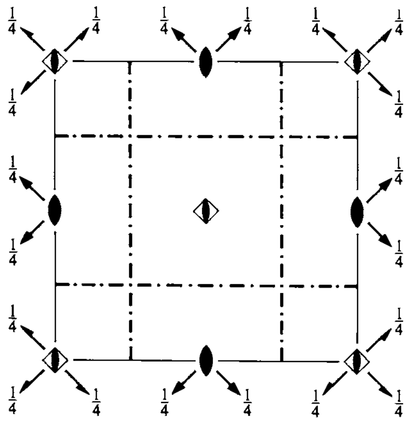
I [2] $P4/nbm$ (125); [2] $P4/mbm$ (127); [2] $P4_2/nbc$ (133); [2] $P4_2/mbc$ (135)

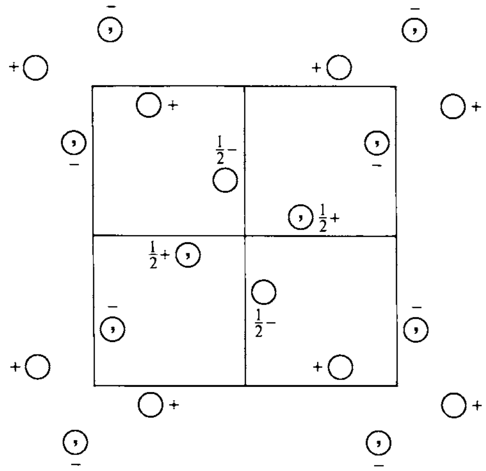
II [2] $C\bar{4}m2$ ($P\bar{4}2m$, 111); [2] $I\bar{4}c2$ (120)

International Tables for Crystallography (2006). Vol. A, Space group 118, pp. 420–421.

$P\bar{4}n2$ $\quad D_{2d}^{8}$ $\quad \bar{4}m2$ $\quad$ Tetragonal

No. 118 $\quad P\bar{4}n2$ $\quad$ Patterson symmetry $P4/mmm$





Origin at $\bar{4}$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $\bar{4}^{+}\quad 0,0,z;\ \ 0,0,0$	(4) $\bar{4}^{-}\quad 0,0,z;\ \ 0,0,0$
(5) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(6) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$	(7) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x,\frac{1}{4}$	(8) $2\quad x,\bar{x}+\frac{1}{2},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	i	1	(1) x,y,z (5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(3) $y,\bar{x},\bar{z}$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $\bar{y},x,\bar{z}$ (8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0kl$: $k+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
4	h	$2\,.\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl : $h+k+l=2n$
4	g	$.\,.\,2$	$x,x+\frac{1}{2},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x,\frac{3}{4}$	no extra conditions
4	f	$.\,.\,2$	$x,\bar{x}+\frac{1}{2},\frac{1}{4}$	$\bar{x},x+\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\bar{x},\frac{3}{4}$	$x+\frac{1}{2},x,\frac{3}{4}$	no extra conditions
4	e	$2\,.\,.$	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl : $h+k+l=2n$
2	d	$2\,.\,22$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$			hkl : $h+k+l=2n$
2	c	$2\,.\,22$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$			hkl : $h+k+l=2n$
2	b	$\bar{4}\,.\,.$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k+l=2n$
2	a	$\bar{4}\,.\,.$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{1}{4}$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
[2] $P2n1$ ($Pnn2$, 34) 1; 2; 5; 6
[2] $P212$ ($C222$, 21) 1; 2; 7; 8

IIa none

IIb [2] $F\bar{4}d2$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I\bar{4}2d$, 122)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{4}n2$ ($\mathbf{c}'=3\mathbf{c}$) (118); [9] $P\bar{4}n2$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (118)

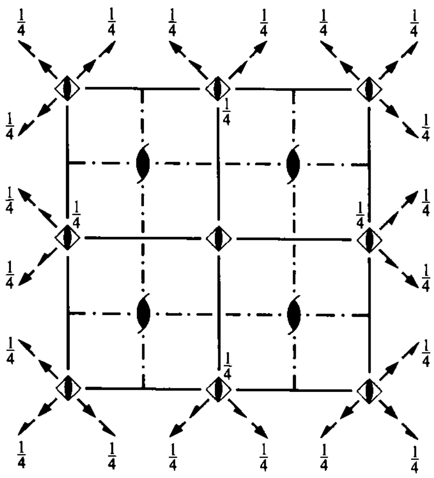
Minimal non-isomorphic supergroups

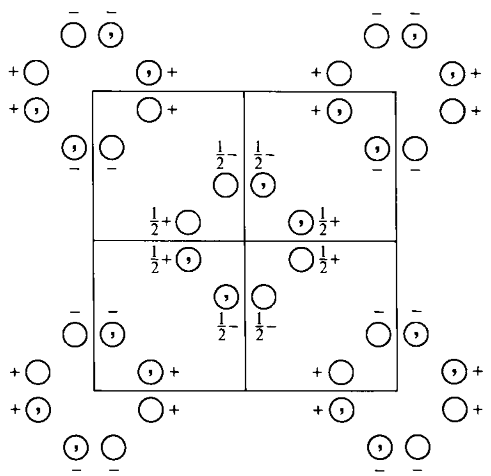
I [2] $P4/nnc$ (126); [2] $P4/mnc$ (128); [2] $P4_2/nnm$ (134); [2] $P4_2/mnm$ (136)

II [2] $C\bar{4}c2$ ($P\bar{4}2c$, 112); [2] $I\bar{4}m2$ (119); [2] $P\bar{4}b2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (117)

$I\bar{4}m2$ D_{2d}^{9} $\bar{4}m2$ Tetragonal

No. 119 $I\bar{4}m2$ Patterson symmetry $I4/mmm$





Origin at $\bar{4}m2$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2 \quad 0,0,z$	(3) $\bar{4}^{+} \quad 0,0,z; \quad 0,0,0$	(4) $\bar{4}^{-} \quad 0,0,z; \quad 0,0,0$
(5) $m \quad x,0,z$	(6) $m \quad 0,y,z$	(7) $2 \quad x,x,0$	(8) $2 \quad x,\bar{x},0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4},\frac{1}{4},z$	(3) $\bar{4}^{+} \quad \frac{1}{2},0,z; \quad \frac{1}{2},0,\frac{1}{4}$	(4) $\bar{4}^{-} \quad 0,\frac{1}{2},z; \quad 0,\frac{1}{2},\frac{1}{4}$
(5) $n(\frac{1}{2},0,\frac{1}{2}) \quad x,\frac{1}{4},z$	(6) $n(0,\frac{1}{2},\frac{1}{2}) \quad \frac{1}{4},y,z$	(7) $2(\frac{1}{2},\frac{1}{2},0) \quad x,x,\frac{1}{4}$	(8) $2 \quad x,\bar{x}+\frac{1}{2},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			General:
16	j	1	(1) x,y,z (5) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z$	(3) $y,\bar{x},\bar{z}$ (7) $y,x,\bar{z}$	(4) $\bar{y},x,\bar{z}$ (8) $\bar{y},\bar{x},\bar{z}$	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$ Special: no extra conditions
8	i	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,\bar{x},\bar{z}$	$0,x,\bar{z}$	
8	h	$..2$	$x,x+\frac{1}{2},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x,\frac{3}{4}$	
8	g	$..2$	$x,x,0$	$\bar{x},\bar{x},0$	$x,\bar{x},0$	$\bar{x},x,0$	
4	f	$2mm.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			
4	e	$2mm.$	$0,0,z$	$0,0,\bar{z}$			
2	d	$\bar{4}m2$	$0,\frac{1}{2},\frac{3}{4}$				
2	c	$\bar{4}m2$	$0,\frac{1}{2},\frac{1}{4}$				
2	b	$\bar{4}m2$	$0,0,\frac{1}{2}$				
2	a	$\bar{4}m2$	$0,0,0$				

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}11$ ($I\bar{4}$, 82)	(1; 2; 3; 4)+
	[2] $I2m1$ ($Imm2$, 44)	(1; 2; 5; 6)+
	[2] $I212$ ($F222$, 22)	(1; 2; 7; 8)+
IIa	[2] $P\bar{4}n2$ (118)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P\bar{4}m2$ (115)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P\bar{4}m2$ (115)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I\bar{4}m2$ ($\mathbf{c}'=3\mathbf{c}$) (119); [9] $I\bar{4}m2$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (119)

Minimal non-isomorphic supergroups

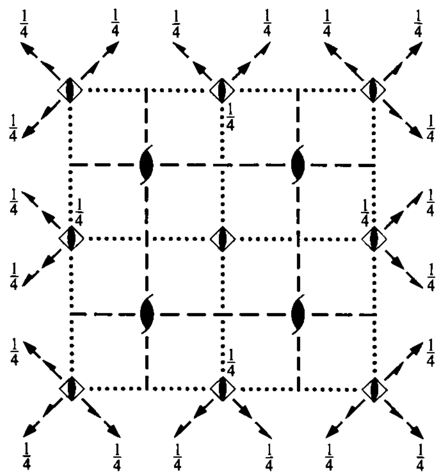
I [2] $I4/mmm$ (139); [2] $I4_1/amd$ (141); [3] $F\bar{4}3m$ (216)

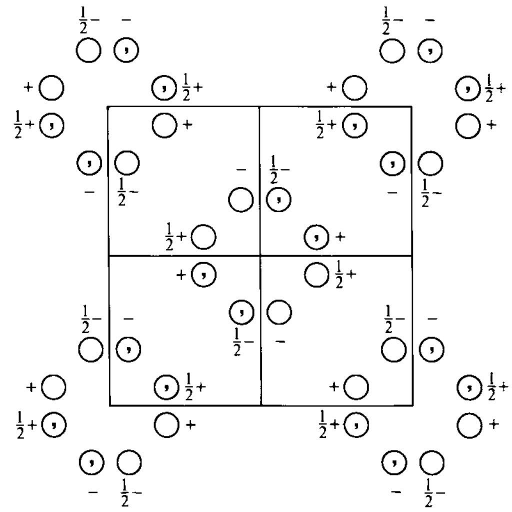
II [2] $C\bar{4}m2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P\bar{4}2m$, 111)

International Tables for Crystallography (2006). Vol. A, Space group 120, pp. 424–425.

$I\bar{4}c2$ $\quad$ D_{2d}^{10} $\quad$ $\bar{4}m2$ $\quad$ Tetragonal

No. 120 $\quad$ $I\bar{4}c2$ $\quad$ Patterson symmetry $I4/mmm$





Origin at $\bar{4}c2_1$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $\bar{4}^{+}\quad 0,0,z;\ \ 0,0,0$	(4) $\bar{4}^{-}\quad 0,0,z;\ \ 0,0,0$
(5) $c\quad x,0,z$	(6) $c\quad 0,y,z$	(7) $2\quad x,x,\frac{1}{4}$	(8) $2\quad x,\bar{x},\frac{1}{4}$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},\frac{1}{4},z$	(3) $\bar{4}^{+}\quad \frac{1}{2},0,z;\ \ \frac{1}{2},0,\frac{1}{4}$	(4) $\bar{4}^{-}\quad 0,\frac{1}{2},z;\ \ 0,\frac{1}{2},\frac{1}{4}$
(5) $a\quad x,\frac{1}{4},z$	(6) $b\quad \frac{1}{4},y,z$	(7) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x,0$	(8) $2\quad x,\bar{x}+\frac{1}{2},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
16	i	1	(1) x,y,z (5) $x,\bar{y},z+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z+\frac{1}{2}$	(3) $y,\bar{x},\bar{z}$ (7) $y,x,\bar{z}+\frac{1}{2}$	(4) $\bar{y},x,\bar{z}$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k,l=2n$ hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
8	h	..2	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x},0$	$\bar{x}+\frac{1}{2},x,0$	no extra conditions
8	g	2..	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	hkl : $l=2n$
8	f	2..	$0,0,z$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$	hkl : $l=2n$
8	e	..2	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	no extra conditions
4	d	2.22	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $l=2n$
4	c	$\bar{4}$..	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl : $l=2n$
4	b	$\bar{4}$..	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$
4	a	2.22	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}11$ ($I\bar{4}$, 82)	(1; 2; 3; 4)+
	[2] $I2c1$ ($Iba2$, 45)	(1; 2; 5; 6)+
	[2] $I212$ ($F222$, 22)	(1; 2; 7; 8)+
IIa	[2] $P\bar{4}b2$ (117)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P\bar{4}c2$ (116)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P\bar{4}c2$ (116)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I\bar{4}c2$ ($\mathbf{c}'=3\mathbf{c}$) (120); [9] $I\bar{4}c2$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (120)

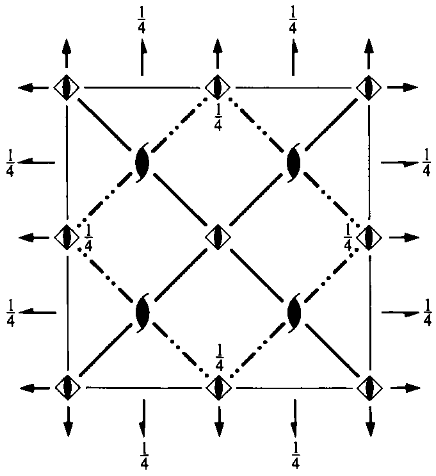
Minimal non-isomorphic supergroups

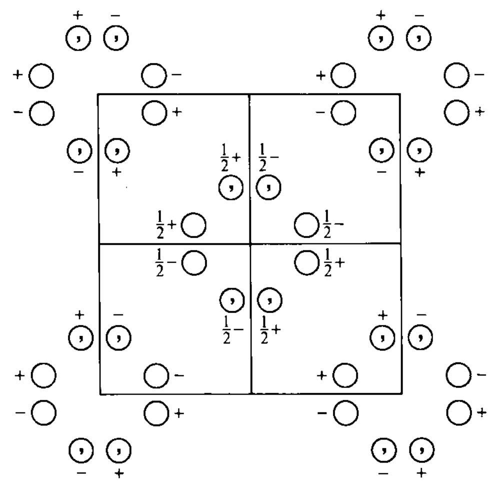
I [2] $I4/mcm$ (140); [2] $I4_1/acd$ (142); [3] $F\bar{4}3c$ (219)

II [2] $C\bar{4}m2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P\bar{4}2m$, 111)

International Tables for Crystallography (2006). Vol. A, Space group 121, pp. 426–427.

$I\bar{4}2m$	D_{2d}^{11}	$\bar{4}2m$	Tetragonal
No. 121	$I\bar{4}2m$		Patterson symmetry $I4/mmm$





Origin at $\bar{4}2m$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $x \le y$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) $\bar{4}^+$ $0,0,z$; $0,0,0$	(4) $\bar{4}^-$ $0,0,z$; $0,0,0$
(5) 2 $0,y,0$	(6) 2 $x,0,0$	(7) m $x,\bar{x},z$	(8) m x,x,z

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(4) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$	(7) c $x+\frac{1}{2},\bar{x},z$	(8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
16	j	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$	(3) $y,\bar{x},\bar{z}$ (7) $\bar{y},\bar{x},z$	(4) $\bar{y},x,\bar{z}$ (8) y,x,z	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
8	i	$..m$	x,x,z	$\bar{x},\bar{x},z$	$x,\bar{x},\bar{z}$	$\bar{x},x,\bar{z}$	no extra conditions
8	h	$2..$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$	hkl : $l=2n$
8	g	$.2.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$0,x,\frac{1}{2}$	no extra conditions
8	f	$.2.$	$x,0,0$	$\bar{x},0,0$	$0,\bar{x},0$	$0,x,0$	no extra conditions
4	e	$2.mm$	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	d	$\bar{4}..$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl : $l=2n$
4	c	$222.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $l=2n$
2	b	$\bar{4}2m$	$0,0,\frac{1}{2}$				no extra conditions
2	a	$\bar{4}2m$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}11$ ($I\bar{4}$, 82)	(1; 2; 3; 4)+
	[2] $I21m$ ($Fmm2$, 42)	(1; 2; 7; 8)+
	[2] $I221$ ($I222$, 23)	(1; 2; 5; 6)+
IIa	[2] $P\bar{4}2_1c$ (114)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P\bar{4}2_1m$ (113)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P\bar{4}2m$ (111)	1; 2; 3; 4; 5; 6; 7; 8
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I\bar{4}2m$ ($\mathbf{c}'=3\mathbf{c}$) (121); [9] $I\bar{4}2m$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (121)

Minimal non-isomorphic supergroups

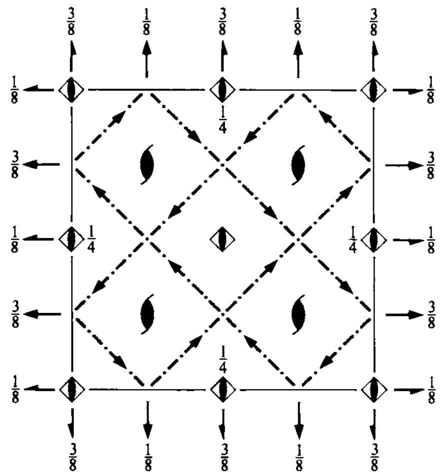
I [2] $I4/mmm$ (139); [2] $I4/mcm$ (140); [3] $I\bar{4}3m$ (217)

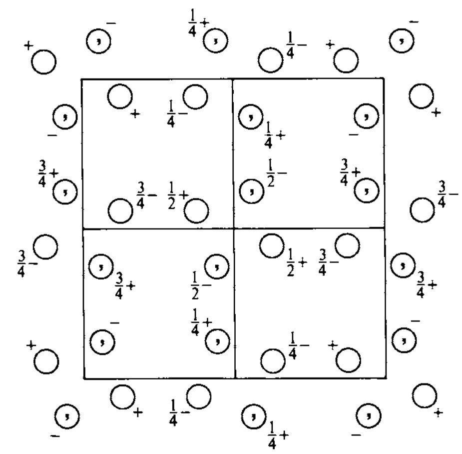
II [2] $C\bar{4}2m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P\bar{4}m2$, 115)

International Tables for Crystallography (2006). Vol. A, Space group 122, pp. 428–429.

$I\bar{4}2d$ $\quad D_{2d}^{12}$ $\quad \bar{4}2m$ $\quad$ Tetragonal

No. 122 $\quad I\bar{4}2d$ $\quad$ Patterson symmetry $I4/mmm$





Origin at $\bar{4}$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2 \quad 0,0,z$	(3) $\bar{4}^{+} \quad 0,0,z; \quad 0,0,0$	(4) $\bar{4}^{-} \quad 0,0,z; \quad 0,0,0$
(5) $2 \quad \frac{1}{4},y,\frac{3}{8}$	(6) $2(\frac{1}{2},0,0) \quad x,0,\frac{3}{8}$	(7) $d(\frac{1}{4},-\frac{1}{4},\frac{3}{4}) \quad x+\frac{1}{4},\bar{x},z$	(8) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4}) \quad x+\frac{1}{4},x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2}) \quad \frac{1}{4},\frac{1}{4},z$	(3) $\bar{4}^{+} \quad \frac{1}{2},0,z; \quad \frac{1}{2},0,\frac{1}{4}$	(4) $\bar{4}^{-} \quad 0,\frac{1}{2},z; \quad 0,\frac{1}{2},\frac{1}{4}$
(5) $2(0,\frac{1}{2},0) \quad 0,y,\frac{1}{8}$	(6) $2 \quad x,\frac{1}{4},\frac{1}{8}$	(7) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4}) \quad x+\frac{1}{4},\bar{x},z$	(8) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4}) \quad x-\frac{1}{4},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
16	e	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{3}{4}$	(3) $y,\bar{x},\bar{z}$ (7) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{3}{4}$	(4) $\bar{y},x,\bar{z}$ (8) $y+\frac{1}{2},x,z+\frac{3}{4}$	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl : $2h+l=4n$ $00l$: $l=4n$ $h00$: $h=2n$ $h\bar{h}0$: $h=2n$
							Special: as above, plus
8	d	. 2 .	$x,\frac{1}{4},\frac{1}{8}$	$\bar{x},\frac{3}{4},\frac{1}{8}$	$\frac{1}{4},\bar{x},\frac{7}{8}$	$\frac{3}{4},x,\frac{7}{8}$	no extra conditions
8	c	2 . .	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{3}{4}$	$\frac{1}{2},0,z+\frac{3}{4}$	hkl : $l=2n+1$ or $2h+l=4n$
4	b	$\bar{4}$ . .	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{4}$			hkl : $l=2n+1$ or $2h+l=4n$
4	a	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},0,\frac{3}{4}$			hkl : $l=2n+1$ or $2h+l=4n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,\frac{3}{8}$

Along [110] $c1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $I\bar{4}11$ ($I\bar{4}$, 82) (1; 2; 3; 4)+
[2] $I21d$ ($Fdd2$, 43) (1; 2; 7; 8)+
[2] $I221$ ($I2_12_12_1$, 24) (1; 2; 5; 6)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I\bar{4}2d$ ($\mathbf{c}'=3\mathbf{c}$) (122); [9] $I\bar{4}2d$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (122)

Minimal non-isomorphic supergroups

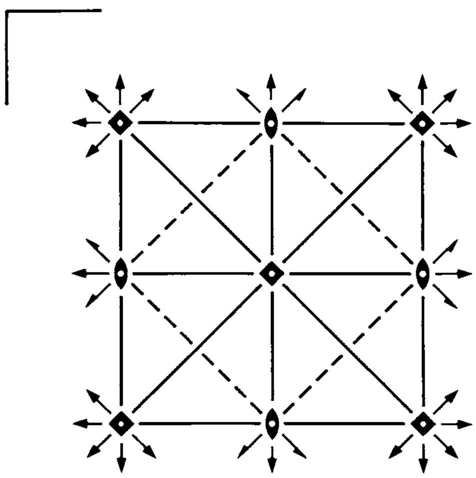
I [2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $I\bar{4}3d$ (220)

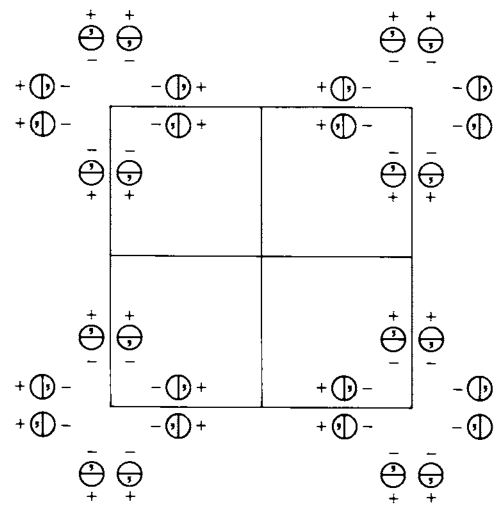
II [2] $C\bar{4}2d$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P\bar{4}n2$, 118)

International Tables for Crystallography (2006). Vol. A, Space group 123, pp. 430–431.

$P4/mmm$ D_{4h}^{1} $4/mmm$ Tetragonal

No. 123 $P\ 4/m\ 2/m\ 2/m$ Patterson symmetry $P4/mmm$





Origin at centre ($4/mmm$)

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $x \le y$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^{+} $0,0,z$	(4) 4^{-} $0,0,z$
(5) 2 $0,y,0$	(6) 2 $x,0,0$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x},0$
(9) $\bar{1}$ $0,0,0$	(10) m $x,y,0$	(11) $\bar{4}^{+}$ $0,0,z$; $0,0,0$	(12) $\bar{4}^{-}$ $0,0,z$; $0,0,0$
(13) m $x,0,z$	(14) m $0,y,z$	(15) m $x,\bar{x},z$	(16) m x,x,z

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4mm$ (99)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/m11$ ($P4/m$, 83)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/m12/m$ ($Cmmm$, 65)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/m2/m1$ ($Pmmm$, 47)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $P4_2/mcm$ ($\mathbf{c}' = 2\mathbf{c}$) (132); [2] $P4_2/mmc$ ($\mathbf{c}' = 2\mathbf{c}$) (131); [2] $P4/mcc$ ($\mathbf{c}' = 2\mathbf{c}$) (124); [2] $C4/emm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4/nmm$, 129); [2] $C4/mmd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4/mbm$, 127); [2] $C4/emd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4/nbm$, 125); [2] $F4/mmc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4/mcm$, 140); [2] $F4/mmm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4/mmm$, 139)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/mmm$ ($\mathbf{c}' = 2\mathbf{c}$) (123); [2] $C4/mmm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4/mmm$, 123)

Minimal non-isomorphic supergroups

I [3] $Pm\bar{3}m$ (221)

II [2] $I4/mmm$ (139)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	u	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	no conditions
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	
			(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y},\bar{x},z$	(16) y,x,z	
							Special:
8	t	$.\,m\,.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z$	$\frac{1}{2},\bar{x},z$	no extra conditions
			$\bar{x},\frac{1}{2},\bar{z}$	$x,\frac{1}{2},\bar{z}$	$\frac{1}{2},x,\bar{z}$	$\frac{1}{2},\bar{x},\bar{z}$	
8	s	$.\,m\,.$	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$	no extra conditions
			$\bar{x},0,\bar{z}$	$x,0,\bar{z}$	$0,x,\bar{z}$	$0,\bar{x},\bar{z}$	
8	r	$.\,.\,m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
			$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
8	q	$m\,.\,.$	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
			$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	$y,x,\frac{1}{2}$	$\bar{y},\bar{x},\frac{1}{2}$	
8	p	$m\,.\,.$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
			$\bar{x},y,0$	$x,\bar{y},0$	$y,x,0$	$\bar{y},\bar{x},0$	
4	o	$m\,2\,m\,.$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	no extra conditions
4	n	$m\,2\,m\,.$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	no extra conditions
4	m	$m\,2\,m\,.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	no extra conditions
4	l	$m\,2\,m\,.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	no extra conditions
4	k	$m\,.\,2m$	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	no extra conditions
4	j	$m\,.\,2m$	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	no extra conditions
4	i	$2\,m\,m\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hkl : $h+k=2n$
2	h	$4\,m\,m$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	g	$4\,m\,m$	$0,0,z$	$0,0,\bar{z}$			no extra conditions
2	f	$m\,m\,m\,.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $h+k=2n$
2	e	$m\,m\,m\,.$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k=2n$
1	d	$4/m\,m\,m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				no extra conditions
1	c	$4/m\,m\,m$	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	b	$4/m\,m\,m$	$0,0,\frac{1}{2}$				no extra conditions
1	a	$4/m\,m\,m$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

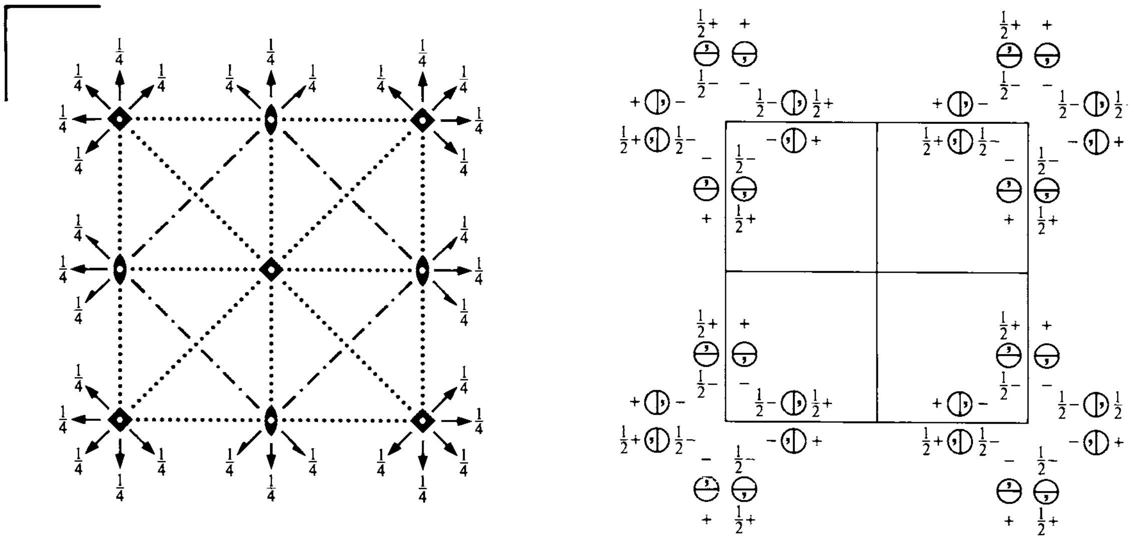
Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

(*Continued on preceding page*)

International Tables for Crystallography (2006). Vol. A, Space group 124, pp. 432–433.

$P4/mcc$ D_{4h}^{2} $4/mmm$ Tetragonal

No. 124 $P\ 4/m\ 2/c\ 2/c$ Patterson symmetry $P4/mmm$



Origin at centre $(4/m)$ at $4/mcc$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\ \ 0,0,z$	(3) $4^{+}\ \ 0,0,z$	(4) $4^{-}\ \ 0,0,z$
(5) $2\ \ 0,y,\frac{1}{4}$	(6) $2\ \ x,0,\frac{1}{4}$	(7) $2\ \ x,x,\frac{1}{4}$	(8) $2\ \ x,\bar{x},\frac{1}{4}$
(9) $\bar{1}\ \ 0,0,0$	(10) $m\ \ x,y,0$	(11) $\bar{4}^{+}\ \ 0,0,z;\ \ 0,0,0$	(12) $\bar{4}^{-}\ \ 0,0,z;\ \ 0,0,0$
(13) $c\ \ x,0,z$	(14) $c\ \ 0,y,z$	(15) $c\ \ x,\bar{x},z$	(16) $c\ \ x,x,z$

Maximal isomorphic subgroups of lowest index

IIc [2] $C4/mcc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4/mcc$, 124); [3] $P4/mcc$ ($\mathbf{c}' = 3\mathbf{c}$) (124)

Minimal non-isomorphic supergroups

I none

II [2] $I4/mcm$ (140); [2] $P4/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (123)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	n	1	(1) x,y,z (5) $\bar{x},y,\bar{z}+\frac{1}{2}$ (9) $\bar{x},\bar{y},\bar{z}$ (13) $x,\bar{y},z+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}+\frac{1}{2}$ (10) $x,y,\bar{z}$ (14) $\bar{x},y,z+\frac{1}{2}$	(3) $\bar{y},x,z$ (7) $y,x,\bar{z}+\frac{1}{2}$ (11) $y,\bar{x},\bar{z}$ (15) $\bar{y},\bar{x},z+\frac{1}{2}$	(4) $y,\bar{x},z$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$ (12) $\bar{y},x,\bar{z}$ (16) $y,x,z+\frac{1}{2}$	$0kl$: $l=2n$ hhl : $l=2n$ $00l$: $l=2n$
							Special: as above, plus
8	m	m . .	$x,y,0$ $\bar{x},y,\frac{1}{2}$	$\bar{x},\bar{y},0$ $x,\bar{y},\frac{1}{2}$	$\bar{y},x,0$ $y,x,\frac{1}{2}$	$y,\bar{x},0$ $\bar{y},\bar{x},\frac{1}{2}$	no extra conditions
8	l	. 2 .	$x,\frac{1}{2},\frac{1}{4}$ $\bar{x},\frac{1}{2},\frac{3}{4}$	$\bar{x},\frac{1}{2},\frac{1}{4}$ $x,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},x,\frac{1}{4}$ $\frac{1}{2},\bar{x},\frac{3}{4}$	$\frac{1}{2},\bar{x},\frac{1}{4}$ $\frac{1}{2},x,\frac{3}{4}$	hkl : $l=2n$
8	k	. 2 .	$x,0,\frac{1}{4}$ $\bar{x},0,\frac{3}{4}$	$\bar{x},0,\frac{1}{4}$ $x,0,\frac{3}{4}$	$0,x,\frac{1}{4}$ $0,\bar{x},\frac{3}{4}$	$0,\bar{x},\frac{1}{4}$ $0,x,\frac{3}{4}$	hkl : $l=2n$
8	j	. . 2	$x,x,\frac{1}{4}$ $\bar{x},\bar{x},\frac{3}{4}$	$\bar{x},\bar{x},\frac{1}{4}$ $x,x,\frac{3}{4}$	$\bar{x},x,\frac{1}{4}$ $x,\bar{x},\frac{3}{4}$	$x,\bar{x},\frac{1}{4}$ $\bar{x},x,\frac{3}{4}$	hkl : $l=2n$
8	i	2 . .	$0,\frac{1}{2},z$ $0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$ $\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$ $0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$ $\frac{1}{2},0,z+\frac{1}{2}$	hkl : $h+k,l=2n$
4	h	4 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl : $l=2n$
4	g	4 . .	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl : $l=2n$
4	f	2 2 2 .	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{3}{4}$	hkl : $h+k,l=2n$
4	e	$2/m$ . .	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl : $h+k,l=2n$
2	d	$4/m$ . .	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
2	c	4 2 2	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl : $l=2n$
2	b	$4/m$ . .	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$
2	a	4 2 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4cc$ (103)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/m11$ ($P4/m$, 83)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/m12/c$ ($Cccm$, 66)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/m2/c1$ ($Pccm$, 49)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $C4/ecc$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4/ncc$, 130); [2] $C4/mcd$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4/mnc$, 128); [2] $C4/ecd$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4/nnc$, 126)

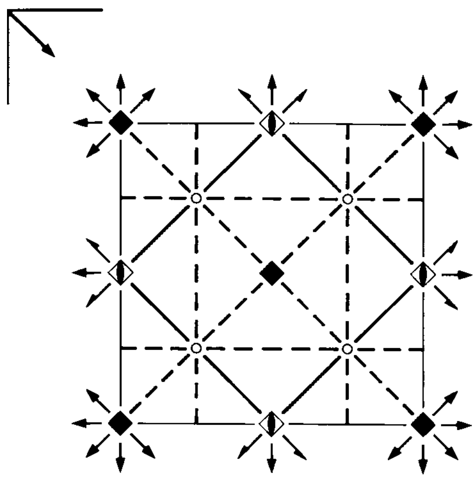
(*Continued on preceding page*)

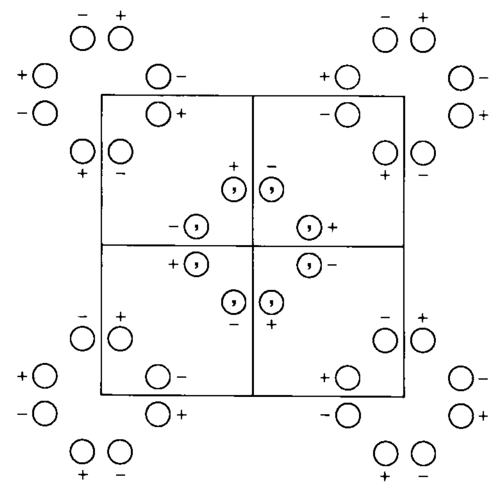
International Tables for Crystallography (2006). Vol. A, Space group 125, pp. 434–437.

$P4/nbm$ D_{4h}^{3} $4/mmm$ Tetragonal

No. 125 $P\ 4/n\ 2/b\ 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at 422 at $4/n22/g$, at $-\frac{1}{4},-\frac{1}{4},0$ from centre ($2/m$)

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le \frac{1}{2}-x$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^{+}\quad 0,0,z$	(4) $4^{-}\quad 0,0,z$
(5) $2\quad 0,y,0$	(6) $2\quad x,0,0$	(7) $2\quad x,x,0$	(8) $2\quad x,\bar{x},0$
(9) $\bar{1}\quad \frac{1}{4},\frac{1}{4},0$	(10) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,0$	(11) $\bar{4}^{+}\quad \frac{1}{2},0,z;\ \ \frac{1}{2},0,0$	(12) $\bar{4}^{-}\quad 0,\frac{1}{2},z;\ \ 0,\frac{1}{2},0$
(13) $a\quad x,\frac{1}{4},z$	(14) $b\quad \frac{1}{4},y,z$	(15) $m\quad x+\frac{1}{2},\bar{x},z$	(16) $g(\frac{1}{2},\frac{1}{2},0)\quad x,x,z$

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/nbm$ ($\mathbf{c}'=2\mathbf{c}$) (125); [9] $P4/nbm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (125)

Minimal non-isomorphic supergroups

I none

II [2] $C4/mmm$ ($P4/mmm$, 123); [2] $I4/mcm$ (140)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	n	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$hk0$: $h+k=2n$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	$0kl$: $k=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$h00$: $h=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	
							Special: as above, plus
8	m	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	no extra conditions
			$\bar{x},x+\frac{1}{2},\bar{z}$	$x,\bar{x}+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},x,\bar{z}$	$\bar{x}+\frac{1}{2},\bar{x},\bar{z}$	
8	l	$.2.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	hkl : $h+k=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	
8	k	$.2.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	hkl : $h+k=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\frac{1}{2},x+\frac{1}{2},0$	
8	j	$..2$	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	hkl : $h+k=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	
8	i	$..2$	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	hkl : $h+k=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$	
4	h	$2.mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hkl : $h+k=2n$
4	g	$4..$	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl : $h+k=2n$
4	f	$..2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	hkl : $h,k=2n$
4	e	$..2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$	hkl : $h,k=2n$
2	d	$\bar{4}2m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k=2n$
2	c	$\bar{4}2m$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $h+k=2n$
2	b	422	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	a	422	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ ($Cmme$, 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/b1$ ($Pban$, 50)	1; 2; 5; 6; 9; 10; 13; 14

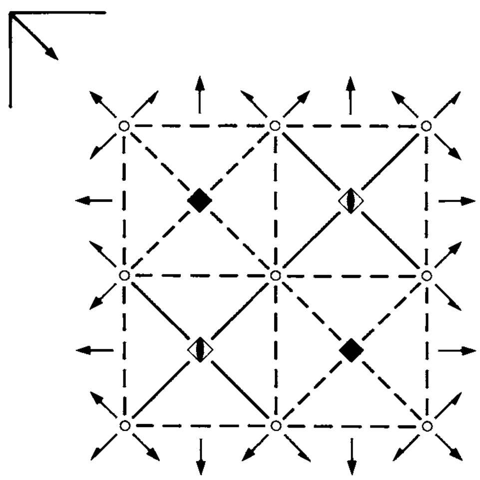
IIa none

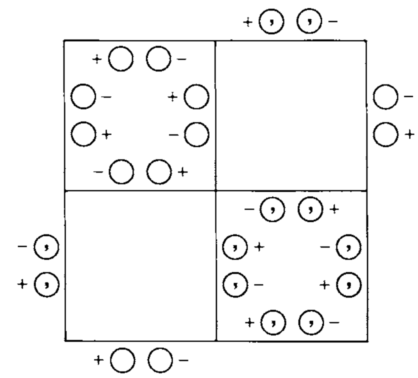
IIb [2] $P4_2/nnm$ ($\mathbf{c}'=2\mathbf{c}$) (134); [2] $P4_2/nbc$ ($\mathbf{c}'=2\mathbf{c}$) (133); [2] $P4/nnc$ ($\mathbf{c}'=2\mathbf{c}$) (126)

(*Continued on preceding page*)

$P4/nbm$	D_{4h}^{3}	$4/mmm$	Tetragonal
No. 125	$P\ 4/n\ 2/b\ 2/m$		Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2





Origin at centre $(2/m)$ at $n(b,a)(2_1/g,2/m)$, at $\frac{1}{4},\frac{1}{4},0$ from 422

Asymmetric unit $\quad -\frac{1}{4} \le x \le \frac{1}{4};\quad -\frac{1}{4} \le y \le \frac{1}{4};\quad 0 \le z \le \frac{1}{2};\quad x \le -y$

Symmetry operations

(1) 1	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $4^{+}\quad \frac{1}{4},\frac{1}{4},z$	(4) $4^{-}\quad \frac{1}{4},\frac{1}{4},z$
(5) $2\quad \frac{1}{4},y,0$	(6) $2\quad x,\frac{1}{4},0$	(7) $2\quad x,x,0$	(8) $2\quad x,\bar{x}+\frac{1}{2},0$
(9) $\bar{1}\quad 0,0,0$	(10) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,0$	(11) $\bar{4}^{+}\quad \frac{1}{4},-\frac{1}{4},z;\ \ \frac{1}{4},-\frac{1}{4},0$	(12) $\bar{4}^{-}\quad -\frac{1}{4},\frac{1}{4},z;\ \ -\frac{1}{4},\frac{1}{4},0$
(13) $a\quad x,0,z$	(14) $b\quad 0,y,z$	(15) $m\quad x,\bar{x},z$	(16) $g(\frac{1}{2},\frac{1}{2},0)\quad x,x,z$

Maximal isomorphic subgroups of lowest index

IIc $\quad$ [2] $P4/nbm$ ($\mathbf{c}' = 2\mathbf{c}$) (125); [9] $P4/nbm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (125)

Minimal non-isomorphic supergroups

I $\quad$ none

II $\quad$ [2] $C4/mmm$ ($P4/mmm$, 123); [2] $I4/mcm$ (140)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	Reflection conditions
				General:
16	n	1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (3) $\bar{y}+\frac{1}{2},x,z$ (4) $y,\bar{x}+\frac{1}{2},z$ (5) $\bar{x}+\frac{1}{2},y,\bar{z}$ (6) $x,\bar{y}+\frac{1}{2},\bar{z}$ (7) $y,x,\bar{z}$ (8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$ (9) $\bar{x},\bar{y},\bar{z}$ (10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (11) $y+\frac{1}{2},\bar{x},\bar{z}$ (12) $\bar{y},x+\frac{1}{2},\bar{z}$ (13) $x+\frac{1}{2},\bar{y},z$ (14) $\bar{x},y+\frac{1}{2},z$ (15) $\bar{y},\bar{x},z$ (16) $y+\frac{1}{2},x+\frac{1}{2},z$	$hk0: h+k=2n$ $0kl: k=2n$ $h00: h=2n$
				Special: as above, plus
8	m	$..m$	$x,\bar{x},z$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},z$ $x+\frac{1}{2},x,z$ $\bar{x},\bar{x}+\frac{1}{2},z$ $\bar{x}+\frac{1}{2},\bar{x},\bar{z}$ $x,x+\frac{1}{2},\bar{z}$ $\bar{x},x,\bar{z}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	no extra conditions
8	l	$.2.$	$x,\frac{1}{4},\frac{1}{2}$ $\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{2}$ $\frac{1}{4},x,\frac{1}{2}$ $\frac{1}{4},\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x},\frac{3}{4},\frac{1}{2}$ $x+\frac{1}{2},\frac{3}{4},\frac{1}{2}$ $\frac{3}{4},\bar{x},\frac{1}{2}$ $\frac{3}{4},x+\frac{1}{2},\frac{1}{2}$	$hkl: h+k=2n$
8	k	$.2.$	$x,\frac{1}{4},0$ $\bar{x}+\frac{1}{2},\frac{1}{4},0$ $\frac{1}{4},x,0$ $\frac{1}{4},\bar{x}+\frac{1}{2},0$ $\bar{x},\frac{3}{4},0$ $x+\frac{1}{2},\frac{3}{4},0$ $\frac{3}{4},\bar{x},0$ $\frac{3}{4},x+\frac{1}{2},0$	$hkl: h+k=2n$
8	j	$..2$	$x,x,\frac{1}{2}$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x}+\frac{1}{2},x,\frac{1}{2}$ $x,\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x},\bar{x},\frac{1}{2}$ $x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},\bar{x},\frac{1}{2}$ $\bar{x},x+\frac{1}{2},\frac{1}{2}$	$hkl: h+k=2n$
8	i	$..2$	$x,x,0$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},0$ $\bar{x}+\frac{1}{2},x,0$ $x,\bar{x}+\frac{1}{2},0$ $\bar{x},\bar{x},0$ $x+\frac{1}{2},x+\frac{1}{2},0$ $x+\frac{1}{2},\bar{x},0$ $\bar{x},x+\frac{1}{2},0$	$hkl: h+k=2n$
4	h	$2.mm$	$\frac{3}{4},\frac{1}{4},z$ $\frac{1}{4},\frac{3}{4},z$ $\frac{3}{4},\frac{1}{4},\bar{z}$ $\frac{1}{4},\frac{3}{4},\bar{z}$	$hkl: h+k=2n$
4	g	$4..$	$\frac{1}{4},\frac{1}{4},z$ $\frac{1}{4},\frac{1}{4},\bar{z}$ $\frac{3}{4},\frac{3}{4},\bar{z}$ $\frac{3}{4},\frac{3}{4},z$	$hkl: h+k=2n$
4	f	$..2/m$	$0,0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$	$hkl: h,k=2n$
4	e	$..2/m$	$0,0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},0,0$ $0,\frac{1}{2},0$	$hkl: h,k=2n$
2	d	$\bar{4}2m$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$ $\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$hkl: h+k=2n$
2	c	$\bar{4}2m$	$\frac{3}{4},\frac{1}{4},0$ $\frac{1}{4},\frac{3}{4},0$	$hkl: h+k=2n$
2	b	422	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$ $\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$hkl: h+k=2n$
2	a	422	$\frac{1}{4},\frac{1}{4},0$ $\frac{3}{4},\frac{3}{4},0$	$hkl: h+k=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I
[2] $P\bar{4}b2$ (117) 1; 2; 7; 8; 11; 12; 13; 14
[2] $P\bar{4}2m$ (111) 1; 2; 5; 6; 11; 12; 15; 16
[2] $P4bm$ (100) 1; 2; 3; 4; 13; 14; 15; 16
[2] $P422$ (89) 1; 2; 3; 4; 5; 6; 7; 8
[2] $P4/n11$ ($P4/n$, 85) 1; 2; 3; 4; 9; 10; 11; 12
[2] $P2/n12/m$ ($Cmme$, 67) 1; 2; 7; 8; 9; 10; 15; 16
[2] $P2/n2/b1$ ($Pban$, 50) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $P4_2/nnm$ ($\mathbf{c}'=2\mathbf{c}$) (134); [2] $P4_2/nbc$ ($\mathbf{c}'=2\mathbf{c}$) (133); [2] $P4/nnc$ ($\mathbf{c}'=2\mathbf{c}$) (126)

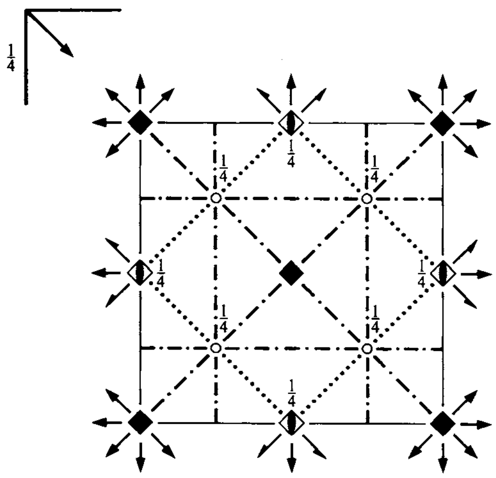
(*Continued on preceding page*)

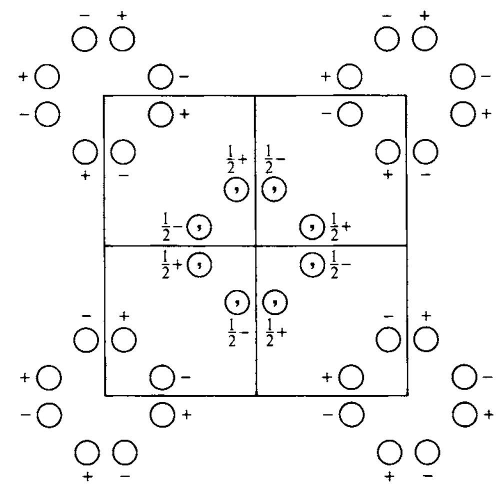
International Tables for Crystallography (2006). Vol. A, Space group 126, pp. 438–441.

$P4/nnc$ D_{4h}^{4} $4/mmm$ Tetragonal

No. 126 $P\ 4/n\ 2/n\ 2/c$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at $422/n$, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^{+}\quad 0,0,z$	(4) $4^{-}\quad 0,0,z$
(5) $2\quad 0,y,0$	(6) $2\quad x,0,0$	(7) $2\quad x,x,0$	(8) $2\quad x,\bar{x},0$
(9) $\bar{1}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,\frac{1}{4}$	(11) $\bar{4}^{+}\quad \frac{1}{2},0,z;\ \ \frac{1}{2},0,\frac{1}{4}$	(12) $\bar{4}^{-}\quad 0,\frac{1}{2},z;\ \ 0,\frac{1}{2},\frac{1}{4}$
(13) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(14) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$	(15) $c\quad x+\frac{1}{2},\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$hk0$: $h+k=2n$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	$0kl$: $k+l=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	hhl : $l=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$00l$: $l=2n$
							$h00$: $h=2n$
							Special: as above, plus
8	j	. 2 .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	hkl : $h+k+l=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\frac{1}{2},x+\frac{1}{2},0$	
8	i	. 2 .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	hkl : $h+k+l=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	
8	h	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	hkl : $h+k+l=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	
8	g	2 . .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	hkl : $h+k,l=2n$
			$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	
8	f	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$ $\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$	hkl : $h,k,l=2n$
4	e	4 . .	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl : $h+k+l=2n$
4	d	$\bar{4}$ . .	$\frac{1}{2},0,\frac{1}{4}$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	$0,\frac{1}{2},\frac{3}{4}$	hkl : $h+k,l=2n$
4	c	2 2 2 .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl : $h+k,l=2n$
2	b	4 2 2	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k+l=2n$
2	a	4 2 2	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4nc$ (104)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/n1$ ($Pnnn$, 48)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4/nnc$ ($\mathbf{c}'=3\mathbf{c}$) (126); [9] $P4/nnc$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (126)

Minimal non-isomorphic supergroups

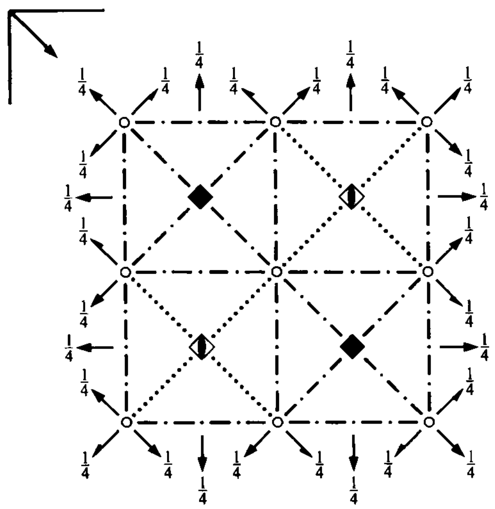
I [3] $Pn\bar{3}n$ (222)

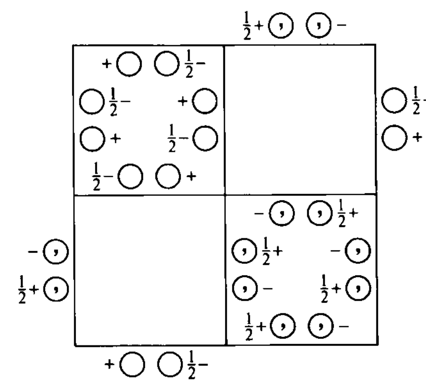
II [2] $I4/mmm$ (139); [2] $C4/mcc$ ($P4/mcc$, 124); [2] $P4/nbm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (125)

$P4/nnc$ D_{4h}^{4} $4/mmm$ Tetragonal

No. 126 $P\ 4/n\ 2/n\ 2/c$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2





Origin at $\bar{1}$ at $nn(n,c)$, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from 422

Asymmetric unit $-\frac{1}{4} \le x \le \frac{1}{4}$; $-\frac{1}{4} \le y \le \frac{1}{4}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\ \ \frac{1}{4},\frac{1}{4},z$	(3) $4^{+}\ \ \frac{1}{4},\frac{1}{4},z$	(4) $4^{-}\ \ \frac{1}{4},\frac{1}{4},z$
(5) $2\ \ \frac{1}{4},y,\frac{1}{4}$	(6) $2\ \ x,\frac{1}{4},\frac{1}{4}$	(7) $2\ \ x,x,\frac{1}{4}$	(8) $2\ \ x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}\ \ 0,0,0$	(10) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$	(11) $\bar{4}^{+}\ \ \frac{1}{4},-\frac{1}{4},z;\ \ \frac{1}{4},-\frac{1}{4},0$	(12) $\bar{4}^{-}\ \ -\frac{1}{4},\frac{1}{4},z;\ \ -\frac{1}{4},\frac{1}{4},0$
(13) $n(\frac{1}{2},0,\frac{1}{2})\ \ x,0,z$	(14) $n(0,\frac{1}{2},\frac{1}{2})\ \ 0,y,z$	(15) $c\ \ x,\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	Reflection conditions
				General:
16	k	1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (3) $\bar{y}+\frac{1}{2},x,z$ (4) $y,\bar{x}+\frac{1}{2},z$ (5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$ (6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $y,x,\bar{z}+\frac{1}{2}$ (8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (9) $\bar{x},\bar{y},\bar{z}$ (10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (11) $y+\frac{1}{2},\bar{x},\bar{z}$ (12) $\bar{y},x+\frac{1}{2},\bar{z}$ (13) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (14) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$ (15) $\bar{y},\bar{x},z+\frac{1}{2}$ (16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
				Special: as above, plus
8	j	. 2 .	$x,\frac{3}{4},\frac{1}{4}$ $\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},x,\frac{1}{4}$ $\frac{3}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$ $\bar{x},\frac{1}{4},\frac{3}{4}$ $x+\frac{1}{2},\frac{1}{4},\frac{3}{4}$ $\frac{1}{4},\bar{x},\frac{3}{4}$ $\frac{1}{4},x+\frac{1}{2},\frac{3}{4}$	hkl : $h+k+l=2n$
8	i	. 2 .	$x,\frac{1}{4},\frac{1}{4}$ $\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},x,\frac{1}{4}$ $\frac{1}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$ $\bar{x},\frac{3}{4},\frac{3}{4}$ $x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$ $\frac{3}{4},\bar{x},\frac{3}{4}$ $\frac{3}{4},x+\frac{1}{2},\frac{3}{4}$	hkl : $h+k+l=2n$
8	h	. . 2	$x,x,\frac{1}{4}$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{4}$ $\bar{x}+\frac{1}{2},x,\frac{1}{4}$ $x,\bar{x}+\frac{1}{2},\frac{1}{4}$ $\bar{x},\bar{x},\frac{3}{4}$ $x+\frac{1}{2},x+\frac{1}{2},\frac{3}{4}$ $x+\frac{1}{2},\bar{x},\frac{3}{4}$ $\bar{x},x+\frac{1}{2},\frac{3}{4}$	hkl : $h+k+l=2n$
8	g	2 . .	$\frac{1}{4},\frac{3}{4},z$ $\frac{3}{4},\frac{1}{4},z$ $\frac{1}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$ $\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$ $\frac{3}{4},\frac{1}{4},\bar{z}$ $\frac{1}{4},\frac{3}{4},\bar{z}$ $\frac{3}{4},\frac{1}{4},z+\frac{1}{2}$ $\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl : $h+k,l=2n$
8	f	$\bar{1}$	$0,0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},0,0$ $0,\frac{1}{2},0$ $\frac{1}{2},0,\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$ $0,0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h,k,l=2n$
4	e	4 . .	$\frac{1}{4},\frac{1}{4},z$ $\frac{1}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$ $\frac{3}{4},\frac{3}{4},\bar{z}$ $\frac{3}{4},\frac{3}{4},z+\frac{1}{2}$	hkl : $h+k+l=2n$
4	d	$\bar{4}$ . .	$\frac{1}{4},\frac{3}{4},0$ $\frac{3}{4},\frac{1}{4},0$ $\frac{1}{4},\frac{3}{4},\frac{1}{2}$ $\frac{3}{4},\frac{1}{4},\frac{1}{2}$	hkl : $h+k,l=2n$
4	c	2 2 2 .	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$ $\frac{3}{4},\frac{1}{4},\frac{3}{4}$ $\frac{3}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{3}{4},\frac{1}{4}$	hkl : $h+k,l=2n$
2	b	4 2 2	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$	hkl : $h+k+l=2n$
2	a	4 2 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$	hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}n2$ (118) 1; 2; 7; 8; 11; 12; 13; 14
[2] $P\bar{4}2c$ (112) 1; 2; 5; 6; 11; 12; 15; 16
[2] $P4nc$ (104) 1; 2; 3; 4; 13; 14; 15; 16
[2] $P422$ (89) 1; 2; 3; 4; 5; 6; 7; 8
[2] $P4/n11$ ($P4/n$, 85) 1; 2; 3; 4; 9; 10; 11; 12
[2] $P2/n12/c$ ($Ccce$, 68) 1; 2; 7; 8; 9; 10; 15; 16
[2] $P2/n2/n1$ ($Pnnn$, 48) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4/nnc$ ($\mathbf{c}'=3\mathbf{c}$) (126); [9] $P4/nnc$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (126)

Minimal non-isomorphic supergroups

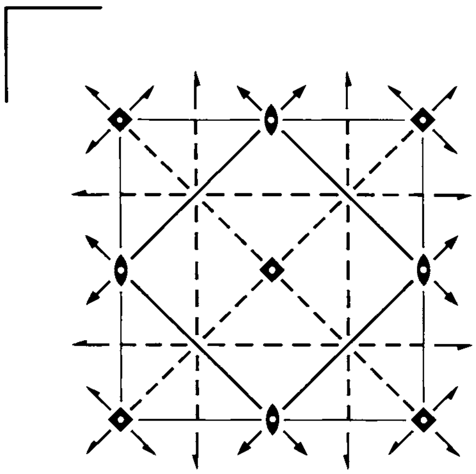
I [3] $Pn\bar{3}n$ (222)

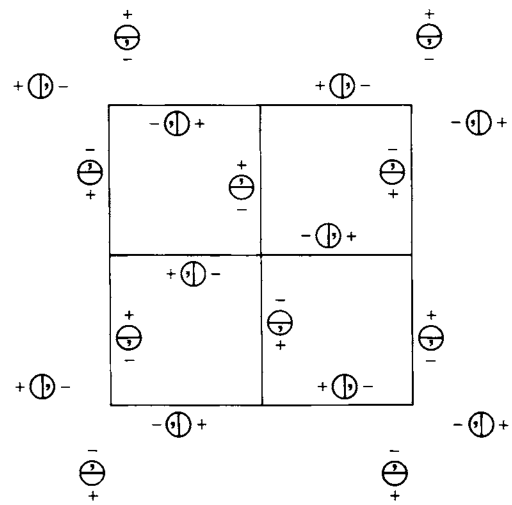
II [2] $I4/mmm$ (139); [2] $C4/mcc$ ($P4/mcc$, 124); [2] $P4/nbm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (125)

International Tables for Crystallography (2006). Vol. A, Space group 127, pp. 442–443.

$P4/mbm$ D_{4h}^5 $4/mmm$ Tetragonal

No. 127 $P\ 4/m\ 2_1/b\ 2/m$ Patterson symmetry $P4/mmm$





Origin at centre $(4/m)$ at $4/m\,1\,2_1/g$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le \frac{1}{2} - x$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^+\ 0,0,z$	(4) $4^-\ 0,0,z$
(5) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$	(7) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x,0$	(8) $2\quad x,\bar{x}+\frac{1}{2},0$
(9) $\bar{1}\quad 0,0,0$	(10) $m\quad x,y,0$	(11) $\bar{4}^+\ 0,0,z;\ 0,0,0$	(12) $\bar{4}^-\ 0,0,z;\ 0,0,0$
(13) $a\quad x,\frac{1}{4},z$	(14) $b\quad \frac{1}{4},y,z$	(15) $m\quad x+\frac{1}{2},\bar{x},z$	(16) $g(\frac{1}{2},\frac{1}{2},0)\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$0kl$: $k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$h00$: $h=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	
							Special: as above, plus
8	k	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	no extra conditions
			$\bar{x}+\frac{1}{2},x,\bar{z}$	$x+\frac{1}{2},\bar{x},\bar{z}$	$x,x+\frac{1}{2},\bar{z}$	$\bar{x},\bar{x}+\frac{1}{2},\bar{z}$	
8	j	$m..$	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	
8	i	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	$y+\frac{1}{2},x+\frac{1}{2},0$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	
4	h	$m.2m$	$x,x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,\frac{1}{2}$	$x+\frac{1}{2},\bar{x},\frac{1}{2}$	no extra conditions
4	g	$m.2m$	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x+\frac{1}{2},\bar{x},0$	no extra conditions
4	f	$2.mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	hkl : $h+k=2n$
4	e	$4..$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl : $h+k=2n$
2	d	$m.mm$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $h+k=2n$
2	c	$m.mm$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k=2n$
2	b	$4/m..$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	a	$4/m..$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}b2$ (117) 1; 2; 7; 8; 11; 12; 13; 14
[2] $P\bar{4}2_1m$ (113) 1; 2; 5; 6; 11; 12; 15; 16
[2] $P4bm$ (100) 1; 2; 3; 4; 13; 14; 15; 16
[2] $P42_12$ (90) 1; 2; 3; 4; 5; 6; 7; 8
[2] $P4/m11$ ($P4/m$, 83) 1; 2; 3; 4; 9; 10; 11; 12
[2] $P2/m12/m$ ($Cmmm$, 65) 1; 2; 7; 8; 9; 10; 15; 16
[2] $P2/m2_1/b1$ ($Pbam$, 55) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $P4_2/mnm$ ($\mathbf{c}'=2\mathbf{c}$) (136); [2] $P4_2/mbc$ ($\mathbf{c}'=2\mathbf{c}$) (135); [2] $P4/mnc$ ($\mathbf{c}'=2\mathbf{c}$) (128)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/mbm$ ($\mathbf{c}'=2\mathbf{c}$) (127); [9] $P4/mbm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (127)

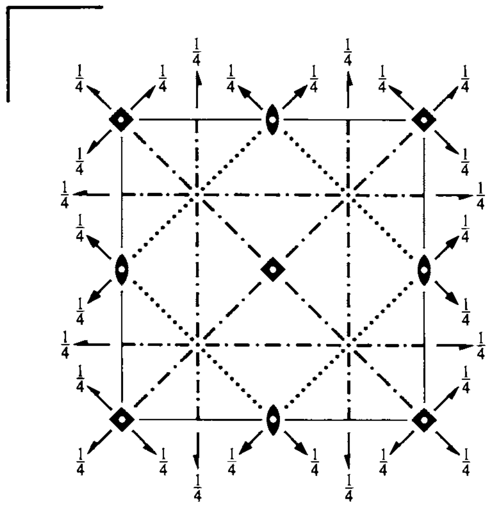
Minimal non-isomorphic supergroups

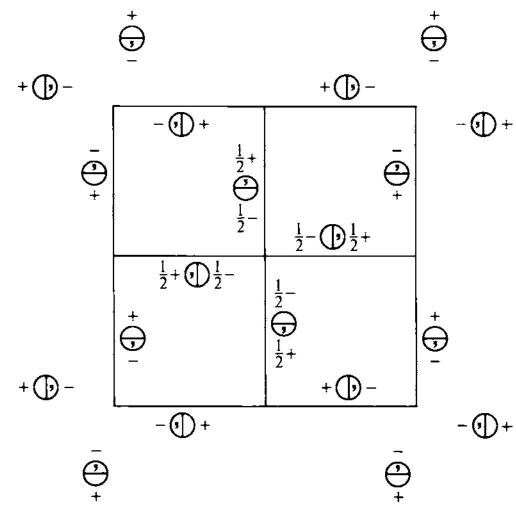
I none

II [2] $C4/mmm$ ($P4/mmm$, 123); [2] $I4/mcm$ (140)

$P4/mnc$ D_{4h}^{6} $4/mmm$ Tetragonal

No. 128 $P\ 4/m\ 2_1/n\ 2/c$ Patterson symmetry $P4/mmm$





Origin at centre $(4/m)$ at $4/m1n$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^+\ 0,0,z$	(4) $4^-\ 0,0,z$
(5) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x,\frac{1}{4}$	(8) $2\quad x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}\quad 0,0,0$	(10) $m\quad x,y,0$	(11) $\bar{4}^+\ 0,0,z;\ 0,0,0$	(12) $\bar{4}^-\ 0,0,z;\ 0,0,0$
(13) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(14) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$	(15) $c\quad x+\frac{1}{2},\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$0kl$: $k+l=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	hhl : $l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	$00l$: $l=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$h00$: $h=2n$
							Special: as above, plus
8	h	$m\,.\,.$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	
8	g	$.\,.\,2$	$x,x+\frac{1}{2},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x,\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{1}{4}$	hkl : $l=2n$
			$\bar{x},\bar{x}+\frac{1}{2},\frac{3}{4}$	$x,x+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x,\frac{3}{4}$	
8	f	$2\,.\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl : $h+k,l=2n$
			$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$	
4	e	$4\,.\,.$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl : $h+k+l=2n$
4	d	$2\,.\,22$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{3}{4}$	hkl : $h+k,l=2n$
4	c	$2/m\,.\,.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl : $h+k,l=2n$
2	b	$4/m\,.\,.$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k+l=2n$
2	a	$4/m\,.\,.$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I
[2] $P\bar{4}n2$ (118) 1; 2; 7; 8; 11; 12; 13; 14
[2] $P\bar{4}2_1c$ (114) 1; 2; 5; 6; 11; 12; 15; 16
[2] $P4nc$ (104) 1; 2; 3; 4; 13; 14; 15; 16
[2] $P42_12$ (90) 1; 2; 3; 4; 5; 6; 7; 8
[2] $P4/m11$ ($P4/m$, 83) 1; 2; 3; 4; 9; 10; 11; 12
[2] $P2/m12/c$ ($Cccm$, 66) 1; 2; 7; 8; 9; 10; 15; 16
[2] $P2/m2_1/n1$ ($Pnnm$, 58) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4/mnc$ ($\mathbf{c}'=3\mathbf{c}$) (128); [9] $P4/mnc$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (128)

Minimal non-isomorphic supergroups

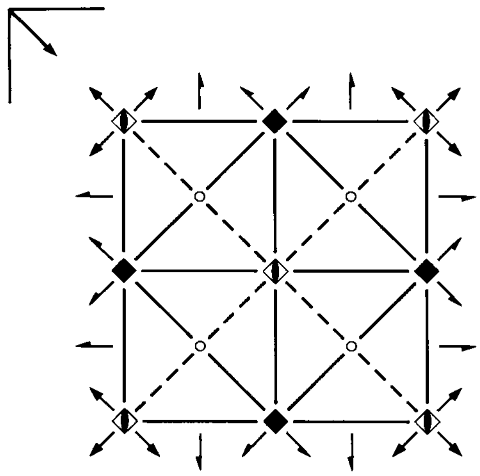
I none

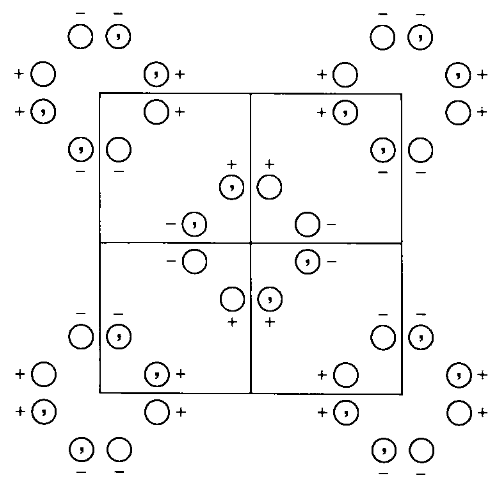
II [2] $C4/mcc$ ($P4/mcc$, 124); [2] $I4/mmm$ (139); [2] $P4/mbm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (127)

$P4/nmm$ D_{4h}^{7} $4/mmm$ Tetragonal

No. 129 $P\ 4/n\ 2_1/m\ 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}m2$ at $\bar{4}/nm2/g$, at $-\frac{1}{4},\frac{1}{4},0$ from centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le \frac{1}{2} - x$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^{+}\quad 0,\frac{1}{2},z$	(4) $4^{-}\quad \frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$	(7) $2\quad x,x,0$	(8) $2\quad x,\bar{x},0$
(9) $\bar{1}\quad \frac{1}{4},\frac{1}{4},0$	(10) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,0$	(11) $\bar{4}^{+}\quad 0,0,z;\ 0,0,0$	(12) $\bar{4}^{-}\quad 0,0,z;\ 0,0,0$
(13) $m\quad x,0,z$	(14) $m\quad 0,y,z$	(15) $m\quad x+\frac{1}{2},\bar{x},z$	(16) $g(\frac{1}{2},\frac{1}{2},0)\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	k	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (13) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (14) $\bar{x},y,z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z$ (7) $y,x,\bar{z}$ (11) $y,\bar{x},\bar{z}$ (15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z$ (8) $\bar{y},\bar{x},\bar{z}$ (12) $\bar{y},x,\bar{z}$ (16) $y+\frac{1}{2},x+\frac{1}{2},z$	$hk0$: $h+k=2n$ $h00$: $h=2n$
							Special: as above, plus
8	j	$..m$	$x,x+\frac{1}{2},z$ $\bar{x}+\frac{1}{2},x,\bar{z}$	$\bar{x},\bar{x}+\frac{1}{2},z$ $x+\frac{1}{2},\bar{x},\bar{z}$	$\bar{x},x+\frac{1}{2},z$ $x+\frac{1}{2},x,\bar{z}$	$x,\bar{x}+\frac{1}{2},z$ $\bar{x}+\frac{1}{2},\bar{x},\bar{z}$	no extra conditions
8	i	$.m.$	$0,y,z$ $\frac{1}{2},y+\frac{1}{2},\bar{z}$	$0,\bar{y},z$ $\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$\bar{y}+\frac{1}{2},\frac{1}{2},z$ $y,0,\bar{z}$	$y+\frac{1}{2},\frac{1}{2},z$ $\bar{y},0,\bar{z}$	no extra conditions
8	h	$..2$	$x,x,\frac{1}{2}$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$ $x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $x,\bar{x},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x},x,\frac{1}{2}$	hkl : $h+k=2n$
8	g	$..2$	$x,x,0$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\bar{x},\bar{x},0$ $x+\frac{1}{2},x+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$ $x,\bar{x},0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},0$ $\bar{x},x,0$	hkl : $h+k=2n$
4	f	$2mm.$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	hkl : $h+k=2n$
4	e	$..2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	hkl : $h,k=2n$
4	d	$..2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl : $h,k=2n$
2	c	$4mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			no extra conditions
2	b	$\bar{4}m2$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	a	$\bar{4}m2$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4mm$ (99)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ ($Cmme$, 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2_1/m1$ ($Pmmn$, 59)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $P4_2/ncm$ ($\mathbf{c}'=2\mathbf{c}$) (138); [2] $P4_2/nmc$ ($\mathbf{c}'=2\mathbf{c}$) (137); [2] $P4/ncc$ ($\mathbf{c}'=2\mathbf{c}$) (130)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/nmm$ ($\mathbf{c}'=2\mathbf{c}$) (129); [9] $P4/nmm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (129)

Minimal non-isomorphic supergroups

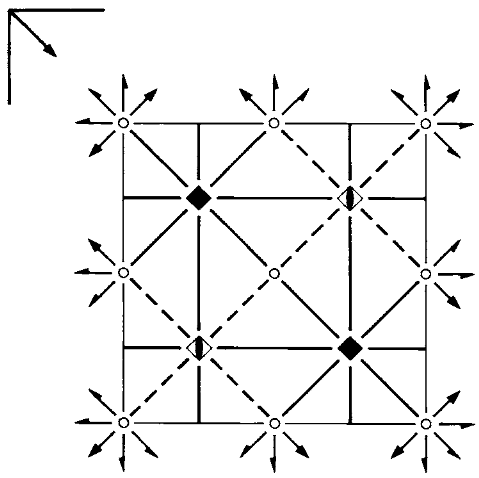
I none

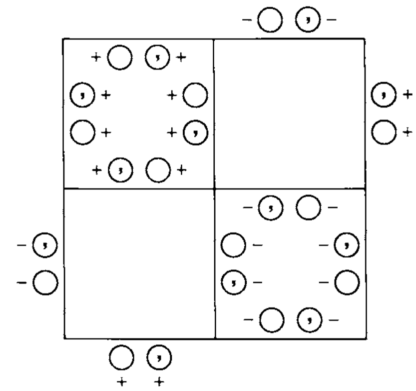
II [2] $C4/mmm$ ($P4/mmm$, 123); [2] $I4/mmm$ (139)

$P4/nmm$ D_{4h}^{7} $4/mmm$ Tetragonal

No. 129 $P\ 4/n\ 2_1/m\ 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2





Origin at centre $(2/m)$ at $n2_1$ $(2/m, 2_1/g)$, at $\frac{1}{4}, -\frac{1}{4}, 0$ from $\bar{4}m2$

Asymmetric unit $-\frac{1}{4} \le x \le \frac{1}{4}$; $-\frac{1}{4} \le y \le \frac{1}{4}$; $0 \le z \le \frac{1}{2}$; $x \le y$

Symmetry operations

(1) 1	(2) $2\ \ \frac{1}{4}, \frac{1}{4}, z$	(3) $4^{+}\ \ \frac{1}{4}, \frac{1}{4}, z$	(4) $4^{-}\ \ \frac{1}{4}, \frac{1}{4}, z$
(5) $2(0, \frac{1}{2}, 0)\ \ 0, y, 0$	(6) $2(\frac{1}{2}, 0, 0)\ \ x, 0, 0$	(7) $2(\frac{1}{2}, \frac{1}{2}, 0)\ \ x, x, 0$	(8) $2\ \ x, \bar{x}, 0$
(9) $\bar{1}\ \ 0, 0, 0$	(10) $n(\frac{1}{2}, \frac{1}{2}, 0)\ \ x, y, 0$	(11) $\bar{4}^{+}\ \ \frac{1}{4}, -\frac{1}{4}, z;\ \ \frac{1}{4}, -\frac{1}{4}, 0$	(12) $\bar{4}^{-}\ \ -\frac{1}{4}, \frac{1}{4}, z;\ \ -\frac{1}{4}, \frac{1}{4}, 0$
(13) $m\ \ x, \frac{1}{4}, z$	(14) $m\ \ \frac{1}{4}, y, z$	(15) $m\ \ x+\frac{1}{2}, \bar{x}, z$	(16) $m\ \ x, x, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	k	1	(1) x,y,z (5) $\bar{x},y+\frac{1}{2},\bar{z}$ (9) $\bar{x},\bar{y},\bar{z}$ (13) $x,\bar{y}+\frac{1}{2},z$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},\bar{y},\bar{z}$ (10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (14) $\bar{x}+\frac{1}{2},y,z$	(3) $\bar{y}+\frac{1}{2},x,z$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$ (11) $y+\frac{1}{2},\bar{x},\bar{z}$ (15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(4) $y,\bar{x}+\frac{1}{2},z$ (8) $\bar{y},\bar{x},\bar{z}$ (12) $\bar{y},x+\frac{1}{2},\bar{z}$ (16) y,x,z	$hk0$: $h+k=2n$ $h00$: $h=2n$
							Special: as above, plus
8	j	$..m$	x,x,z $\bar{x},x+\frac{1}{2},\bar{z}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},z$ $x+\frac{1}{2},\bar{x},\bar{z}$	$\bar{x}+\frac{1}{2},x,z$ $x+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$x,\bar{x}+\frac{1}{2},z$ $\bar{x},\bar{x},\bar{z}$	no extra conditions
8	i	$.m.$	$\frac{1}{4},y,z$ $\frac{3}{4},y+\frac{1}{2},\bar{z}$	$\frac{1}{4},\bar{y}+\frac{1}{2},z$ $\frac{3}{4},\bar{y},\bar{z}$	$\bar{y}+\frac{1}{2},\frac{1}{4},z$ $y+\frac{1}{2},\frac{3}{4},\bar{z}$	$y,\frac{1}{4},z$ $\bar{y},\frac{3}{4},\bar{z}$	no extra conditions
8	h	$..2$	$x,\bar{x},\frac{1}{2}$ $\bar{x},x,\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},x,\frac{1}{2}$ $\bar{x}+\frac{1}{2},\bar{x},\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{2}$ $x,x+\frac{1}{2},\frac{1}{2}$	hkl : $h+k=2n$
8	g	$..2$	$x,\bar{x},0$ $\bar{x},x,0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},x,0$ $\bar{x}+\frac{1}{2},\bar{x},0$	$\bar{x},\bar{x}+\frac{1}{2},0$ $x,x+\frac{1}{2},0$	hkl : $h+k=2n$
4	f	$2mm.$	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	hkl : $h+k=2n$
4	e	$..2/m$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl : $h,k=2n$
4	d	$..2/m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hkl : $h,k=2n$
2	c	$4mm$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}$			no extra conditions
2	b	$\bar{4}m2$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$			hkl : $h+k=2n$
2	a	$\bar{4}m2$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I
[2] $P\bar{4}m2$ (115) 1; 2; 7; 8; 11; 12; 13; 14
[2] $P\bar{4}2_1m$ (113) 1; 2; 5; 6; 11; 12; 15; 16
[2] $P4mm$ (99) 1; 2; 3; 4; 13; 14; 15; 16
[2] $P42_12$ (90) 1; 2; 3; 4; 5; 6; 7; 8
[2] $P4/n11$ ($P4/n$, 85) 1; 2; 3; 4; 9; 10; 11; 12
[2] $P2/n12/m$ ($Cmme$, 67) 1; 2; 7; 8; 9; 10; 15; 16
[2] $P2/n2_1/m1$ ($Pmmn$, 59) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $P4_2/ncm$ ($\mathbf{c}'=2\mathbf{c}$) (138); [2] $P4_2/nmc$ ($\mathbf{c}'=2\mathbf{c}$) (137); [2] $P4/ncc$ ($\mathbf{c}'=2\mathbf{c}$) (130)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/nmm$ ($\mathbf{c}'=2\mathbf{c}$) (129); [9] $P4/nmm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (129)

Minimal non-isomorphic supergroups

I none

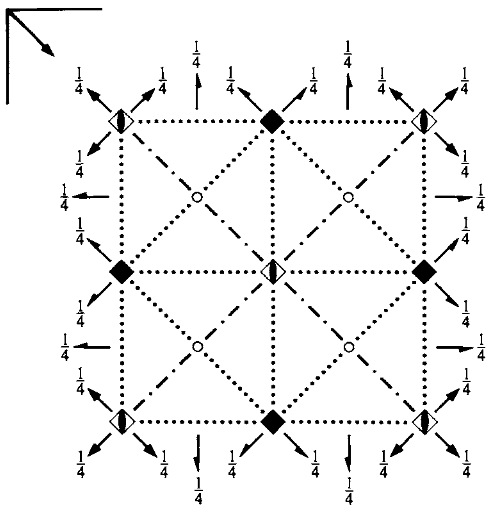
II [2] $C4/mmm$ ($P4/mmm$, 123); [2] $I4/mmm$ (139)

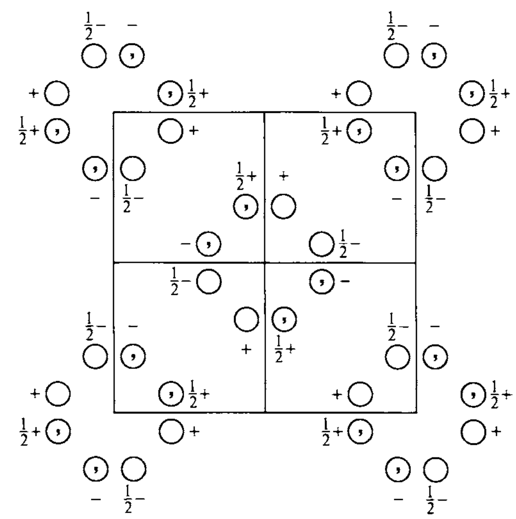
International Tables for Crystallography (2006). Vol. A, Space group 130, pp. 450–453.

$P4/ncc$ D_{4h}^{8} $4/mmm$ Tetragonal

No. 130 $P\ 4/n\ 2_1/c\ 2/c$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}/ncn$, at $-\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^{+}\quad 0,\frac{1}{2},z$	(4) $4^{-}\quad \frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{1}{4}$	(7) $2\quad x,x,\frac{1}{4}$	(8) $2\quad x,\bar{x},\frac{1}{4}$
(9) $\bar{1}\quad \frac{1}{4},\frac{1}{4},0$	(10) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,0$	(11) $\bar{4}^{+}\quad 0,0,z;\ \ 0,0,0$	(12) $\bar{4}^{-}\quad 0,0,z;\ \ 0,0,0$
(13) $c\quad x,0,z$	(14) $c\quad 0,y,z$	(15) $c\quad x+\frac{1}{2},\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z$	$hk0: h+k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$0kl: l=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	$hhl: l=2n$
			(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$00l: l=2n$
							$h00: h=2n$
							Special: as above, plus
8	f	$..2$	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{4}$	$hkl: h+k+l=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{3}{4}$	$x,\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	
8	e	$2..$	$0,0,z$ $\quad \frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$		$hkl: h+k,l=2n$
			$\frac{1}{2},\frac{1}{2},\bar{z}$ $\quad 0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$		
8	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$ $\quad \frac{3}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{3}{4},0$ $\quad \frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$ $\quad \frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$ $\quad \frac{3}{4},\frac{3}{4},\frac{1}{2}$	$hkl: h,k,l=2n$
4	c	$4..$	$0,\frac{1}{2},z$ $\quad \frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$		$hkl: l=2n$
4	b	$\bar{4}..$	$0,0,0$ $\quad \frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$		$hkl: h+k,l=2n$
4	a	2.22	$0,0,\frac{1}{4}$ $\quad \frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$0,0,\frac{3}{4}$		$hkl: h+k,l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\quad \mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\quad \mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad \mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4cc$ (103)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2_1/c1$ ($Pccn$, 56)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4/ncc$ ($\mathbf{c}'=3\mathbf{c}$) (130); [9] $P4/ncc$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (130)

Minimal non-isomorphic supergroups

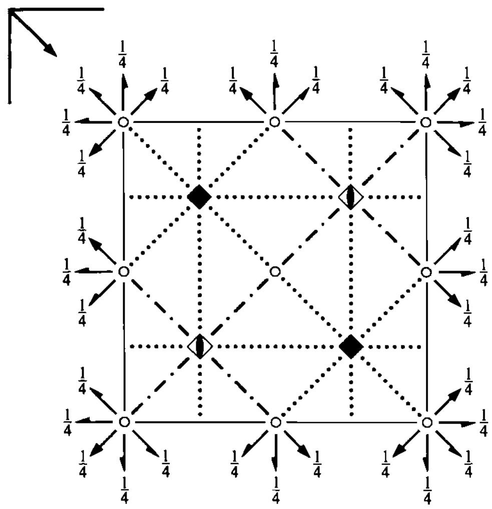
I none

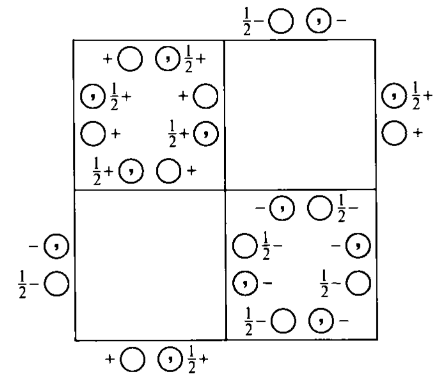
II [2] $C4/mcc$ ($P4/mcc$, 124); [2] $I4/mcm$ (140); [2] $P4/nmm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (129)

$P4/ncc$ D_{4h}^{8} $4/mmm$ Tetragonal

No. 130 $P\ 4/n\ 2_1/c\ 2/c$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2





Origin at $\bar{1}$ at $n1\,(c,n)$, at $\frac{1}{4},-\frac{1}{4},0$ from $\bar{4}$

Asymmetric unit $-\frac{1}{4} \le x \le \frac{1}{4}$; $-\frac{1}{4} \le y \le \frac{1}{4}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\ \ \frac{1}{4},\frac{1}{4},z$	(3) $4^{+}\ \ \frac{1}{4},\frac{1}{4},z$	(4) $4^{-}\ \ \frac{1}{4},\frac{1}{4},z$
(5) $2(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\ \ x,0,\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x,\frac{1}{4}$	(8) $2\ \ x,\bar{x},\frac{1}{4}$
(9) $\bar{1}\ \ 0,0,0$	(10) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$	(11) $\bar{4}^{+}\ \ \frac{1}{4},-\frac{1}{4},z$; $\frac{1}{4},-\frac{1}{4},0$	(12) $\bar{4}^{-}\ \ -\frac{1}{4},\frac{1}{4},z$; $-\frac{1}{4},\frac{1}{4},0$
(13) $c\ \ x,\frac{1}{4},z$	(14) $c\ \ \frac{1}{4},y,z$	(15) $c\ \ x+\frac{1}{2},\bar{x},z$	(16) $c\ \ x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z$	(4) $y,\bar{x}+\frac{1}{2},z$	$hk0$: $h+k=2n$
			(5) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$0kl$: $l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}$	hhl : $l=2n$
			(13) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$	$00l$: $l=2n$
							$h00$: $h=2n$
							Special: as above, plus
8	f	..2	$x,\bar{x},\frac{1}{4}$ $\quad$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$ $\quad$ $x+\frac{1}{2},x,\frac{1}{4}$ $\quad$ $\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$				hkl : $h+k+l=2n$
			$\bar{x},x,\frac{3}{4}$ $\quad$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$ $\quad$ $\bar{x}+\frac{1}{2},\bar{x},\frac{3}{4}$ $\quad$ $x,x+\frac{1}{2},\frac{3}{4}$				
8	e	2..	$\frac{3}{4},\frac{1}{4},z$ $\quad$ $\frac{1}{4},\frac{3}{4},z$ $\quad$ $\frac{1}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$ $\quad$ $\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$				hkl : $h+k,l=2n$
			$\frac{1}{4},\frac{3}{4},\bar{z}$ $\quad$ $\frac{3}{4},\frac{1}{4},\bar{z}$ $\quad$ $\frac{3}{4},\frac{1}{4},z+\frac{1}{2}$ $\quad$ $\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$				
8	d	$\bar{1}$	$0,0,0$ $\quad$ $\frac{1}{2},\frac{1}{2},0$ $\quad$ $\frac{1}{2},0,0$ $\quad$ $0,\frac{1}{2},0$ $\quad$ $0,\frac{1}{2},\frac{1}{2}$ $\quad$ $\frac{1}{2},0,\frac{1}{2}$ $\quad$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\quad$ $0,0,\frac{1}{2}$				hkl : $h,k,l=2n$
4	c	4..	$\frac{1}{4},\frac{1}{4},z$ $\quad$ $\frac{3}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$ $\quad$ $\frac{3}{4},\frac{3}{4},\bar{z}$ $\quad$ $\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$				hkl : $l=2n$
4	b	$\bar{4}$..	$\frac{3}{4},\frac{1}{4},0$ $\quad$ $\frac{1}{4},\frac{3}{4},0$ $\quad$ $\frac{1}{4},\frac{3}{4},\frac{1}{2}$ $\quad$ $\frac{3}{4},\frac{1}{4},\frac{1}{2}$				hkl : $h+k,l=2n$
4	a	2.22	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$ $\quad$ $\frac{1}{4},\frac{3}{4},\frac{1}{4}$ $\quad$ $\frac{1}{4},\frac{3}{4},\frac{3}{4}$ $\quad$ $\frac{3}{4},\frac{1}{4},\frac{3}{4}$				hkl : $h+k,l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\quad$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\quad$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4cc$ (103)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2_1/c1$ ($Pccn$, 56)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4/ncc$ ($\mathbf{c}'=3\mathbf{c}$) (130); [9] $P4/ncc$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (130)

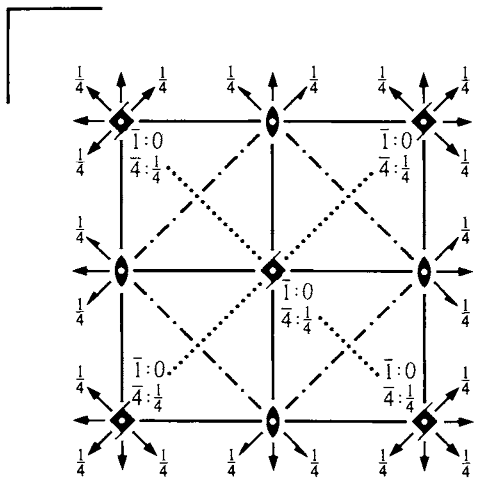
Minimal non-isomorphic supergroups

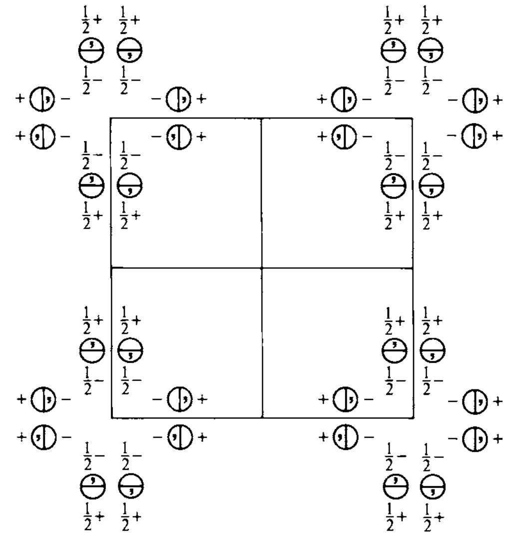
I none

II [2] $C4/mcc$ ($P4/mcc$, 124); [2] $I4/mcm$ (140); [2] $P4/nmm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (129)

$P4_2/mmc$ $\quad D_{4h}^{9}$ $\quad 4/mmm$ $\quad$ Tetragonal

No. 131 $\quad P\ 4_2/m\ 2/m\ 2/c$ $\quad$ Patterson symmetry $P4/mmm$





Origin at centre (mmm) at $4_2/m2/mc$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\ \ 0,0,z$	(3) $4^{+}(0,0,\frac{1}{2})\ \ 0,0,z$	(4) $4^{-}(0,0,\frac{1}{2})\ \ 0,0,z$
(5) $2\ \ 0,y,0$	(6) $2\ \ x,0,0$	(7) $2\ \ x,x,\frac{1}{4}$	(8) $2\ \ x,\bar{x},\frac{1}{4}$
(9) $\bar{1}\ \ 0,0,0$	(10) $m\ \ x,y,0$	(11) $\bar{4}^{+}\ \ 0,0,z;\ \ 0,0,\frac{1}{4}$	(12) $\bar{4}^{-}\ \ 0,0,z;\ \ 0,0,\frac{1}{4}$
(13) $m\ \ x,0,z$	(14) $m\ \ 0,y,z$	(15) $c\ \ x,\bar{x},z$	(16) $c\ \ x,x,z$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2mc$ (105)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/m11$ ($P4_2/m$, 84)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/m12/c$ ($Cccm$, 66)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/m2/m1$ ($Pmmm$, 47)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $C4_2/emc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/ncm$, 138); [2] $C4_2/mmd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/mnm$, 136); [2] $C4_2/emd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/nnm$, 134); [2] $C4_2/mmc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/mcm$, 132)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/mmc$ ($\mathbf{c}' = 3\mathbf{c}$) (131); [9] $P4_2/mmc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (131)

Minimal non-isomorphic supergroups

I [3] $Pm\bar{3}n$ (223)

II [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mmm$ (139); [2] $P4/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (123)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	r	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$ (9) $\bar{x},\bar{y},\bar{z}$ (13) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$ (10) $x,y,\bar{z}$ (14) $\bar{x},y,z$	(3) $\bar{y},x,z+\frac{1}{2}$ (7) $y,x,\bar{z}+\frac{1}{2}$ (11) $y,\bar{x},\bar{z}+\frac{1}{2}$ (15) $\bar{y},\bar{x},z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$ (12) $\bar{y},x,\bar{z}+\frac{1}{2}$ (16) $y,x,z+\frac{1}{2}$	hhl : $l=2n$ $00l$: $l=2n$
							Special: as above, plus
8	q	$m\,.\,.$	$x,y,0$ $\bar{x},y,0$	$\bar{x},\bar{y},0$ $x,\bar{y},0$	$\bar{y},x,\frac{1}{2}$ $y,x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$ $\bar{y},\bar{x},\frac{1}{2}$	no extra conditions
8	p	$.\,m\,.$	$\frac{1}{2},y,z$ $\frac{1}{2},y,\bar{z}$	$\frac{1}{2},\bar{y},z$ $\frac{1}{2},\bar{y},\bar{z}$	$\bar{y},\frac{1}{2},z+\frac{1}{2}$ $y,\frac{1}{2},\bar{z}+\frac{1}{2}$	$y,\frac{1}{2},z+\frac{1}{2}$ $\bar{y},\frac{1}{2},\bar{z}+\frac{1}{2}$	no extra conditions
8	o	$.\,m\,.$	$0,y,z$ $0,y,\bar{z}$	$0,\bar{y},z$ $0,\bar{y},\bar{z}$	$\bar{y},0,z+\frac{1}{2}$ $y,0,\bar{z}+\frac{1}{2}$	$y,0,z+\frac{1}{2}$ $\bar{y},0,\bar{z}+\frac{1}{2}$	no extra conditions
8	n	$.\,.\,2$	$x,x,\frac{1}{4}$ $\bar{x},\bar{x},\frac{3}{4}$	$\bar{x},\bar{x},\frac{1}{4}$ $x,x,\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$ $x,\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{3}{4}$ $\bar{x},x,\frac{1}{4}$	hkl : $l=2n$
4	m	$m\,2\,m\,.$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	no extra conditions
4	l	$m\,2\,m\,.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,0$	$0,\bar{x},0$	no extra conditions
4	k	$m\,2\,m\,.$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	no extra conditions
4	j	$m\,2\,m\,.$	$x,0,0$	$\bar{x},0,0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	no extra conditions
4	i	$2\,m\,m\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	hkl : $h+k+l=2n$
4	h	$2\,m\,m\,.$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl : $l=2n$
4	g	$2\,m\,m\,.$	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	hkl : $l=2n$
2	f	$\bar{4}\,m\,2$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl : $l=2n$
2	e	$\bar{4}\,m\,2$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl : $l=2n$
2	d	$m\,m\,m\,.$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$			hkl : $h+k+l=2n$
2	c	$m\,m\,m\,.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k+l=2n$
2	b	$m\,m\,m\,.$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
2	a	$m\,m\,m\,.$	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

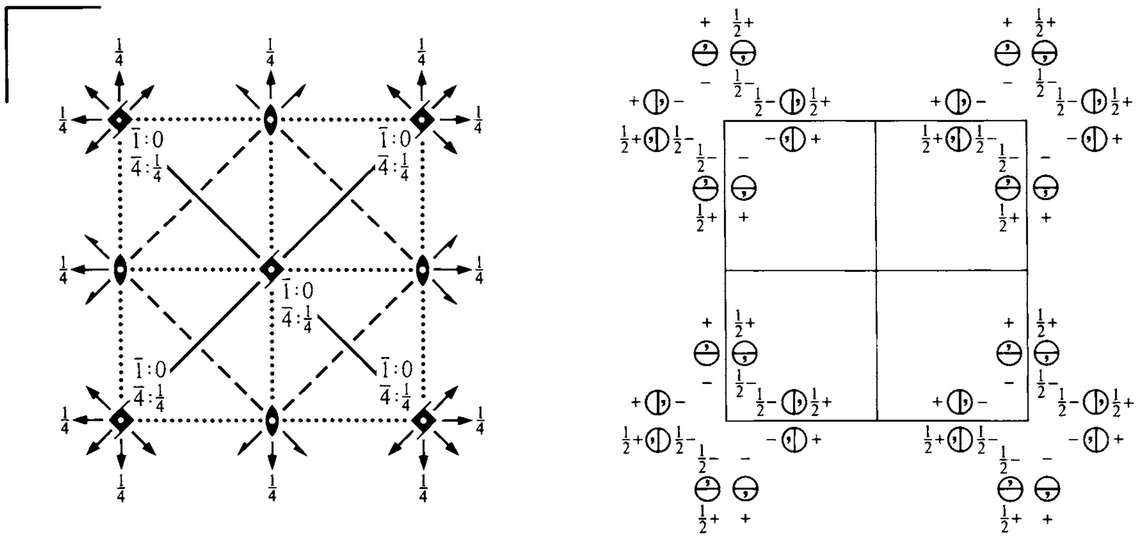
Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

(*Continued on preceding page*)

International Tables for Crystallography (2006). Vol. A, Space group 132, pp. 456–457.

$P4_2/mcm$ D_{4h}^{10} $4/mmm$ Tetragonal

No. 132 $P\ 4_2/m\ 2/c\ 2/m$ Patterson symmetry $P4/mmm$



Origin at centre (mmm) at $4_2/mc2/m$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $x \le y$

Symmetry operations

(1) 1	(2) $2\ \ 0,0,z$	(3) $4^{+}(0,0,\frac{1}{2})\ \ 0,0,z$	(4) $4^{-}(0,0,\frac{1}{2})\ \ 0,0,z$
(5) $2\ \ 0,y,\frac{1}{4}$	(6) $2\ \ x,0,\frac{1}{4}$	(7) $2\ \ x,x,0$	(8) $2\ \ x,\bar{x},0$
(9) $\bar{1}\ \ 0,0,0$	(10) $m\ \ x,y,0$	(11) $\bar{4}^{+}\ \ 0,0,z;\ \ 0,0,\frac{1}{4}$	(12) $\bar{4}^{-}\ \ 0,0,z;\ \ 0,0,\frac{1}{4}$
(13) $c\ \ x,0,z$	(14) $c\ \ 0,y,z$	(15) $m\ \ x,\bar{x},z$	(16) $m\ \ x,x,z$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2cm$ (101)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/m11$ ($P4_2/m$, 84)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/m12/m$ ($Cmmm$, 65)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/m2/c1$ ($Pccm$, 49)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $C4_2/ecm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/nmc$, 137); [2] $C4_2/mcd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/mbc$, 135); [2] $C4_2/ecd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/nbc$, 133); [2] $C4_2/mcm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_2/mmc$, 131)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/mcm$ ($\mathbf{c}' = 3\mathbf{c}$) (132); [9] $P4_2/mcm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (132)

Minimal non-isomorphic supergroups

I none

II [2] $C4_2/mcm$ ($P4_2/mmc$, 131); [2] $I4/mcm$ (140); [2] $P4/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (123)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	p	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	$0kl$: $l=2n$
			(5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	$00l$: $l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x,\bar{z}+\frac{1}{2}$	
			(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z$	(16) y,x,z	
							Special: as above, plus
8	o	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z+\frac{1}{2}$	$x,\bar{x},z+\frac{1}{2}$	no extra conditions
			$\bar{x},x,\bar{z}+\frac{1}{2}$	$x,\bar{x},\bar{z}+\frac{1}{2}$	$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
8	n	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
			$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	$y,x,0$	$\bar{y},\bar{x},0$	
8	m	$.2.$	$x,\frac{1}{2},\frac{1}{4}$	$\bar{x},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},x,\frac{3}{4}$	$\frac{1}{2},\bar{x},\frac{3}{4}$	hkl : $l=2n$
			$\bar{x},\frac{1}{2},\frac{3}{4}$	$x,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\bar{x},\frac{1}{4}$	$\frac{1}{2},x,\frac{1}{4}$	
8	l	$.2.$	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$0,x,\frac{3}{4}$	$0,\bar{x},\frac{3}{4}$	hkl : $l=2n$
			$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	$0,\bar{x},\frac{1}{4}$	$0,x,\frac{1}{4}$	
8	k	$2..$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	hkl : $h+k,l=2n$
			$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,z$	
4	j	$m.2m$	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,0$	$x,\bar{x},0$	no extra conditions
4	i	$m.2m$	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	no extra conditions
4	h	$2.mm$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	hkl : $l=2n$
4	g	$2.mm$	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	hkl : $l=2n$
4	f	$2/m..$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$	hkl : $h+k,l=2n$
4	e	$222.$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	hkl : $h+k,l=2n$
2	d	$\bar{4}2m$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl : $l=2n$
2	c	$m.mm$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
2	b	$\bar{4}2m$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl : $l=2n$
2	a	$m.mm$	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

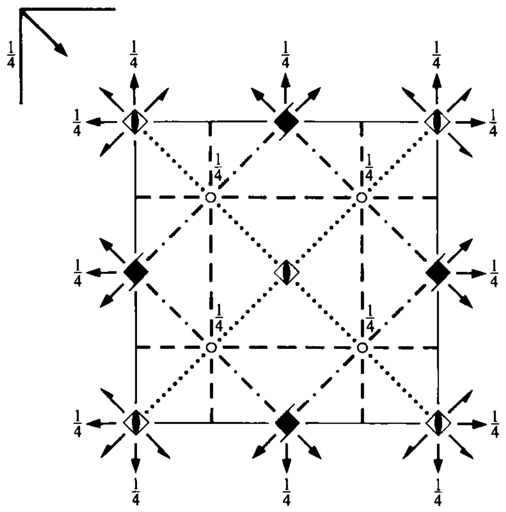
(*Continued on preceding page*)

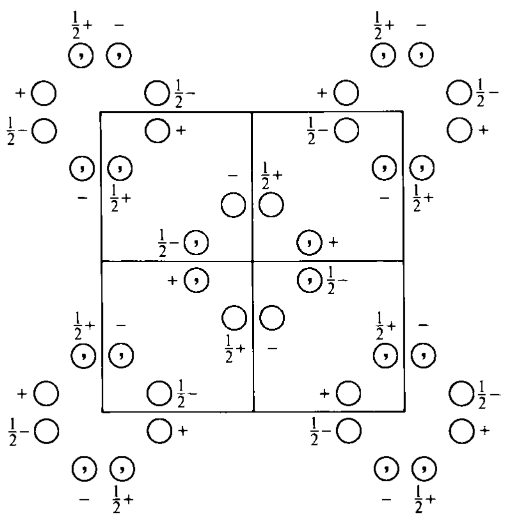
International Tables for Crystallography (2006). Vol. A, Space group 133, pp. 458–461.

$P4_2/nbc$ D_{4h}^{11} $4/mmm$ Tetragonal

No. 133 $P\ 4_2/n\ 2/b\ 2/c$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}12_1/c$, at $-\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^+(0,0,\frac{1}{2})\quad 0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})\quad \frac{1}{2},0,z$
(5) $2\quad 0,y,\frac{1}{4}$	(6) $2\quad x,0,\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x,0$	(8) $2\quad x,\bar{x}+\frac{1}{2},0$
(9) $\bar{1}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,\frac{1}{4}$	(11) $\bar{4}^+\quad 0,0,z;\ 0,0,0$	(12) $\bar{4}^-\quad 0,0,z;\ 0,0,0$
(13) $a\quad x,\frac{1}{4},z$	(14) $b\quad \frac{1}{4},y,z$	(15) $c\quad x,\bar{x},z$	(16) $c\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates								Reflection conditions
											General:
16	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$					$hk0:\ h+k=2n$
			(5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$					$0kl:\ k=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$					$hhl:\ l=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$					$00l:\ l=2n$
											$h00:\ h=2n$
											Special: as above, plus
8	j	. . 2	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x},x+\frac{1}{2},\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},\frac{1}{2}$					$hkl:\ h+k+l=2n$
			$\bar{x}+\frac{1}{2},\bar{x},\frac{1}{2}$	$x+\frac{1}{2},x,\frac{1}{2}$	$x+\frac{1}{2},\bar{x},0$	$\bar{x}+\frac{1}{2},x,0$					
8	i	. 2 .	$x,0,\frac{3}{4}$	$\bar{x},0,\frac{3}{4}$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{4}$					$hkl:\ h+k=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$0,\bar{x},\frac{1}{4}$	$0,x,\frac{1}{4}$					
8	h	. 2 .	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\frac{1}{2},x+\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$					$hkl:\ h+k=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$0,\bar{x},\frac{3}{4}$	$0,x,\frac{3}{4}$					
8	g	2 . .	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$					$hkl:\ h+k,l=2n$
			$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	$0,0,z+\frac{1}{2}$					
8	f	2 . .	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$					$hkl:\ h+k,l=2n$
			$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z$	$\frac{1}{2},0,z+\frac{1}{2}$					
8	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$hkl:\ h,k,l=2n$
4	d	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$					$hkl:\ h+k,l=2n$
4	c	2 . 22	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},0,0$					$hkl:\ h+k,l=2n$
4	b	2 2 2 .	$0,0,\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkl:\ h+k,l=2n$
4	a	2 2 2 .	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$					$hkl:\ h+k,l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,\frac{1}{4}$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2bc$ (106)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/n11$ ($P4_2/n$, 86)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/b1$ ($Pban$, 50)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/nbc$ ($\mathbf{c}'=3\mathbf{c}$) (133); [9] $P4_2/nbc$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (133)

Minimal non-isomorphic supergroups

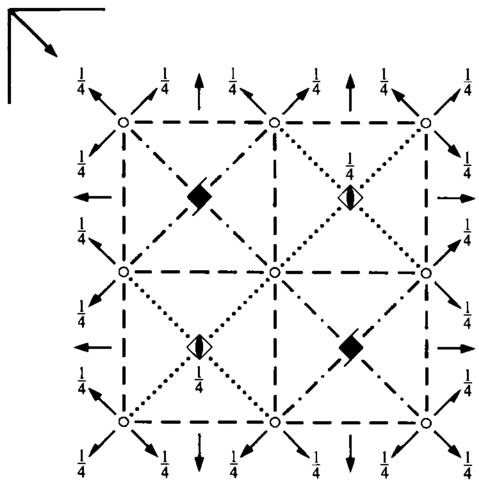
I none

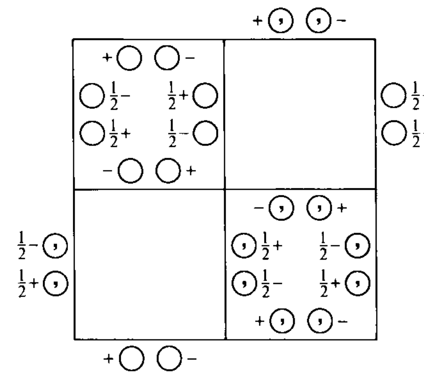
II [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mcm$ (140); [2] $P4/nbm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (125)

$P4_2/nbc$ $\quad D_{4h}^{11}$ $\quad 4/mmm$ $\quad$ Tetragonal

No. 133 $\quad P\ 4_2/n\ 2/b\ 2/c$ $\quad$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2





Origin at $\bar{1}$ at $n(b,a)(n,c)$, at $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ from $\bar{4}$

Asymmetric unit $\quad -\frac{1}{4} \le x \le \frac{1}{4};\quad -\frac{1}{4} \le y \le \frac{1}{4};\quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\ \ \frac{1}{4},\frac{1}{4},z$	(3) $4^{+}(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$	(4) $4^{-}(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$
(5) $2\ \ \frac{1}{4},y,0$	(6) $2\ \ x,\frac{1}{4},0$	(7) $2\ \ x,x,\frac{1}{4}$	(8) $2\ \ x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}\ \ 0,0,0$	(10) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$	(11) $\bar{4}^{+}\ \frac{1}{4},-\frac{1}{4},z;\ \ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$	(12) $\bar{4}^{-}\ -\frac{1}{4},\frac{1}{4},z;\ \ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(13) $a\ \ x,0,z$	(14) $b\ \ 0,y,z$	(15) $c\ \ x,\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	Reflection conditions
				General:
16	k	1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (3) $\bar{y}+\frac{1}{2},x,z+\frac{1}{2}$ (4) $y,\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (5) $\bar{x}+\frac{1}{2},y,\bar{z}$ (6) $x,\bar{y}+\frac{1}{2},\bar{z}$ (7) $y,x,\bar{z}+\frac{1}{2}$ (8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (9) $\bar{x},\bar{y},\bar{z}$ (10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (11) $y+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$ (12) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (13) $x+\frac{1}{2},\bar{y},z$ (14) $\bar{x},y+\frac{1}{2},z$ (15) $\bar{y},\bar{x},z+\frac{1}{2}$ (16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h+k=2n$ $0kl$: $k=2n$ hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
				Special: as above, plus
8	j	..2	$x,x,\frac{1}{4}$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{4}$ $\bar{x}+\frac{1}{2},x,\frac{3}{4}$ $x,\bar{x}+\frac{1}{2},\frac{3}{4}$ $\bar{x},\bar{x},\frac{3}{4}$ $x+\frac{1}{2},x+\frac{1}{2},\frac{3}{4}$ $x+\frac{1}{2},\bar{x},\frac{1}{4}$ $\bar{x},x+\frac{1}{2},\frac{1}{4}$	hkl : $h+k+l=2n$
8	i	.2.	$x,\frac{1}{4},\frac{1}{2}$ $\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{2}$ $\frac{1}{4},x,0$ $\frac{1}{4},\bar{x}+\frac{1}{2},0$ $\bar{x},\frac{3}{4},\frac{1}{2}$ $x+\frac{1}{2},\frac{3}{4},\frac{1}{2}$ $\frac{3}{4},\bar{x},0$ $\frac{3}{4},x+\frac{1}{2},0$	hkl : $h+k=2n$
8	h	.2.	$x,\frac{1}{4},0$ $\bar{x}+\frac{1}{2},\frac{1}{4},0$ $\frac{1}{4},x,\frac{1}{2}$ $\frac{1}{4},\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x},\frac{3}{4},0$ $x+\frac{1}{2},\frac{3}{4},0$ $\frac{3}{4},\bar{x},\frac{1}{2}$ $\frac{3}{4},x+\frac{1}{2},\frac{1}{2}$	hkl : $h+k=2n$
8	g	2..	$\frac{3}{4},\frac{1}{4},z$ $\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$ $\frac{3}{4},\frac{1}{4},\bar{z}$ $\frac{1}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$ $\frac{1}{4},\frac{3}{4},\bar{z}$ $\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$ $\frac{1}{4},\frac{3}{4},z$ $\frac{3}{4},\frac{1}{4},z+\frac{1}{2}$	hkl : $h+k,l=2n$
8	f	2..	$\frac{1}{4},\frac{1}{4},z$ $\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$ $\frac{1}{4},\frac{1}{4},\bar{z}$ $\frac{1}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$ $\frac{3}{4},\frac{3}{4},\bar{z}$ $\frac{3}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$ $\frac{3}{4},\frac{3}{4},z$ $\frac{3}{4},\frac{3}{4},z+\frac{1}{2}$	hkl : $h+k,l=2n$
8	e	$\bar{1}$	$0,0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},0,\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,0$ $0,\frac{1}{2},0$ $0,0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h,k,l=2n$
4	d	$\bar{4}$..	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$ $\frac{1}{4},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{3}{4},\frac{3}{4}$	hkl : $h+k,l=2n$
4	c	2.22	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},\frac{3}{4}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$	hkl : $h+k,l=2n$
4	b	222.	$\frac{3}{4},\frac{1}{4},0$ $\frac{1}{4},\frac{3}{4},\frac{1}{2}$ $\frac{1}{4},\frac{3}{4},0$ $\frac{3}{4},\frac{1}{4},\frac{1}{2}$	hkl : $h+k,l=2n$
4	a	222.	$\frac{1}{4},\frac{1}{4},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{2}$ $\frac{3}{4},\frac{3}{4},0$ $\frac{3}{4},\frac{3}{4},\frac{1}{2}$	hkl : $h+k,l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2bc$ (106)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/n11$ ($P4_2/n$, 86)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/b1$ ($Pban$, 50)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/nbc$ ($\mathbf{c}'=3\mathbf{c}$) (133); [9] $P4_2/nbc$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (133)

Minimal non-isomorphic supergroups

I none

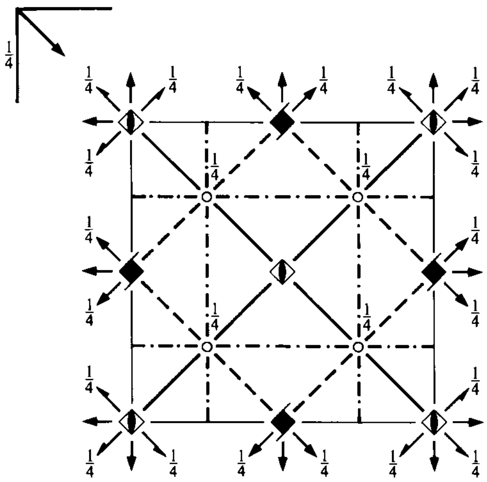
II [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mcm$ (140); [2] $P4/nbm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (125)

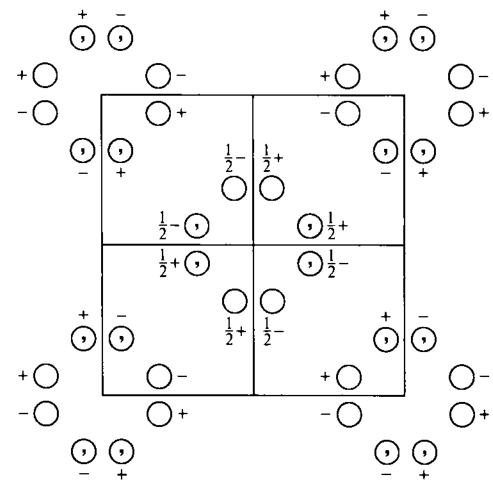
International Tables for Crystallography (2006). Vol. A, Space group 134, pp. 462–465.

$P4_2/nnm$ D_{4h}^{12} $4/mmm$ Tetragonal

No. 134 $P\ 4_2/n\ 2/n\ 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}2m$, at $-\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ from centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{4};\quad x \le y;\quad y \le 1-x$

Symmetry operations

(1) 1	(2) $2\ \ 0,0,z$	(3) $4^+(0,0,\frac{1}{2})\ \ 0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})\ \ \frac{1}{2},0,z$
(5) $2\ \ 0,y,0$	(6) $2\ \ x,0,0$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x,\frac{1}{4}$	(8) $2\ \ x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}\ \ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,\frac{1}{4}$	(11) $\bar{4}^+\ \ 0,0,z;\ \ 0,0,0$	(12) $\bar{4}^-\ \ 0,0,z;\ \ 0,0,0$
(13) $n(\frac{1}{2},0,\frac{1}{2})\ \ x,\frac{1}{4},z$	(14) $n(0,\frac{1}{2},\frac{1}{2})\ \ \frac{1}{4},y,z$	(15) $m\ \ x,\bar{x},z$	(16) $m\ \ x,x,z$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2nm$ (102)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/n11$ ($P4_2/n$, 86)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ ($Cmme$, 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/n1$ ($Pnnn$, 48)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $F4_1/ddc$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4_1/acd$, 142); [2] $F4_1/ddm$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4_1/amd$, 141)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/nnm$ ($\mathbf{c}'=3\mathbf{c}$) (134); [9] $P4_2/nnm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (134)

Minimal non-isomorphic supergroups

I [3] $Pn\bar{3}m$ (224)

II [2] $C4_2/mcm$ ($P4_2/mmc$, 131); [2] $I4/mmm$ (139); [2] $P4/nbm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (125)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	n	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$hk0: h+k=2n$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0kl: k+l=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	$00l: l=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z$	(16) y,x,z	$h00: h=2n$
							Special: as above, plus
8	m	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	no extra conditions
			$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	
8	l	$..2$	$x,x+\frac{1}{2},\frac{3}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\bar{x},x+\frac{1}{2},\frac{1}{4}$	$x,\bar{x}+\frac{1}{2},\frac{1}{4}$	$hkl: h+k=2n$
			$\bar{x}+\frac{1}{2},\bar{x},\frac{3}{4}$	$x+\frac{1}{2},x,\frac{3}{4}$	$x+\frac{1}{2},\bar{x},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x,\frac{1}{4}$	
8	k	$..2$	$x,x+\frac{1}{2},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\bar{x},x+\frac{1}{2},\frac{3}{4}$	$x,\bar{x}+\frac{1}{2},\frac{3}{4}$	$hkl: h+k=2n$
			$\bar{x}+\frac{1}{2},\bar{x},\frac{1}{4}$	$x+\frac{1}{2},x,\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x,\frac{3}{4}$	
8	j	$.2.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\frac{1}{2},x+\frac{1}{2},0$	$\frac{1}{2},\bar{x}+\frac{1}{2},0$	$hkl: h+k+l=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},0$	$0,\bar{x},\frac{1}{2}$	$0,x,\frac{1}{2}$	
8	i	$.2.$	$x,0,0$	$\bar{x},0,0$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$hkl: h+k+l=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\bar{x},0$	$0,x,0$	
8	h	$2..$	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$hkl: h+k,l=2n$
			$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z+\frac{1}{2}$	$\frac{1}{2},0,z$	
4	g	$2.mm$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$hkl: h+k+l=2n$
4	f	$..2/m$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$hkl: h+k,h+l,k+l=2n$
4	e	$..2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$hkl: h+k,h+l,k+l=2n$
4	d	2.22	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	$hkl: h+k,l=2n$
4	c	$222.$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},0,0$	$hkl: h+k,l=2n$
2	b	$\bar{4}2m$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			$hkl: h+k+l=2n$
2	a	$\bar{4}2m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$hkl: h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

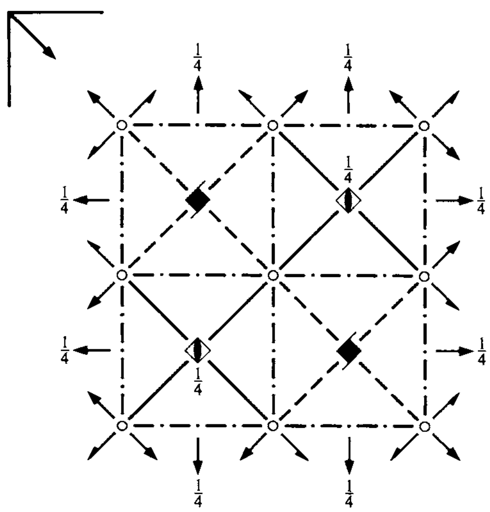
Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{1}{4}$

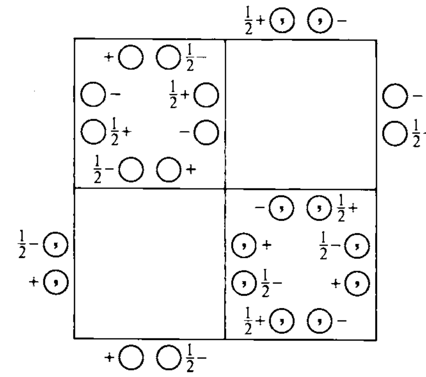
(*Continued on preceding page*)

$P4_2/nnm$ D_{4h}^{12} $4/mmm$ Tetragonal

No. 134 $P\ 4_2/n\ 2/n\ 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2





Origin at centre ($2/m$) at $nn(2_1/g,2/m)$, at $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ from $\bar{4}2m$

Asymmetric unit $-\frac{1}{4} \le x \le \frac{1}{4};\quad -\frac{1}{4} \le y \le \frac{1}{4};\quad 0 \le z \le \frac{1}{2};\quad x \le -y$

Symmetry operations

(1) 1	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})\quad \frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{2})\quad \frac{1}{4},\frac{1}{4},z$
(5) $2\quad \frac{1}{4},y,\frac{1}{4}$	(6) $2\quad x,\frac{1}{4},\frac{1}{4}$	(7) $2\quad x,x,0$	(8) $2\quad x,\bar{x}+\frac{1}{2},0$
(9) $\bar{1}\quad 0,0,0$	(10) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,0$	(11) $\bar{4}^+\quad \frac{1}{4},-\frac{1}{4},z;\quad \frac{1}{4},-\frac{1}{4},\frac{1}{4}$	(12) $\bar{4}^-\quad -\frac{1}{4},\frac{1}{4},z;\quad -\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(13) $n(\frac{1}{2},0,\frac{1}{2})\quad x,0,z$	(14) $n(0,\frac{1}{2},\frac{1}{2})\quad 0,y,z$	(15) $m\quad x,\bar{x},z$	(16) $g(\frac{1}{2},\frac{1}{2},0)\quad x,x,z$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2nm$ (102)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/n11$ ($P4_2/n$, 86)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ ($Cmme$, 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/n1$ ($Pnnn$, 48)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $F4_1/ddc$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4_1/acd$, 142); [2] $F4_1/ddm$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4_1/amd$, 141)

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/nnm$ ($\mathbf{c}'=3\mathbf{c}$) (134); [9] $P4_2/nnm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (134)

Minimal non-isomorphic supergroups

I [3] $Pn\bar{3}m$ (224)

II [2] $C4_2/mcm$ ($P4_2/mmc$, 131); [2] $I4/mmm$ (139); [2] $P4/nbm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (125)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	n	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$ (9) $\bar{x},\bar{y},\bar{z}$ (13) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (14) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y}+\frac{1}{2},x,z+\frac{1}{2}$ (7) $y,x,\bar{z}$ (11) $y+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$ (15) $\bar{y},\bar{x},z$	(4) $y,\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$ (12) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (16) $y+\frac{1}{2},x+\frac{1}{2},z$	$hk0: h+k=2n$ $0kl: k+l=2n$ $00l: l=2n$ $h00: h=2n$
							Special: as above, plus
8	m	$..m$	$x,\bar{x},z$ $\bar{x}+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},z$ $x,x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$x+\frac{1}{2},x,z+\frac{1}{2}$ $\bar{x},x,\bar{z}$	$\bar{x},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	no extra conditions
8	l	$..2$	$x,x,\frac{1}{2}$ $\bar{x},\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,0$ $x+\frac{1}{2},\bar{x},0$	$x,\bar{x}+\frac{1}{2},0$ $\bar{x},x+\frac{1}{2},0$	$hkl: h+k=2n$
8	k	$..2$	$x,x,0$ $\bar{x},\bar{x},0$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},0$ $x+\frac{1}{2},x+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,\frac{1}{2}$ $x+\frac{1}{2},\bar{x},\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x},x+\frac{1}{2},\frac{1}{2}$	$hkl: h+k=2n$
8	j	$.2.$	$x,\frac{1}{4},\frac{1}{4}$ $\bar{x},\frac{3}{4},\frac{3}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{4}$ $x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},x,\frac{3}{4}$ $\frac{3}{4},\bar{x},\frac{1}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{3}{4}$ $\frac{3}{4},x+\frac{1}{2},\frac{1}{4}$	$hkl: h+k+l=2n$
8	i	$.2.$	$x,\frac{1}{4},\frac{3}{4}$ $\bar{x},\frac{3}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{3}{4}$ $x+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$ $\frac{3}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$ $\frac{3}{4},x+\frac{1}{2},\frac{3}{4}$	$hkl: h+k+l=2n$
8	h	$2..$	$\frac{1}{4},\frac{1}{4},z$ $\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$ $\frac{3}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	$\frac{1}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$ $\frac{3}{4},\frac{3}{4},z+\frac{1}{2}$	$\frac{1}{4},\frac{1}{4},\bar{z}$ $\frac{3}{4},\frac{3}{4},z$	$hkl: h+k,l=2n$
4	g	$2.mm$	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$hkl: h+k+l=2n$
4	f	$..2/m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$hkl: h+k,h+l,k+l=2n$
4	e	$..2/m$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$hkl: h+k,h+l,k+l=2n$
4	d	2.22	$\frac{1}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$hkl: h+k,l=2n$
4	c	$222.$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$hkl: h+k,l=2n$
2	b	$\bar{4}2m$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$			$hkl: h+k+l=2n$
2	a	$\bar{4}2m$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$			$hkl: h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

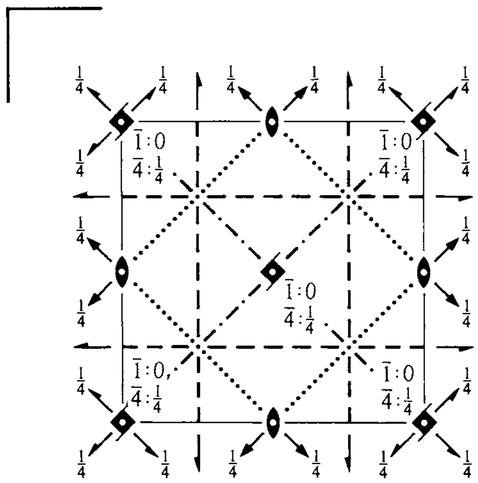
Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

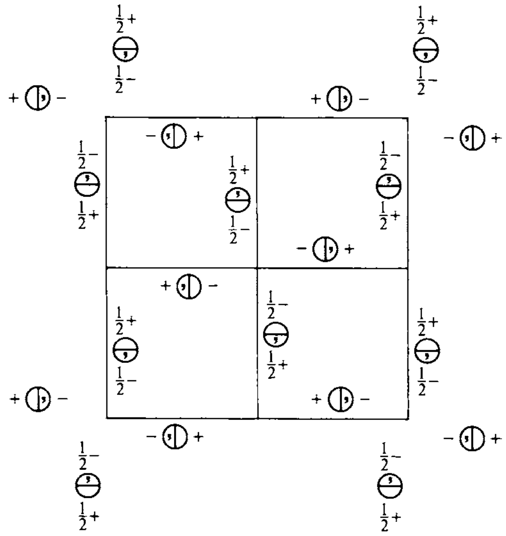
(*Continued on preceding page*)

International Tables for Crystallography (2006). Vol. A, Space group 135, pp. 466–467.

$P4_2/mbc$ $\quad D_{4h}^{13}$ $\quad 4/mmm$ $\quad$ Tetragonal

No. 135 $\quad P\ 4_2/m\ 2_1/b\ 2/c$ $\quad$ Patterson symmetry $P4/mmm$





Origin at centre $(2/m)$ at $4_2/m\,1\,n$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^{+}(0,0,\frac{1}{2})\quad 0,0,z$	(4) $4^{-}(0,0,\frac{1}{2})\quad 0,0,z$
(5) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$	(7) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x,\frac{1}{4}$	(8) $2\quad x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}\quad 0,0,0$	(10) $m\quad x,y,0$	(11) $\bar{4}^{+}\quad 0,0,z;\ \ 0,0,\frac{1}{4}$	(12) $\bar{4}^{-}\quad 0,0,z;\ \ 0,0,\frac{1}{4}$
(13) $a\quad x,\frac{1}{4},z$	(14) $b\quad \frac{1}{4},y,z$	(15) $c\quad x+\frac{1}{2},\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	i	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (9) $\bar{x},\bar{y},\bar{z}$ (13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (10) $x,y,\bar{z}$ (14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(3) $\bar{y},x,z+\frac{1}{2}$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (11) $y,\bar{x},\bar{z}+\frac{1}{2}$ (15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$ (8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (12) $\bar{y},x,\bar{z}+\frac{1}{2}$ (16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k=2n$ hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
8	h	$m\,.\,.$	$x,y,0$ $\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$\bar{x},\bar{y},0$ $x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	$\bar{y},x,\frac{1}{2}$ $y+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$ $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	no extra conditions
8	g	$.\,.\,2$	$x,x+\frac{1}{2},\frac{1}{4}$ $\bar{x},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$ $x,x+\frac{1}{2},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x,\frac{3}{4}$ $x+\frac{1}{2},\bar{x},\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$ $\bar{x}+\frac{1}{2},x,\frac{1}{4}$	hkl : $l=2n$
8	f	$2\,.\,.$	$0,\frac{1}{2},z$ $0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z+\frac{1}{2}$ $\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$ $\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$ $0,\frac{1}{2},z+\frac{1}{2}$	hkl : $h+k,l=2n$
8	e	$2\,.\,.$	$0,0,z$ $0,0,\bar{z}$	$0,0,z+\frac{1}{2}$ $0,0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$ $\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl : $h+k,l=2n$
4	d	$2\,.\,22$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	hkl : $h+k,l=2n$
4	c	$2/m\,.\,.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	hkl : $h+k,l=2n$
4	b	$\bar{4}\,.\,.$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	hkl : $h+k,l=2n$
4	a	$2/m\,.\,.$	$0,0,0$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+k,l=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I
[2] $P\bar{4}b2$ (117) 1; 2; 7; 8; 11; 12; 13; 14
[2] $P\bar{4}2_1c$ (114) 1; 2; 5; 6; 11; 12; 15; 16
[2] $P4_2bc$ (106) 1; 2; 3; 4; 13; 14; 15; 16
[2] $P4_22_12$ (94) 1; 2; 3; 4; 5; 6; 7; 8
[2] $P4_2/m11$ ($P4_2/m$, 84) 1; 2; 3; 4; 9; 10; 11; 12
[2] $P2/m12/c$ ($Cccm$, 66) 1; 2; 7; 8; 9; 10; 15; 16
[2] $P2/m2_1/b1$ ($Pbam$, 55) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/mbc$ ($\mathbf{c}'=3\mathbf{c}$) (135); [9] $P4_2/mbc$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (135)

Minimal non-isomorphic supergroups

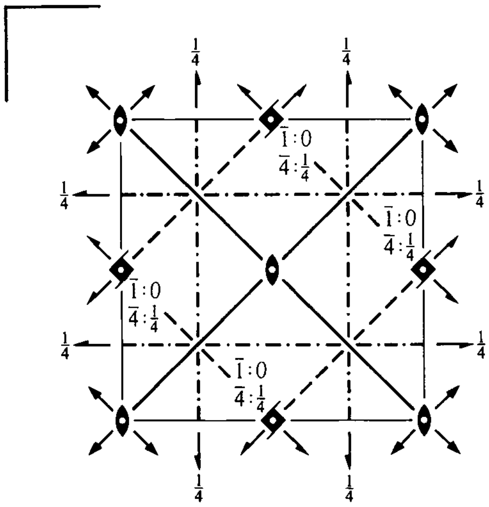
I none

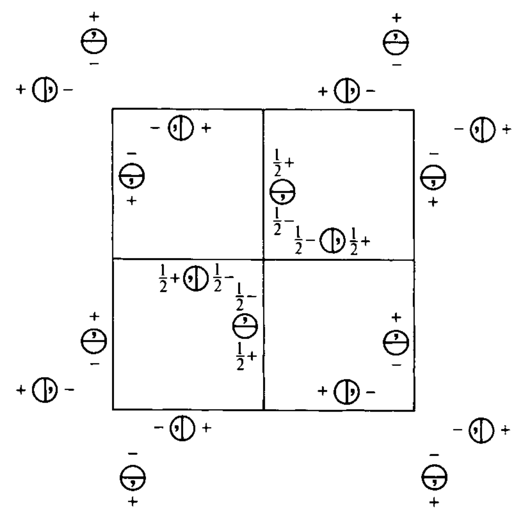
II [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mcm$ (140); [2] $P4/mbm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (127)

International Tables for Crystallography (2006). Vol. A, Space group 136, pp. 468–469.

$P4_2/mnm$ $\quad D_{4h}^{14}$ $\quad 4/mmm$ $\quad$ Tetragonal

No. 136 $\quad P\ 4_2/m\ 2_1/n\ 2/m$ $\quad$ Patterson symmetry $P4/mmm$





Origin at centre (mmm) at $2/m12/m$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}; \quad x \le y$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^+(0,0,\frac{1}{2})\quad 0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})\quad \frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{1}{4}$	(7) $2\quad x,x,0$	(8) $2\quad x,\bar{x},0$
(9) $\bar{1}\quad 0,0,0$	(10) $m\quad x,y,0$	(11) $\bar{4}^+\quad \frac{1}{2},0,z;\quad \frac{1}{2},0,\frac{1}{4}$	(12) $\bar{4}^-\quad 0,\frac{1}{2},z;\quad 0,\frac{1}{2},\frac{1}{4}$
(13) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(14) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$	(15) $m\quad x,\bar{x},z$	(16) $m\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	$00l$: $l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$h00$: $h=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z$	(16) y,x,z	
							Special: as above, plus
8	j	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
8	i	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$y,x,0$	$\bar{y},\bar{x},0$	
8	h	$2..$	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	hkl : $h+k,l=2n$
			$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	$\frac{1}{2},0,z$	
4	g	$m.2m$	$x,\bar{x},0$	$\bar{x},x,0$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	no extra conditions
4	f	$m.2m$	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	no extra conditions
4	e	$2.mm$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	hkl : $h+k+l=2n$
4	d	$\bar{4}..$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	hkl : $h+k,l=2n$
4	c	$2/m..$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},0,0$	hkl : $h+k,l=2n$
2	b	$m.mm$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k+l=2n$
2	a	$m.mm$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,\frac{1}{2},z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2nm$ (102)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22_12$ (94)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/m11$ ($P4_2/m$, 84)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/m12/m$ ($Cmmm$, 65)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/m2_1/n1$ ($Pnnm$, 58)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/mnm$ ($\mathbf{c}'=3\mathbf{c}$) (136); [9] $P4_2/mnm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (136)

Minimal non-isomorphic supergroups

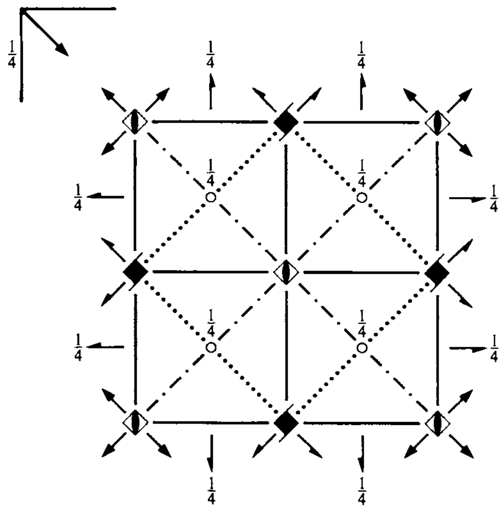
I none

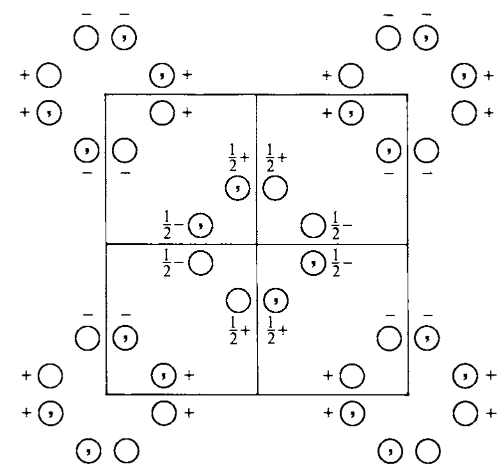
II [2] $C4_2/mcm$ ($P4_2/mmc$, 131); [2] $I4/mmm$ (139); [2] $P4/mbm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (127)

$P4_2/nmc$ $\quad D_{4h}^{15}$ $\quad 4/mmm$ $\quad$ Tetragonal

No. 137 $\quad P\ 4_2/n\ 2_1/m\ 2/c$ $\quad$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}m2/n$, at $-\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^+(0,0,\frac{1}{2})\quad 0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})\quad \frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{1}{4}$	(7) $2\quad x,x,0$	(8) $2\quad x,\bar{x},0$
(9) $\bar{1}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,\frac{1}{4}$	(11) $\bar{4}^+\quad 0,0,z;\ \ 0,0,0$	(12) $\bar{4}^-\quad 0,0,z;\ \ 0,0,0$
(13) $m\quad x,0,z$	(14) $m\quad 0,y,z$	(15) $c\quad x+\frac{1}{2},\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	h	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (13) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (14) $\bar{x},y,z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ (7) $y,x,\bar{z}$ (11) $y,\bar{x},\bar{z}$ (15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (8) $\bar{y},\bar{x},\bar{z}$ (12) $\bar{y},x,\bar{z}$ (16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h+k=2n$ hhl: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
8	g	$.m.$	$0,y,z$ $\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\bar{y},z$ $\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$\bar{y}+\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$ $y,0,\bar{z}$	$y+\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$ $\bar{y},0,\bar{z}$	no extra conditions
8	f	$..2$	$x,x,0$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{x},0$ $x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $x,\bar{x},0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x},x,0$	hkl: $h+k+l=2n$
8	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$ $\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$	hkl: $h,k,l=2n$
4	d	$2mm.$	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	hkl: $l=2n$
4	c	$2mm.$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	hkl: $h+k+l=2n$
2	b	$\bar{4}m2$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	a	$\bar{4}m2$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2mc$ (105)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22_12$ (94)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/n11$ ($P4_2/n$, 86)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2_1/m1$ ($Pmmn$, 59)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/nmc$ ($\mathbf{c}'=3\mathbf{c}$) (137); [9] $P4_2/nmc$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (137)

Minimal non-isomorphic supergroups

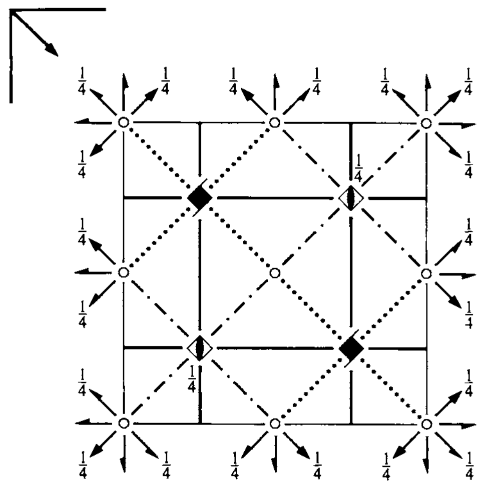
I none

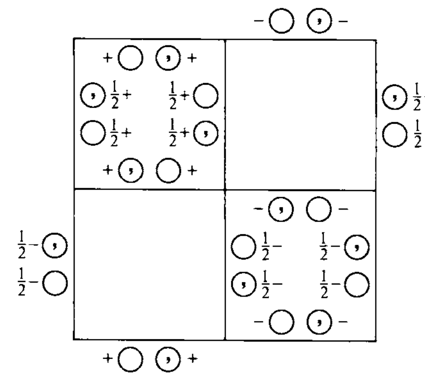
II [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mmm$ (139); [2] $P4/nmm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (129)

$P4_2/nmc$ $\quad D_{4h}^{15}$ $\quad 4/mmm$ $\quad$ Tetragonal

No. 137 $\quad P\ 4_2/n\ 2_1/m\ 2/c$ $\quad$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2





Origin at $\bar{1}$ at $n2_1(c,n)$, at $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ from $\bar{4}m2$

Asymmetric unit $\quad -\frac{1}{4} \le x \le \frac{1}{4};\quad -\frac{1}{4} \le y \le \frac{1}{4};\quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\ \ \frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$
(5) $2(0,\frac{1}{2},0)\ \ 0,y,0$	(6) $2(\frac{1}{2},0,0)\ \ x,0,0$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x,\frac{1}{4}$	(8) $2\ \ x,\bar{x},\frac{1}{4}$
(9) $\bar{1}\ \ 0,0,0$	(10) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$	(11) $\bar{4}^+\ \ \frac{1}{4},-\frac{1}{4},z;\ \ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$	(12) $\bar{4}^-\ \ -\frac{1}{4},\frac{1}{4},z;\ \ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(13) $m\ \ x,\frac{1}{4},z$	(14) $m\ \ \frac{1}{4},y,z$	(15) $c\ \ x+\frac{1}{2},\bar{x},z$	(16) $c\ \ x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	h	1	(1) x,y,z (5) $\bar{x},y+\frac{1}{2},\bar{z}$ (9) $\bar{x},\bar{y},\bar{z}$ (13) $x,\bar{y}+\frac{1}{2},z$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},\bar{y},\bar{z}$ (10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (14) $\bar{x}+\frac{1}{2},y,z$	(3) $\bar{y}+\frac{1}{2},x,z+\frac{1}{2}$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (11) $y+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$ (15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(4) $y,\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$ (12) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (16) $y,x,z+\frac{1}{2}$	$hk0:\ h+k=2n$ $hhl:\ l=2n$ $00l:\ l=2n$ $h00:\ h=2n$
							Special: as above, plus
8	g	$.m.$	$\frac{1}{4},y,z$ $\frac{3}{4},y+\frac{1}{2},\bar{z}$	$\frac{1}{4},\bar{y}+\frac{1}{2},z$ $\frac{3}{4},\bar{y},\bar{z}$	$\bar{y}+\frac{1}{2},\frac{1}{4},z+\frac{1}{2}$ $y+\frac{1}{2},\frac{3}{4},\bar{z}+\frac{1}{2}$	$y,\frac{1}{4},z+\frac{1}{2}$ $\bar{y},\frac{3}{4},\bar{z}+\frac{1}{2}$	no extra conditions
8	f	$..2$	$x,\bar{x},\frac{1}{4}$ $\bar{x},x,\frac{3}{4}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},x,\frac{3}{4}$ $\bar{x}+\frac{1}{2},\bar{x},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{3}{4}$ $x,x+\frac{1}{2},\frac{1}{4}$	$hkl:\ h+k+l=2n$
8	e	$\bar{1}$	$0,0,0$ $\quad \frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$ $\quad 0,\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$ $\quad \frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\quad 0,0,\frac{1}{2}$	$hkl:\ h,k,l=2n$
4	d	$2mm.$	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	$hkl:\ l=2n$
4	c	$2mm.$	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$hkl:\ h+k+l=2n$
2	b	$\bar{4}m2$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$			$hkl:\ h+k+l=2n$
2	a	$\bar{4}m2$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$			$hkl:\ h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\quad \mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\quad \mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad \mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}m2$ (115) 1; 2; 7; 8; 11; 12; 13; 14
[2] $P\bar{4}2_1c$ (114) 1; 2; 5; 6; 11; 12; 15; 16
[2] $P4_2mc$ (105) 1; 2; 3; 4; 13; 14; 15; 16
[2] $P4_22_12$ (94) 1; 2; 3; 4; 5; 6; 7; 8
[2] $P4_2/n11$ ($P4_2/n$, 86) 1; 2; 3; 4; 9; 10; 11; 12
[2] $P2/n12/c$ ($Ccce$, 68) 1; 2; 7; 8; 9; 10; 15; 16
[2] $P2/n2_1/m1$ ($Pmmn$, 59) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/nmc$ ($\mathbf{c}'=3\mathbf{c}$) (137); [9] $P4_2/nmc$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (137)

Minimal non-isomorphic supergroups

I none

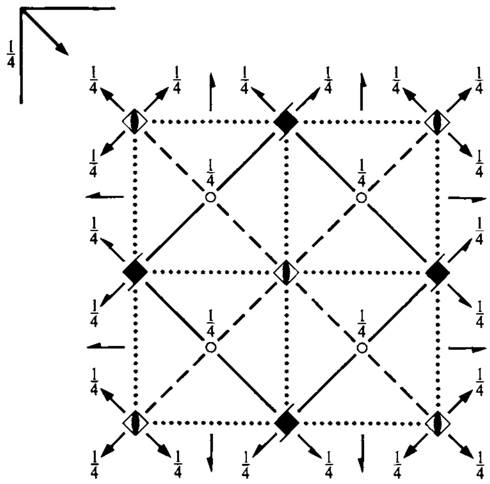
II [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mmm$ (139); [2] $P4/nmm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (129)

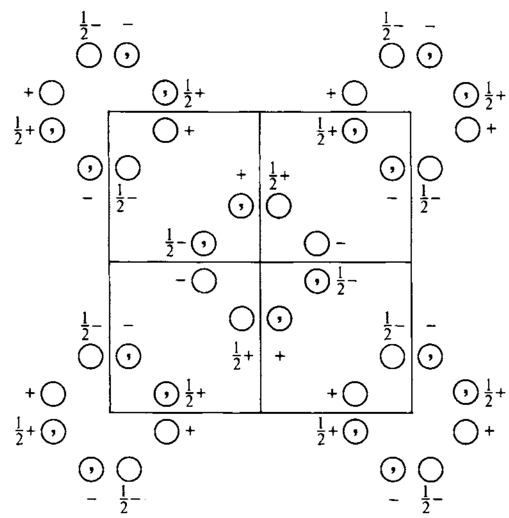
International Tables for Crystallography (2006). Vol. A, Space group 138, pp. 474–477.

$P4_2/ncm$ D_{4h}^{16} $4/mmm$ Tetragonal

No. 138 $P\ 4_2/n\ 2_1/c\ 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}cg$, at $-\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ from centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{4};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le 1;\quad x \le y;\quad y \le \frac{1}{2}-x$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^+(0,0,\frac{1}{2})\quad 0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})\quad \frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$	(7) $2\quad x,x,\frac{1}{4}$	(8) $2\quad x,\bar{x},\frac{1}{4}$
(9) $\bar{1}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,\frac{1}{4}$	(11) $\bar{4}^+\quad 0,0,z;\ 0,0,0$	(12) $\bar{4}^-\quad 0,0,z;\ 0,0,0$
(13) $c\quad x,0,z$	(14) $c\quad 0,y,z$	(15) $m\quad x+\frac{1}{2},\bar{x},z$	(16) $g(\frac{1}{2},\frac{1}{2},0)\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h+k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$0kl$: $l=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	$00l$: $l=2n$
			(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	$h00$: $h=2n$
							Special: as above, plus
8	i	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x},x+\frac{1}{2},z+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},z+\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{2},x,\bar{z}$	$x+\frac{1}{2},\bar{x},\bar{z}$	$x+\frac{1}{2},x,\bar{z}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	
8	h	$..2$	$x,x,\frac{3}{4}$	$\bar{x},\bar{x},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{4}$	hkl : $h+k=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{3}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{1}{4}$	
8	g	$..2$	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$	hkl : $h+k=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$	$x,\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	
8	f	$2..$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	hkl : $h+k,l=2n$
			$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z$	
4	e	$2.mm$	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	hkl : $l=2n$
4	d	$..2/m$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	hkl : $h+k,h+l,k+l=2n$
4	c	$..2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	hkl : $h+k,h+l,k+l=2n$
4	b	$\bar{4}..$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,0,\frac{1}{2}$	hkl : $h+k,l=2n$
4	a	2.22	$0,0,\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$0,0,\frac{3}{4}$	hkl : $h+k,l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{1}{4}$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2cm$ (101)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22_12$ (94)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/n11$ ($P4_2/n$, 86)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ ($Cmme$, 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2_1/c1$ ($Pccn$, 56)	1; 2; 5; 6; 9; 10; 13; 14
IIa	none	
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/ncm$ ($\mathbf{c}'=3\mathbf{c}$) (138); [9] $P4_2/ncm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (138)

Minimal non-isomorphic supergroups

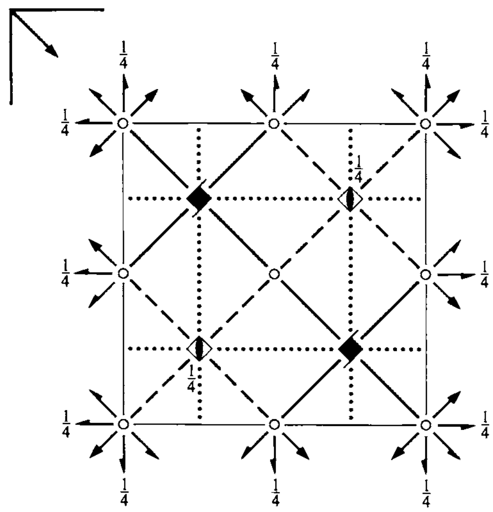
I none

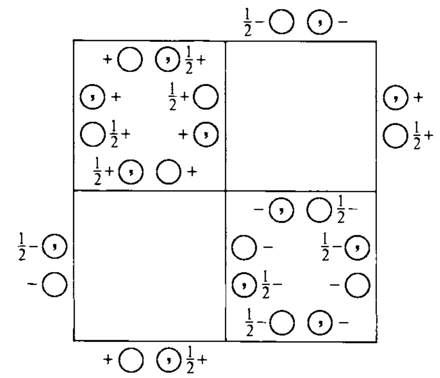
II [2] $C4_2/mcm$ ($P4_2/mmc$, 131); [2] $I4/mcm$ (140); [2] $P4/nmm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (129)

$P4_2/ncm$ $\quad D_{4h}^{16}$ $\quad 4/mmm$ $\quad$ Tetragonal

No. 138 $\quad P\ 4_2/n\ 2_1/c\ 2/m$ $\quad$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2





Origin at centre $(2/m)$ at $n\,1\,(2/m, 2_1/g)$, at $\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ from $\bar{4}$

Asymmetric unit $\quad -\frac{1}{4} \le x \le \frac{1}{4}; \quad -\frac{1}{4} \le y \le \frac{1}{4}; \quad 0 \le z \le \frac{1}{2}; \quad x \le y$

Symmetry operations

(1) 1	(2) $2\ \ \frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$
(5) $2(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\ \ x,0,\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x,0$	(8) $2\ \ x,\bar{x},0$
(9) $\bar{1}\ \ 0,0,0$	(10) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$	(11) $\bar{4}^+\ \ \frac{1}{4},-\frac{1}{4},z;\ \ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$	(12) $\bar{4}^-\ \ -\frac{1}{4},\frac{1}{4},z;\ \ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(13) $c\ \ x,\frac{1}{4},z$	(14) $c\ \ \frac{1}{4},y,z$	(15) $m\ \ x+\frac{1}{2},\bar{x},z$	(16) $m\ \ x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	j	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z+\frac{1}{2}$	(4) $y,\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h+k=2n$
			(5) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	$0kl$: $l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$00l$: $l=2n$
			(13) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) y,x,z	$h00$: $h=2n$
							Special: as above, plus
8	i	$..m$	x,x,z	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},z+\frac{1}{2}$	no extra conditions
			$\bar{x},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
8	h	$..2$	$x,\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},x,\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{2}$	hkl : $h+k=2n$
			$\bar{x},x,0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},\bar{x},\frac{1}{2}$	$x,x+\frac{1}{2},\frac{1}{2}$	
8	g	$..2$	$x,\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},x,0$	$\bar{x},\bar{x}+\frac{1}{2},0$	hkl : $h+k=2n$
			$\bar{x},x,\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x},0$	$x,x+\frac{1}{2},0$	
8	f	$2..$	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	hkl : $h+k,l=2n$
			$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},z+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},z$	
4	e	$2.mm$	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	hkl : $l=2n$
4	d	$..2/m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl : $h+k,h+l,k+l=2n$
4	c	$..2/m$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hkl : $h+k,h+l,k+l=2n$
4	b	$\bar{4}..$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	hkl : $h+k,l=2n$
4	a	2.22	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	hkl : $h+k,l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I
[2] $P\bar{4}c2$ (116) 1; 2; 7; 8; 11; 12; 13; 14
[2] $P\bar{4}2_1m$ (113) 1; 2; 5; 6; 11; 12; 15; 16
[2] $P4_2cm$ (101) 1; 2; 3; 4; 13; 14; 15; 16
[2] $P4_22_12$ (94) 1; 2; 3; 4; 5; 6; 7; 8
[2] $P4_2/n11$ ($P4_2/n$, 86) 1; 2; 3; 4; 9; 10; 11; 12
[2] $P2/n12/m$ ($Cmme$, 67) 1; 2; 7; 8; 9; 10; 15; 16
[2] $P2/n2_1/c1$ ($Pccn$, 56) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/ncm$ ($\mathbf{c}'=3\mathbf{c}$) (138); [9] $P4_2/ncm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (138)

Minimal non-isomorphic supergroups

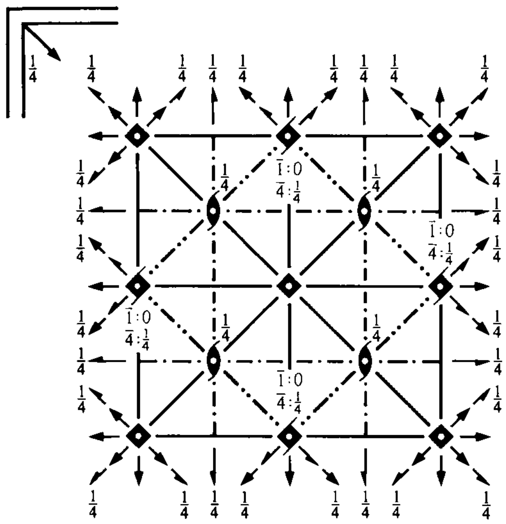
I none

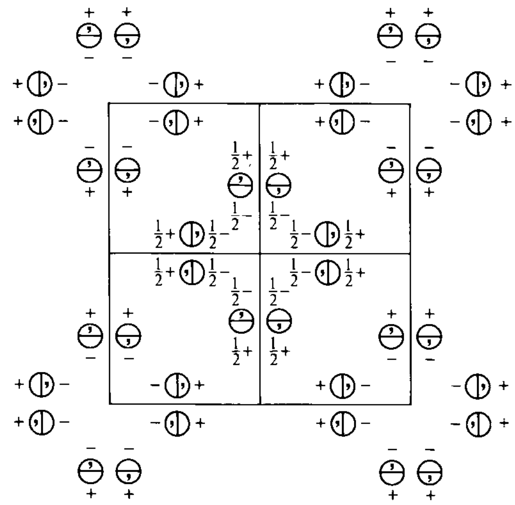
II [2] $C4_2/mcm$ ($P4_2/mmc$, 131); [2] $I4/mcm$ (140); [2] $P4/nmm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (129)

International Tables for Crystallography (2006). Vol. A, Space group 139, pp. 478–479.

$I4/mmm$ $\quad D_{4h}^{17}$ $\quad 4/mmm$ $\quad$ Tetragonal

No. 139 $\quad I\ 4/m\ 2/m\ 2/m$ $\quad$ Patterson symmetry $I4/mmm$





Origin at centre ($4/mmm$)

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{4};\quad x \le y$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $4^+\quad 0,0,z$	(4) $4^-\quad 0,0,z$
(5) $2\quad 0,y,0$	(6) $2\quad x,0,0$	(7) $2\quad x,x,0$	(8) $2\quad x,\bar{x},0$
(9) $\bar{1}\quad 0,0,0$	(10) $m\quad x,y,0$	(11) $\bar{4}^+\quad 0,0,z;\ 0,0,0$	(12) $\bar{4}^-\quad 0,0,z;\ 0,0,0$
(13) $m\quad x,0,z$	(14) $m\quad 0,y,z$	(15) $m\quad x,\bar{x},z$	(16) $m\quad x,x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})\quad 0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})\quad \frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x,\frac{1}{4}$	(8) $2\quad x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,\frac{1}{4}$	(11) $\bar{4}^+\quad \frac{1}{2},0,z;\ \frac{1}{2},0,\frac{1}{4}$	(12) $\bar{4}^-\quad 0,\frac{1}{2},z;\ 0,\frac{1}{2},\frac{1}{4}$
(13) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(14) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$	(15) $c\quad x+\frac{1}{2},\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,z$

Maximal non-isomorphic subgroups *(continued)*

IIa	[2] $P4_2/nmc$ (137)	1; 2; 7; 8; 11; 12; 13; 14; (3; 4; 5; 6; 9; 10; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4_2/mnm$ (136)	1; 2; 7; 8; 9; 10; 15; 16; (3; 4; 5; 6; 11; 12; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4_2/nnm$ (134)	1; 2; 5; 6; 11; 12; 15; 16; (3; 4; 7; 8; 9; 10; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4_2/mmc$ (131)	1; 2; 5; 6; 9; 10; 13; 14; (3; 4; 7; 8; 11; 12; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4/nmm$ (129)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 9; 10; 11; 12) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4/mnc$ (128)	1; 2; 3; 4; 9; 10; 11; 12; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4/nnc$ (126)	1; 2; 3; 4; 5; 6; 7; 8; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4/mmm$ (123)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc $\quad$ [3] $I4/mmm$ ($\mathbf{c}' = 3\mathbf{c}$) (139); [9] $I4/mmm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (139)

Minimal non-isomorphic supergroups

I $\quad$ [3] $Fm\bar{3}m$ (225); [3] $Im\bar{3}m$ (229)

II $\quad$ [2] $C4/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P4/mmm$, 123)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
32	o	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	hkl : $h+k+l=2n$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	$hk0$: $h+k=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	$0kl$: $k+l=2n$
			(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y},\bar{x},z$	(16) y,x,z	hhl : $l=2n$
							$00l$: $l=2n$
							$h00$: $h=2n$
							Special: as above, plus
16	n	$.m.$	$0,y,z$	$0,\bar{y},z$	$\bar{y},0,z$	$y,0,z$	no extra conditions
			$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$y,0,\bar{z}$	$\bar{y},0,\bar{z}$	
16	m	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
			$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
16	l	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
			$\bar{x},y,0$	$x,\bar{y},0$	$y,x,0$	$\bar{y},\bar{x},0$	
16	k	$..2$	$x,x+\frac{1}{2},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x,\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{1}{4}$	hkl : $l=2n$
			$\bar{x},\bar{x}+\frac{1}{2},\frac{3}{4}$	$x,x+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x,\frac{3}{4}$	
8	j	$m2m.$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	no extra conditions
8	i	$m2m.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	no extra conditions
8	h	$m.2m$	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	no extra conditions
8	g	$2mm.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hkl : $l=2n$
8	f	$..2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	hkl : $k,l=2n$
4	e	$4mm$	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	d	$\bar{4}m2$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$			hkl : $l=2n$
4	c	$mmm.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $l=2n$
2	b	$4/mmm$	$0,0,\frac{1}{2}$				no extra conditions
2	a	$4/mmm$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

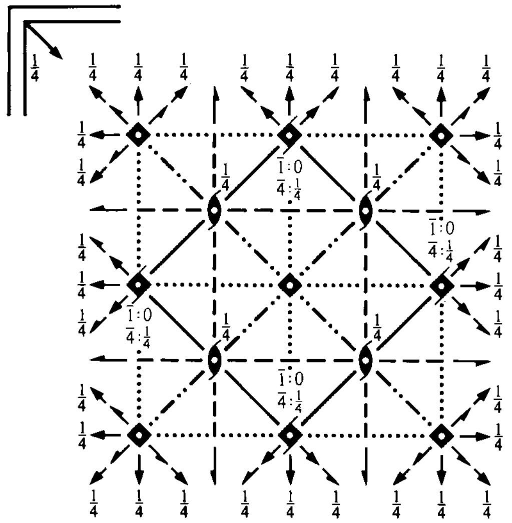
I	[2] $I\bar{4}2m$ (121)	(1; 2; 5; 6; 11; 12; 15; 16)+
	[2] $I\bar{4}m2$ (119)	(1; 2; 7; 8; 11; 12; 13; 14)+
	[2] $I4mm$ (107)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[2] $I422$ (97)	(1; 2; 3; 4; 5; 6; 7; 8)+
	[2] $I4/m11$ ($I4/m$, 87)	(1; 2; 3; 4; 9; 10; 11; 12)+
	[2] $I2/m2/m1$ ($Immm$, 71)	(1; 2; 5; 6; 9; 10; 13; 14)+
	[2] $I2/m12/m$ ($Fmmm$, 69)	(1; 2; 7; 8; 9; 10; 15; 16)+

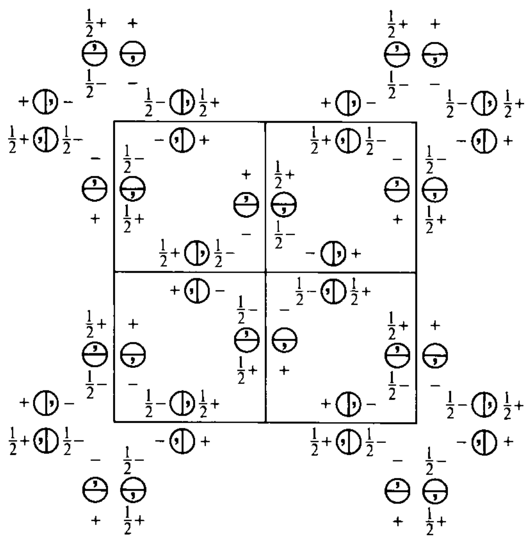
(*Continued on preceding page*)

International Tables for Crystallography (2006). Vol. A, Space group 140, pp. 480–481.

$I4/mcm$ D_{4h}^{18} $4/mmm$ Tetragonal

No. 140 $I\ 4/m\ 2/c\ 2/m$ Patterson symmetry $I4/mmm$





Origin at centre $(4/m)$ at $4/mc2_1/e$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$; $y \le \frac{1}{2} - x$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\ \ 0,0,z$	(3) $4^+\ \ 0,0,z$	(4) $4^-\ \ 0,0,z$
(5) $2\ \ 0,y,\frac{1}{4}$	(6) $2\ \ x,0,\frac{1}{4}$	(7) $2\ \ x,x,\frac{1}{4}$	(8) $2\ \ x,\bar{x},\frac{1}{4}$
(9) $\bar{1}\ \ 0,0,0$	(10) $m\ \ x,y,0$	(11) $\bar{4}^+\ \ 0,0,z;\ 0,0,0$	(12) $\bar{4}^-\ \ 0,0,z;\ 0,0,0$
(13) $c\ \ x,0,z$	(14) $c\ \ 0,y,z$	(15) $c\ \ x,\bar{x},z$	(16) $c\ \ x,x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})\ \ 0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})\ \ \frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)\ \ \frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},0$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x,0$	(8) $2\ \ x,\bar{x}+\frac{1}{2},0$
(9) $\bar{1}\ \ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,\frac{1}{4}$	(11) $\bar{4}^+\ \ \frac{1}{2},0,z;\ \frac{1}{2},0,\frac{1}{4}$	(12) $\bar{4}^-\ \ 0,\frac{1}{2},z;\ 0,\frac{1}{2},\frac{1}{4}$
(13) $a\ \ x,\frac{1}{4},z$	(14) $b\ \ \frac{1}{4},y,z$	(15) $m\ \ x+\frac{1}{2},\bar{x},z$	(16) $g(\frac{1}{2},\frac{1}{2},0)\ \ x,x,z$

Maximal non-isomorphic subgroups *(continued)*

IIa	[2] $P4_2/ncm$ (138)	1; 2; 7; 8; 11; 12; 13; 14; (3; 4; 5; 6; 9; 10; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4_2/mbc$ (135)	1; 2; 7; 8; 9; 10; 15; 16; (3; 4; 5; 6; 11; 12; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4_2/nbc$ (133)	1; 2; 5; 6; 11; 12; 15; 16; (3; 4; 7; 8; 9; 10; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4_2/mcm$ (132)	1; 2; 5; 6; 9; 10; 13; 14; (3; 4; 7; 8; 11; 12; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4/ncc$ (130)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 9; 10; 11; 12) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4/mbm$ (127)	1; 2; 3; 4; 9; 10; 11; 12; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4/nbm$ (125)	1; 2; 3; 4; 5; 6; 7; 8; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4/mcc$ (124)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $I4/mcm$ ($\mathbf{c}' = 3\mathbf{c}$) (140); [9] $I4/mcm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (140)

Minimal non-isomorphic supergroups

I [3] $Fm\bar{3}c$ (226)

II [2] $C4/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P4/mmm$, 123)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
32	m	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	hkl : $h+k+l=2n$
			(5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$hk0$: $h+k=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	$0kl$: $k,l=2n$
			(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$	hhl : $l=2n$
							$00l$: $l=2n$
							$h00$: $h=2n$
							Special: as above, plus
16	l	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	no extra conditions
			$\bar{x},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$x+\frac{1}{2},x,\bar{z}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	
16	k	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
			$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	$y,x,\frac{1}{2}$	$\bar{y},\bar{x},\frac{1}{2}$	
16	j	$.2.$	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$0,x,\frac{1}{4}$	$0,\bar{x},\frac{1}{4}$	hkl : $l=2n$
			$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	$0,\bar{x},\frac{3}{4}$	$0,x,\frac{3}{4}$	
16	i	$..2$	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{1}{4}$	$x,\bar{x},\frac{1}{4}$	hkl : $l=2n$
			$\bar{x},\bar{x},\frac{3}{4}$	$x,x,\frac{3}{4}$	$x,\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	
8	h	$m.2m$	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x+\frac{1}{2},\bar{x},0$	no extra conditions
8	g	$2.mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	hkl : $l=2n$
8	f	$4..$	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl : $l=2n$
8	e	$..2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	hkl : $k,l=2n$
4	d	$m.mm$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $l=2n$
4	c	$4/m..$	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$
4	b	$\bar{4}2m$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$			hkl : $l=2n$
4	a	422	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}2m$ (121)	(1; 2; 5; 6; 11; 12; 15; 16)+
	[2] $I\bar{4}c2$ (120)	(1; 2; 7; 8; 11; 12; 13; 14)+
	[2] $I4cm$ (108)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[2] $I422$ (97)	(1; 2; 3; 4; 5; 6; 7; 8)+
	[2] $I4/m11$ ($I4/m$, 87)	(1; 2; 3; 4; 9; 10; 11; 12)+
	[2] $I2/m2/c1$ ($Ibam$, 72)	(1; 2; 5; 6; 9; 10; 13; 14)+
	[2] $I2/m12/m$ ($Fmmm$, 69)	(1; 2; 7; 8; 9; 10; 15; 16)+

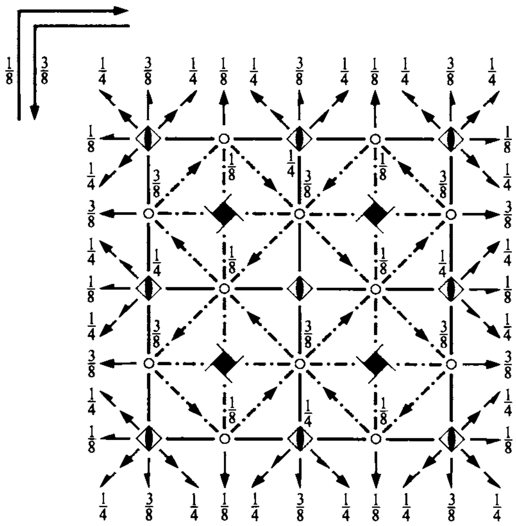
(*Continued on preceding page*)

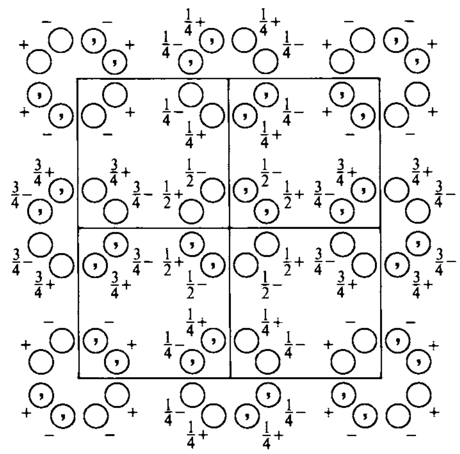
International Tables for Crystallography (2006). Vol. A, Space group 141, pp. 482–485.

$I4_1/amd$ D_{4h}^{19} $4/mmm$ Tetragonal

No. 141 $I\ 4_1/a\ 2/m\ 2/d$ Patterson symmetry $I4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}m2$, at $0, \frac{1}{4}, -\frac{1}{8}$ from centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},-\frac{1}{4},z$
(5) 2 $\frac{1}{4},y,\frac{3}{8}$	(6) 2 $x,\frac{1}{4},\frac{1}{8}$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x},0$
(9) $\bar{1}$ $0,\frac{1}{4},\frac{1}{8}$	(10) a $x,y,\frac{3}{8}$	(11) $\bar{4}^+$ $0,0,z$; $0,0,0$	(12) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(13) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(14) m $0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x-\frac{1}{4},x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,0,z$	(3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},\frac{1}{4},z$
(5) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{8}$	(6) $2(\frac{1}{2},0,0)$ $x,0,\frac{3}{8}$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}$ $\frac{1}{4},0,\frac{3}{8}$	(10) b $x,y,\frac{1}{8}$	(11) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(12) $\bar{4}^-$ $0,0,z$; $0,0,0$
(13) m $x,0,z$	(14) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
32	i	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{3}{4}$ (9) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$ (13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$ (10) $x+\frac{1}{2},y,\bar{z}+\frac{3}{4}$ (14) $\bar{x},y,z$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (11) $y,\bar{x},\bar{z}$ (15) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{3}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$ (8) $\bar{y},\bar{x},\bar{z}$ (12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (16) $y,x+\frac{1}{2},z+\frac{1}{4}$	hkl : $h+k+l=2n$ $hk0$: $h,k=2n$ $0kl$: $k+l=2n$ hhl : $2h+l=4n$ $00l$: $l=4n$ $h00$: $h=2n$ $h\bar{h}0$: $h=2n$
							Special: as above, plus
16	h	$.\,m\,.$	$0,y,z$ $\frac{1}{2},y,\bar{z}+\frac{3}{4}$	$\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ $0,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	$\bar{y},\frac{1}{2},z+\frac{1}{4}$ $y+\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$y+\frac{1}{2},0,z+\frac{3}{4}$ $\bar{y},0,\bar{z}$	no extra conditions
16	g	$.\,.\,2$	$x,x,0$ $\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},x,\frac{3}{4}$	$\bar{x},x+\frac{1}{2},\frac{1}{4}$ $x,\bar{x},0$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	hkl : $l=2n+1$ or $2h+l=4n$
16	f	$.\,2\,.$	$x,\frac{1}{4},\frac{1}{8}$ $\bar{x},\frac{1}{4},\frac{1}{8}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{5}{8}$ $x+\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},x+\frac{1}{2},\frac{3}{8}$ $\frac{1}{4},\bar{x},\frac{7}{8}$	$\frac{3}{4},\bar{x},\frac{7}{8}$ $\frac{1}{4},x+\frac{1}{2},\frac{3}{8}$	hkl : $l=2n+1$ or $h=2n$
8	e	$2\,m\,m\,.$	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$	$\frac{1}{2},0,\bar{z}+\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl : $l=2n+1$ or $2h+l=4n$
8	d	$.\,2/m\,.$	$0,\frac{1}{4},\frac{5}{8}$	$\frac{1}{2},\frac{1}{4},\frac{1}{8}$	$\frac{3}{4},\frac{1}{2},\frac{7}{8}$	$\frac{3}{4},0,\frac{3}{8}$	hkl : $l=2n+1$ or $h,k=2n,\ h+k+l=4n$
8	c	$.\,2/m\,.$	$0,\frac{1}{4},\frac{1}{8}$	$\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},\frac{1}{2},\frac{3}{8}$	$\frac{3}{4},0,\frac{7}{8}$	
4	b	$\bar{4}\,m\,2$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{3}{4}$			hkl : $l=2n+1$ or $2h+l=4n$
4	a	$\bar{4}\,m\,2$	$0,0,0$	$0,\frac{1}{2},\frac{1}{4}$			

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,\frac{3}{8}$

Along [110] $c2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $I\bar{4}2d$ (122) (1; 2; 5; 6; 11; 12; 15; 16)+
[2] $I\bar{4}m2$ (119) (1; 2; 7; 8; 11; 12; 13; 14)+
[2] $I4_1md$ (109) (1; 2; 3; 4; 13; 14; 15; 16)+
[2] $I4_122$ (98) (1; 2; 3; 4; 5; 6; 7; 8)+
[2] $I4_1/a11$ ($I4_1/a$, 88) (1; 2; 3; 4; 9; 10; 11; 12)+
[2] $I2/a2/m1$ ($Imma$, 74) (1; 2; 5; 6; 9; 10; 13; 14)+
[2] $I2/a12/d$ ($Fddd$, 70) (1; 2; 7; 8; 9; 10; 15; 16)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1/amd$ ($\mathbf{c}'=3\mathbf{c}$) (141); [9] $I4_1/amd$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (141)

Minimal non-isomorphic supergroups

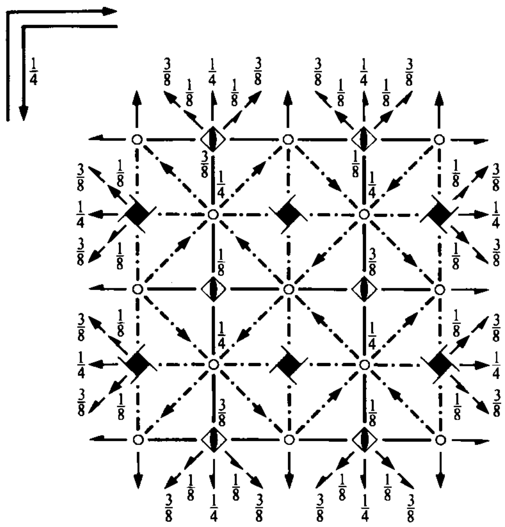
I [3] $Fd\bar{3}m$ (227)

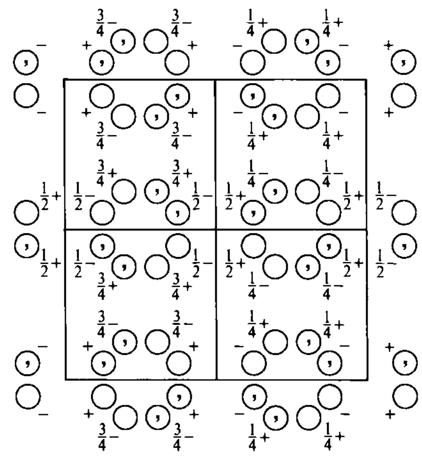
II [2] $C4_2/amd$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P4_2/nnm$, 134)

$I4_1/amd$ D_{4h}^{19} $4/mmm$ Tetragonal

No. 141 $I\ 4_1/a\ 2/m\ 2/d$ Patterson symmetry $I4/mmm$

ORIGIN CHOICE 2





Origin at centre $(2/m)$ at $b\,(2/m,2_1/n)d$, at $0,-\frac{1}{4},\frac{1}{8}$ from $\bar{4}m2$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $-\frac{1}{4} \le y \le \frac{1}{4}$; $0 \le z \le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},0,z$
(5) 2 $\frac{1}{4},y,\frac{1}{4}$	(6) 2 $x,0,0$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{1}{8}$	(8) 2 $x,\bar{x}+\frac{1}{4},\frac{3}{8}$
(9) $\bar{1}$ $0,0,0$	(10) a $x,y,\frac{1}{4}$	(11) $\bar{4}^+$ $\frac{1}{2},-\frac{1}{4},z$; $\frac{1}{2},-\frac{1}{4},\frac{3}{8}$	(12) $\bar{4}^-$ $0,\frac{3}{4},z$; $0,\frac{3}{4},\frac{1}{8}$
(13) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$	(14) m $0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{3}{4},\frac{3}{4},\frac{1}{4})$ x,x,z

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,\frac{1}{4},z$	(3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{4})$ $\frac{3}{4},0,z$
(5) $2(0,\frac{1}{2},0)$ $0,y,0$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{3}{8}$	(8) 2 $x,\bar{x}+\frac{3}{4},\frac{1}{8}$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) b $x,y,0$	(11) $\bar{4}^+$ $\frac{1}{2},\frac{1}{4},z$; $\frac{1}{2},\frac{1}{4},\frac{1}{8}$	(12) $\bar{4}^-$ $0,\frac{1}{4},z$; $0,\frac{1}{4},\frac{3}{8}$
(13) m $x,\frac{1}{4},z$	(14) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac12,\frac12,\frac12)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates: $(0,0,0)+\quad(\frac12,\frac12,\frac12)+$ — Reflection conditions

Mult.	Wyckoff	Site symm.	Coordinates				Reflection conditions
							General:
32	i	1	(1) x,y,z	(2) $\bar{x}+\frac12,\bar{y},z+\frac12$	(3) $\bar{y}+\frac14,x+\frac34,z+\frac14$	(4) $y+\frac14,\bar{x}+\frac14,z+\frac34$	hkl : $h+k+l=2n$
			(5) $\bar{x}+\frac12,y,\bar{z}+\frac12$	(6) $x,\bar{y},\bar{z}$	(7) $y+\frac14,x+\frac34,\bar{z}+\frac14$	(8) $\bar{y}+\frac14,\bar{x}+\frac14,\bar{z}+\frac34$	$hk0$: $h,k=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac12,y,\bar{z}+\frac12$	(11) $y+\frac34,\bar{x}+\frac14,\bar{z}+\frac34$	(12) $\bar{y}+\frac34,x+\frac34,\bar{z}+\frac14$	$0kl$: $k+l=2n$
			(13) $x+\frac12,\bar{y},z+\frac12$	(14) $\bar{x},y,z$	(15) $\bar{y}+\frac34,\bar{x}+\frac14,z+\frac34$	(16) $y+\frac34,x+\frac34,z+\frac14$	hhl : $2h+l=4n$
							$00l$: $l=4n$
							$h00$: $h=2n$
							$h\bar{h}0$: $h=2n$
							Special: as above, plus
16	h	$.m.$	$0,y,z$	$\frac12,\bar{y},z+\frac12$	$\bar{y}+\frac14,\frac34,z+\frac14$	$y+\frac14,\frac14,z+\frac34$	no extra conditions
			$\frac12,y,\bar{z}+\frac12$	$0,\bar{y},\bar{z}$	$y+\frac14,\frac34,\bar{z}+\frac14$	$\bar{y}+\frac14,\frac14,\bar{z}+\frac34$	
16	g	$..2$	$x,x+\frac14,\frac78$	$\bar{x}+\frac12,\bar{x}+\frac34,\frac38$	$\bar{x},x+\frac34,\frac18$	$x+\frac12,\bar{x}+\frac14,\frac58$	hkl : $l=2n+1$ or $2h+l=4n$
			$\bar{x},\bar{x}+\frac34,\frac18$	$x+\frac12,x+\frac14,\frac58$	$x,\bar{x}+\frac14,\frac78$	$\bar{x}+\frac12,x+\frac34,\frac38$	
16	f	$.2.$	$x,0,0$	$\bar{x}+\frac12,0,\frac12$	$\frac14,x+\frac34,\frac14$	$\frac14,\bar{x}+\frac14,\frac34$	hkl : $l=2n+1$ or $h=2n$
			$\bar{x},0,0$	$x+\frac12,0,\frac12$	$\frac34,\bar{x}+\frac14,\frac34$	$\frac34,x+\frac34,\frac14$	
8	e	$2mm.$	$0,\frac14,z$	$0,\frac34,z+\frac14$	$\frac12,\frac14,\bar{z}+\frac12$	$\frac12,\frac34,\bar{z}+\frac14$	hkl : $l=2n+1$ or $2h+l=4n$
8	d	$.2/m.$	$0,0,\frac12$	$\frac12,0,0$	$\frac14,\frac34,\frac34$	$\frac14,\frac14,\frac14$	hkl : $l=2n+1$ or $h,k=2n$, $h+k+l=4n$ (for d and c)
8	c	$.2/m.$	$0,0,0$	$\frac12,0,\frac12$	$\frac14,\frac34,\frac14$	$\frac14,\frac14,\frac34$	
4	b	$\bar{4}m2$	$0,\frac14,\frac38$	$0,\frac34,\frac58$			hkl : $l=2n+1$ or $2h+l=4n$ (for b and a)
4	a	$\bar{4}m2$	$0,\frac34,\frac18$	$\frac12,\frac34,\frac38$			

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac12\mathbf{a}$ $\mathbf{b}'=\frac12\mathbf{b}$
Origin at $\frac14,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac14,\frac14$

Along [110] $c2mm$
$\mathbf{a}'=\frac12(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac12\mathbf{c}$
Origin at $x,x+\frac14,\frac18$

Maximal non-isomorphic subgroups

I
- [2] $I\bar{4}2d$ (122) (1; 2; 5; 6; 11; 12; 15; 16)+
- [2] $I\bar{4}m2$ (119) (1; 2; 7; 8; 11; 12; 13; 14)+
- [2] $I4_1md$ (109) (1; 2; 3; 4; 13; 14; 15; 16)+
- [2] $I4_122$ (98) (1; 2; 3; 4; 5; 6; 7; 8)+
- [2] $I4_1/a11$ ($I4_1/a$, 88) (1; 2; 3; 4; 9; 10; 11; 12)+
- [2] $I2/a2/m1$ ($Imma$, 74) (1; 2; 5; 6; 9; 10; 13; 14)+
- [2] $I2/a12/d$ ($Fddd$, 70) (1; 2; 7; 8; 9; 10; 15; 16)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1/amd$ ($\mathbf{c}'=3\mathbf{c}$) (141); [9] $I4_1/amd$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (141)

Minimal non-isomorphic supergroups

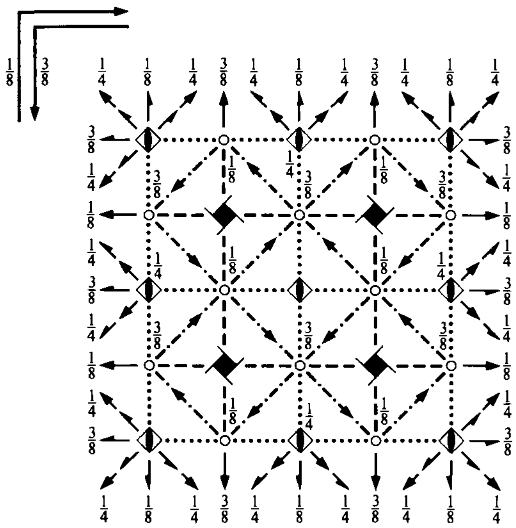
I [3] $Fd\bar{3}m$ (227)

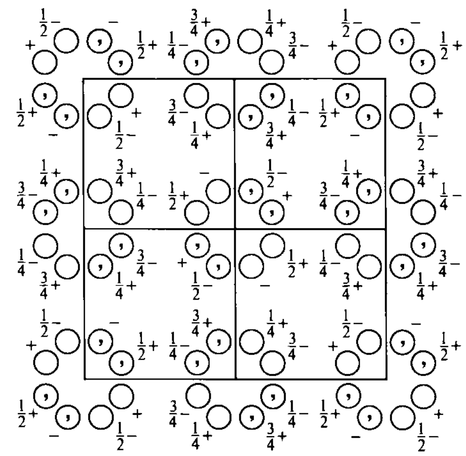
II [2] $C4_2/amd$ ($\mathbf{c}'=\frac12\mathbf{c}$) ($P4_2/nnm$, 134)

$I4_1/acd$ $\quad D_{4h}^{20}$ $\quad 4/mmm$ $\quad$ Tetragonal

No. 142 $\quad I\ 4_1/a\ 2/c\ 2/d$ $\quad$ Patterson symmetry $I4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}c2_1$, at $0,\frac{1}{4},-\frac{1}{8}$ from $\bar{1}$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{4})\ \ -\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{3}{4})\ \ \frac{1}{4},-\frac{1}{4},z$
(5) $2\ \ \frac{1}{4},y,\frac{1}{8}$	(6) $2\ \ x,\frac{1}{4},\frac{3}{8}$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x,0$	(8) $2\ \ x,\bar{x},\frac{1}{4}$
(9) $\bar{1}\ \ 0,\frac{1}{4},\frac{1}{8}$	(10) $a\ \ x,y,\frac{3}{8}$	(11) $\bar{4}^+\ 0,0,z;\ \ 0,0,0$	(12) $\bar{4}^-\ 0,\frac{1}{2},z;\ \ 0,\frac{1}{2},\frac{1}{4}$
(13) $a\ \ x,\frac{1}{4},z$	(14) $c\ \ 0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})\ \ x+\frac{1}{4},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})\ \ x-\frac{1}{4},x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\ \ 0,0,z$	(3) $4^+(0,0,\frac{3}{4})\ \ \frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{4})\ \ \frac{1}{4},\frac{1}{4},z$
(5) $2(0,\frac{1}{2},0)\ \ 0,y,\frac{3}{8}$	(6) $2(\frac{1}{2},0,0)\ \ x,0,\frac{1}{8}$	(7) $2\ \ x,x,\frac{1}{4}$	(8) $2\ \ x,\bar{x}+\frac{1}{2},0$
(9) $\bar{1}\ \ \frac{1}{4},0,\frac{3}{8}$	(10) $b\ \ x,y,\frac{1}{8}$	(11) $\bar{4}^+\ \frac{1}{2},0,z;\ \ \frac{1}{2},0,\frac{1}{4}$	(12) $\bar{4}^-\ 0,0,z;\ \ 0,0,0$
(13) $c\ \ x,0,z$	(14) $b\ \ \frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})\ \ x+\frac{1}{4},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\ \ x+\frac{1}{4},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
32 g 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$	hkl : $h+k+l=2n$
	(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{4}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{3}{4}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$hk0$: $h,k=2n$
	(9) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(10) $x+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0kl$: $k,l=2n$
	(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{1}{4}$	(16) $y,x+\frac{1}{2},z+\frac{3}{4}$	hhl : $2h+l=4n$
					$00l$: $l=4n$
					$h00$: $h=2n$
					$h\bar{h}0$: $h=2n$
					Special: as above, plus
16 f . . 2	$x,x,\frac{1}{4}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\bar{x},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x},0$	hkl : $l=2n+1$
	$\bar{x},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},x,\frac{1}{2}$	$x,\bar{x},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$	or $2h+l=4n$
16 e . 2 .	$\frac{1}{4},y,\frac{1}{8}$	$\frac{1}{4},\bar{y}+\frac{1}{2},\frac{5}{8}$	$\bar{y},\frac{3}{4},\frac{3}{8}$	$y+\frac{1}{2},\frac{3}{4},\frac{7}{8}$	hkl : $l=2n+1$
	$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{1}{8}$	$\frac{3}{4},y,\frac{5}{8}$	$y,\frac{3}{4},\frac{7}{8}$	$\bar{y}+\frac{1}{2},\frac{3}{4},\frac{3}{8}$	or $h=2n$
16 d 2 . .	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$	$\frac{1}{2},0,\bar{z}+\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	hkl : $2h+l=4n$
	$0,\frac{1}{2},\bar{z}+\frac{1}{4}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{4}$	
16 c $\bar{1}$	$0,\frac{1}{4},\frac{1}{8}$ $\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},\frac{1}{2},\frac{3}{8}$ $\frac{3}{4},0,\frac{7}{8}$	$\frac{1}{2},\frac{1}{4},\frac{1}{8}$ $0,\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},\frac{1}{2},\frac{7}{8}$ $\frac{3}{4},0,\frac{3}{8}$	hkl : $h,k=2n$, $h+k+l=4n$
8 b 2 . 22	$0,0,\frac{1}{4}$	$0,\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	$0,0,\frac{3}{4}$	hkl : $2h+l=4n$
8 a $\bar{4}$ . .	$0,0,0$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},0$	hkl : $2h+l=4n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,\frac{1}{8}$

Along [110] $c2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+
	[2] $I\bar{4}c2$ (120)	(1; 2; 7; 8; 11; 12; 13; 14)+
	[2] $I4_1cd$ (110)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[2] $I4_122$ (98)	(1; 2; 3; 4; 5; 6; 7; 8)+
	[2] $I4_1/a11$ ($I4_1/a$, 88)	(1; 2; 3; 4; 9; 10; 11; 12)+
	[2] $I2/a2/c1$ ($Ibca$, 73)	(1; 2; 5; 6; 9; 10; 13; 14)+
	[2] $I2/a12/d$ ($Fddd$, 70)	(1; 2; 7; 8; 9; 10; 15; 16)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1/acd$ ($\mathbf{c}'=3\mathbf{c}$) (142); [9] $I4_1/acd$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (142)

Minimal non-isomorphic supergroups

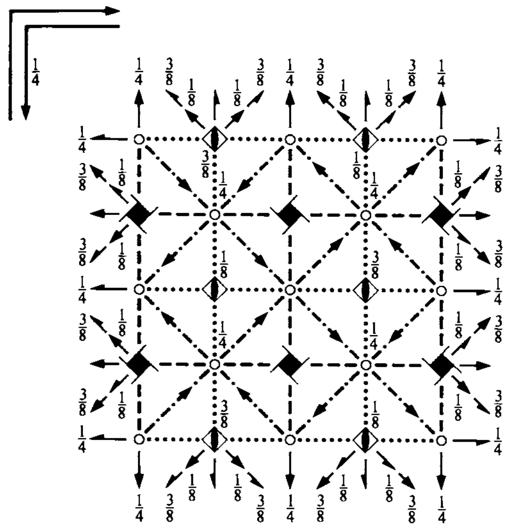
I [3] $Fd\bar{3}c$ (228); [3] $Ia\bar{3}d$ (230)

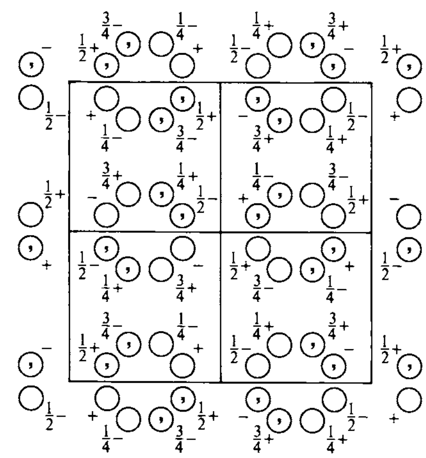
II [2] $C4_2/amd$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P4_2/nnm$, 134)

$I4_1/acd$ $\quad D_{4h}^{20}$ $\quad 4/mmm$ $\quad$ Tetragonal

No. 142 $\quad I\ 4_1/a\ 2/c\ 2/d$ $\quad$ Patterson symmetry $I4/mmm$

ORIGIN CHOICE 2





Origin at $\bar{1}$ at $b(c,a)d$, at $0,-\frac{1}{4},\frac{1}{8}$ from $\bar{4}$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad -\frac{1}{4} \le y \le \frac{1}{4}; \quad 0 \le z \le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $4^+(0,0,\frac{1}{4})\quad -\frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{3}{4})\quad \frac{1}{4},0,z$
(5) $2\quad \frac{1}{4},y,0$	(6) $2\quad x,0,\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x+\frac{1}{4},\frac{3}{8}$	(8) $2\quad x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(9) $\bar{1}\quad 0,0,0$	(10) $a\quad x,y,\frac{1}{4}$	(11) $\bar{4}^+\quad \frac{1}{2},-\frac{1}{4},z;\ \ \frac{1}{2},-\frac{1}{4},\frac{3}{8}$	(12) $\bar{4}^-\quad 0,\frac{3}{4},z;\ \ 0,\frac{3}{4},\frac{1}{8}$
(13) $a\quad x,0,z$	(14) $c\quad 0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})\quad x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})\quad x,x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\quad 0,\frac{1}{4},z$	(3) $4^+(0,0,\frac{3}{4})\quad \frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{4})\quad \frac{3}{4},0,z$
(5) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$	(7) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x-\frac{1}{4},\frac{1}{8}$	(8) $2\quad x,\bar{x}+\frac{3}{4},\frac{3}{8}$
(9) $\bar{1}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $b\quad x,y,0$	(11) $\bar{4}^+\quad \frac{1}{2},\frac{1}{4},z;\ \ \frac{1}{2},\frac{1}{4},\frac{1}{8}$	(12) $\bar{4}^-\quad 0,\frac{1}{4},z;\ \ 0,\frac{1}{4},\frac{3}{8}$
(13) $c\quad x,\frac{1}{4},z$	(14) $b\quad \frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})\quad x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
32	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$	(4) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	hkl : $h+k+l=2n$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{4},x+\frac{3}{4},\bar{z}+\frac{3}{4}$	(8) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	$hk0$: $h,k=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(11) $y+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$	(12) $\bar{y}+\frac{3}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$	$0kl$: $k,l=2n$
			(13) $x+\frac{1}{2},\bar{y},z$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{3}{4},\bar{x}+\frac{1}{4},z+\frac{1}{4}$	(16) $y+\frac{3}{4},x+\frac{3}{4},z+\frac{3}{4}$	hhl : $2h+l=4n$
							$00l$: $l=4n$
							$h00$: $h=2n$
							$h\bar{h}0$: $h=2n$
							Special: as above, plus
16	f	$..2$	$x,x+\frac{1}{4},\frac{1}{8}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{3}{4},\frac{5}{8}$	$\bar{x},x+\frac{3}{4},\frac{3}{8}$	$x+\frac{1}{2},\bar{x}+\frac{1}{4},\frac{7}{8}$	hkl : $l=2n+1$
			$\bar{x},\bar{x}+\frac{3}{4},\frac{7}{8}$	$x+\frac{1}{2},x+\frac{1}{4},\frac{3}{8}$	$x,\bar{x}+\frac{1}{4},\frac{5}{8}$	$\bar{x}+\frac{1}{2},x+\frac{3}{4},\frac{1}{8}$	or $2h+l=4n$
16	e	$.2.$	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{4},x+\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\bar{x}+\frac{1}{4},0$	hkl : $l=2n+1$
			$\bar{x},0,\frac{3}{4}$	$x+\frac{1}{2},0,\frac{1}{4}$	$\frac{3}{4},\bar{x}+\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},x+\frac{3}{4},0$	or $h=2n$
16	d	$2..$	$0,\frac{1}{4},z$	$0,\frac{3}{4},z+\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\bar{z}$	$\frac{1}{2},\frac{3}{4},\bar{z}+\frac{3}{4}$	hkl : $2h+l=4n$
			$0,\frac{3}{4},\bar{z}$	$0,\frac{1}{4},\bar{z}+\frac{3}{4}$	$\frac{1}{2},\frac{3}{4},z$	$\frac{1}{2},\frac{1}{4},z+\frac{1}{4}$	
16	c	$\bar{1}$	$0,0,0$ $\quad\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$ $\quad\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{2},0,0$ $\quad 0,0,\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$ $\quad\frac{1}{4},\frac{1}{4},\frac{1}{4}$	hkl : $h,k=2n,\ h+k+l=4n$
8	b	2.22	$0,\frac{1}{4},\frac{1}{8}$	$0,\frac{3}{4},\frac{3}{8}$	$0,\frac{3}{4},\frac{7}{8}$	$0,\frac{1}{4},\frac{5}{8}$	hkl : $2h+l=4n$
8	a	$\bar{4}..$	$0,\frac{1}{4},\frac{3}{8}$	$0,\frac{3}{4},\frac{5}{8}$	$\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{1}{2},\frac{3}{4},\frac{3}{8}$	hkl : $2h+l=4n$

Symmetry of special projections

Along [001] $p4mm$	Along [100] $p2mm$	Along [110] $c2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\quad\mathbf{b}'=\frac{1}{2}\mathbf{b}$	$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\quad\mathbf{b}'=\frac{1}{2}\mathbf{c}$	$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $\frac{1}{4},0,z$	Origin at $x,0,0$	Origin at $x,x+\frac{1}{4},\frac{1}{8}$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+
	[2] $I\bar{4}c2$ (120)	(1; 2; 7; 8; 11; 12; 13; 14)+
	[2] $I4_1cd$ (110)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[2] $I4_122$ (98)	(1; 2; 3; 4; 5; 6; 7; 8)+
	[2] $I4_1/a11$ ($I4_1/a$, 88)	(1; 2; 3; 4; 9; 10; 11; 12)+
	[2] $I2/a2/c1$ ($Ibca$, 73)	(1; 2; 5; 6; 9; 10; 13; 14)+
	[2] $I2/a12/d$ ($Fddd$, 70)	(1; 2; 7; 8; 9; 10; 15; 16)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1/acd$ ($\mathbf{c}'=3\mathbf{c}$) (142); [9] $I4_1/acd$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (142)

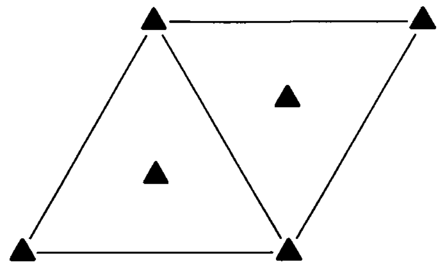
Minimal non-isomorphic supergroups

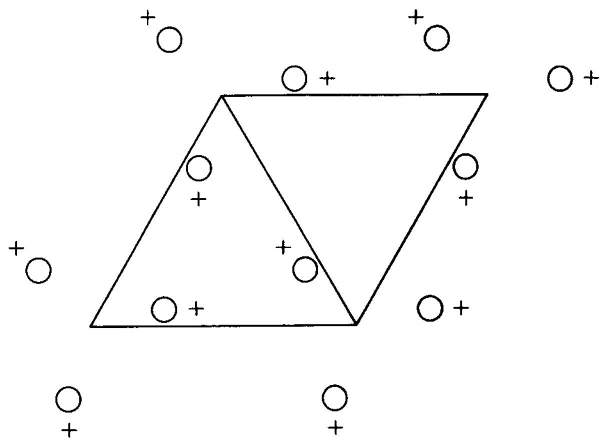
I [3] $Fd\bar{3}c$ (228); [3] $Ia\bar{3}d$ (230)

II [2] $C4_2/amd$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P4_2/nnm$, 134)

International Tables for Crystallography (2006). Vol. A, Space group 143, pp. 490–491.

$P3$	C_3^1	3	Trigonal
No. 143	$P3$		Patterson symmetry $P\bar{3}$





Origin on 3

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le 1$; $x \le (1+y)/2$; $y \le \min(1-x, (1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$

$0,0,1$ $\frac{1}{2},0,1$ $\frac{2}{3},\frac{1}{3},1$ $\frac{1}{3},\frac{2}{3},1$ $0,\frac{1}{2},1$

Symmetry operations

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
3	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
						Special: no extra conditions
1	c	$3\,.\,.$	$\frac{2}{3},\frac{1}{3},z$			
1	b	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$			
1	a	$3\,.\,.$	$0,0,z$			

Symmetry of special projections

Along [001] $p3$
$\mathbf{a}'=\mathbf{a}$ $\quad\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\quad\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\quad\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [3] $P1$ (1) 1

IIa none

IIb [3] $P3_2$ ($\mathbf{c}'=3\mathbf{c}$) (145); [3] $P3_1$ ($\mathbf{c}'=3\mathbf{c}$) (144); [3] $R3$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{a}+2\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (146); [3] $R3$ ($\mathbf{a}'=2\mathbf{a}+\mathbf{b},\mathbf{b}'=-\mathbf{a}+\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (146)

Maximal isomorphic subgroups of lowest index

IIc [2] $P3$ ($\mathbf{c}'=2\mathbf{c}$) (143); [3] $H3$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P3$, 143)

Minimal non-isomorphic supergroups

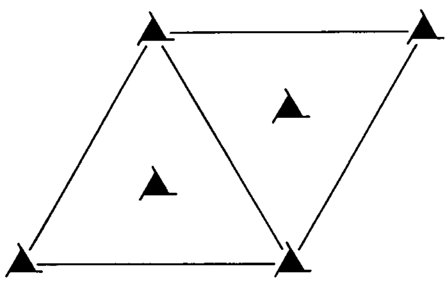
I [2] $P\bar{3}$ (147); [2] $P312$ (149); [2] $P321$ (150); [2] $P3m1$ (156); [2] $P31m$ (157); [2] $P3c1$ (158); [2] $P31c$ (159); [2] $P6$ (168); [2] $P6_3$ (173); [2] $P\bar{6}$ (174)

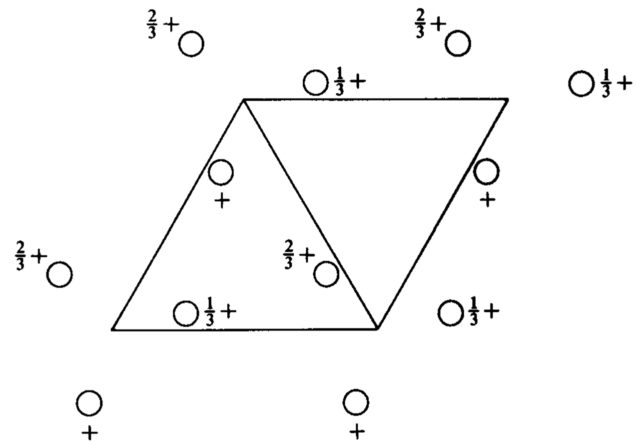
II [3] $R3$ (obverse) (146); [3] $R3$ (reverse) (146)

International Tables for Crystallography (2006). Vol. A, Space group 144, p. 492.

$P3_1$ $\quad C_3^2$ $\quad 3$ $\quad$ Trigonal

No. 144 $\quad P3_1$ $\quad$ Patterson symmetry $P\bar{3}$





Origin on 3_1

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{3}$

Vertices $\quad 0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$

$0,0,\frac{1}{3} \quad 1,0,\frac{1}{3} \quad 1,1,\frac{1}{3} \quad 0,1,\frac{1}{3}$

Symmetry operations

(1) 1 $\qquad$ (2) $3^+(0,0,\frac{1}{3})\ \ 0,0,z$ $\qquad$ (3) $3^-(0,0,\frac{2}{3})\ \ 0,0,z$

Generators selected $\quad$ (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
3 $\ a\ $ 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	$000l$: $l=3n$

Symmetry of special projections

Along [001] $p3$
$\mathbf{a}'=\mathbf{a} \qquad \mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b}) \qquad \mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b} \qquad \mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I $\quad$ [3] $P1$ (1) $\quad$ 1
IIa $\quad$ none
IIb $\quad$ none

Maximal isomorphic subgroups of lowest index

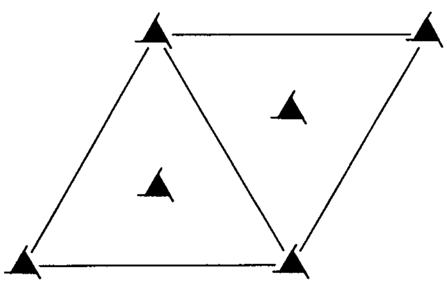
IIc $\quad$ [2] $P3_2$ ($\mathbf{c}'=2\mathbf{c}$) (145); [3] $H3_1$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P3_1$, 144); [7] $P3_1$ ($\mathbf{c}'=7\mathbf{c}$) (144)

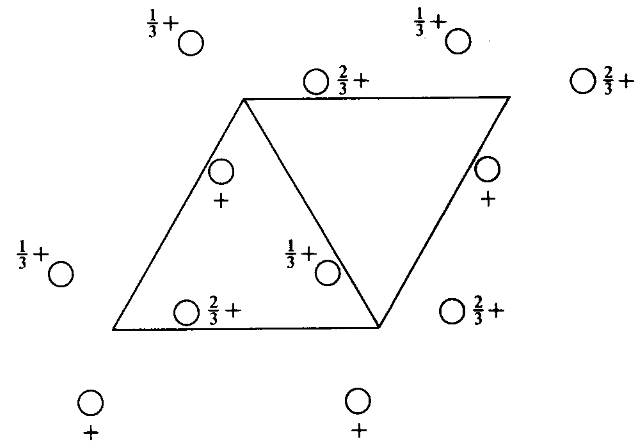
Minimal non-isomorphic supergroups

I $\quad$ [2] $P3_112$ (151); [2] $P3_121$ (152); [2] $P6_1$ (169); [2] $P6_4$ (172)
II $\quad$ [3] $R3$ (obverse) (146); [3] $R3$ (reverse) (146); [3] $P3$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (143)

Trigonal 3 C_3^3 $P3_2$

Patterson symmetry $P\bar{3}$ $P3_2$ No. 145





Origin on 3_2

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{3}$

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$

$0,0,\frac{1}{3} \quad 1,0,\frac{1}{3} \quad 1,1,\frac{1}{3} \quad 0,1,\frac{1}{3}$

Symmetry operations

(1) 1 (2) $3^+(0,0,\frac{2}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{1}{3})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
3 *a* 1	(1) x,y,z (2) $\bar{y},x-y,z+\frac{2}{3}$ (3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$	$000l$: $l=3n$

Symmetry of special projections

Along [001] $p3$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [3] $P1$ (1) 1
IIa none
IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $P3_1$ ($\mathbf{c}'=2\mathbf{c}$) (144); [3] $H3_2$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P3_2$, 145); [7] $P3_2$ ($\mathbf{c}'=7\mathbf{c}$) (145)

Minimal non-isomorphic supergroups

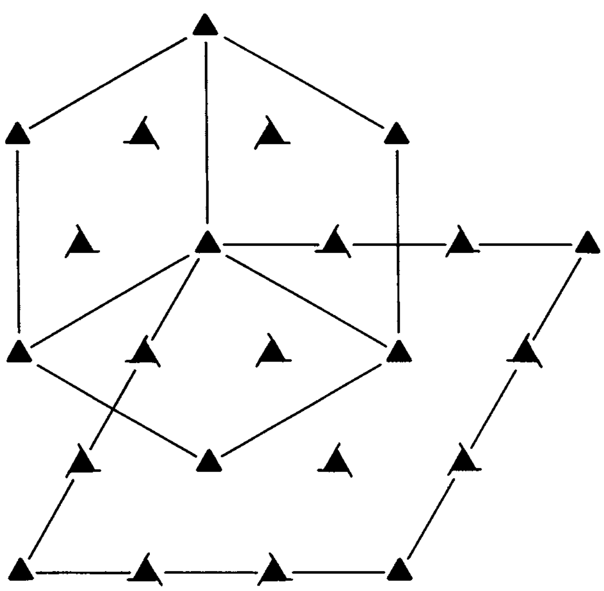
I [2] $P3_212$ (153); [2] $P3_221$ (154); [2] $P6_5$ (170); [2] $P6_2$ (171)
II [3] $R3$ (obverse) (146); [3] $R3$ (reverse) (146); [3] $P3$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (143)

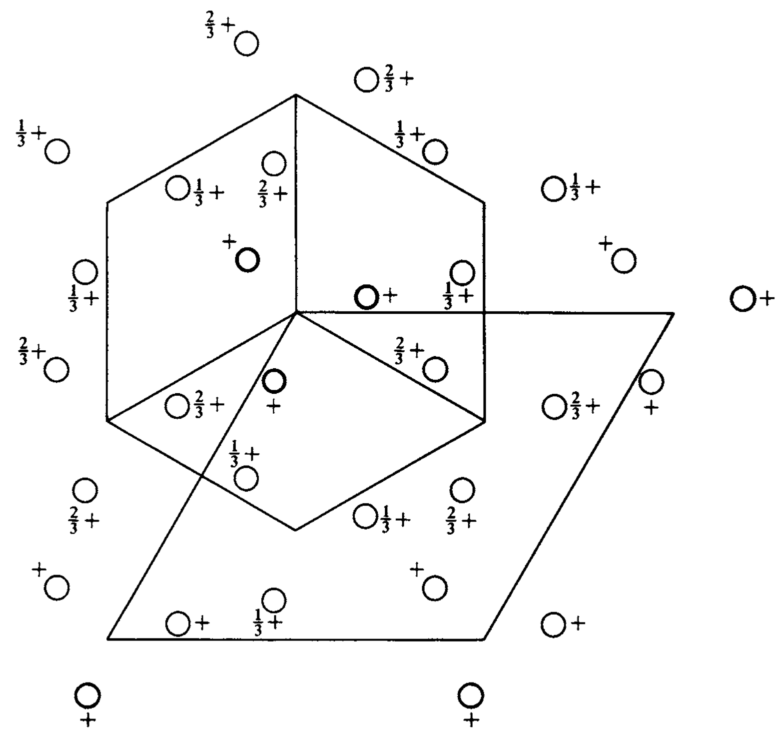
International Tables for Crystallography (2006). Vol. A, Space group 146, pp. 494–497.

$R3$ $\quad C_3^4$ $\quad 3$ $\quad$ Trigonal

No. 146 $\quad R3$ $\quad$ Patterson symmetry $R\bar{3}$

HEXAGONAL AXES





Origin on 3

Asymmetric unit $\quad 0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{2}{3};\quad 0 \le z \le \frac{1}{3};\quad x \le (1+y)/2;\quad y \le \min(1-x,(1+x)/2)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0 \quad 0,\frac{1}{2},0$

$0,0,\frac{1}{3} \quad \frac{1}{2},0,\frac{1}{3} \quad \frac{2}{3},\frac{1}{3},\frac{1}{3} \quad \frac{1}{3},\frac{2}{3},\frac{1}{3} \quad 0,\frac{1}{2},\frac{1}{3}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 $\quad$ (2) $3^+\ 0,0,z$ $\quad$ (3) $3^-\ 0,0,z$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$ $\quad$ (2) $3^+(0,0,\frac{1}{3})\ \ \frac{1}{3},\frac{1}{3},z$ $\quad$ (3) $3^-(0,0,\frac{1}{3})\ \ \frac{1}{3},0,z$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$ $\quad$ (2) $3^+(0,0,\frac{2}{3})\ \ 0,\frac{1}{3},z$ $\quad$ (3) $3^-(0,0,\frac{2}{3})\ \ \frac{1}{3},\frac{1}{3},z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
			$(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$	General:
9	b	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$hkil$: $-h+k+l=3n$ $hki0$: $-h+k=3n$ $hh\overline{2h}l$: $l=3n$ $h\bar{h}0l$: $h+l=3n$ $000l$: $l=3n$ $h\bar{h}00$: $h=3n$
						Special: no extra conditions
3	a	3 .	$0,0,z$			

Symmetry of special projections

Along [001] $p3$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

Along [210] $p1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [3] $R1$ ($P1$, 1) 1+

IIa [3] $P3_2$ (145) 1; $2+(\frac{1}{3},\frac{2}{3},\frac{2}{3})$; $3+(\frac{2}{3},\frac{1}{3},\frac{1}{3})$
[3] $P3_1$ (144) 1; $2+(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $3+(\frac{1}{3},\frac{2}{3},\frac{2}{3})$
[3] $P3$ (143) 1; 2; 3

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $R3$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (146); [4] $R3$ ($\mathbf{a}'=-2\mathbf{a},\mathbf{b}'=-2\mathbf{b}$) (146)

Minimal non-isomorphic supergroups

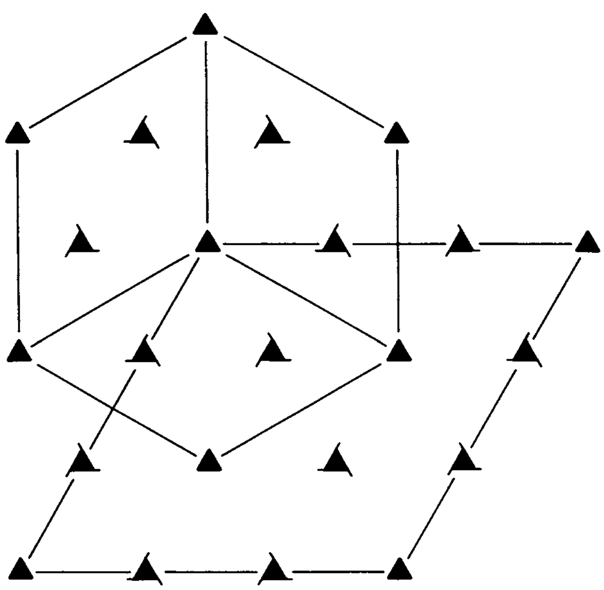
I [2] $R\bar{3}$ (148); [2] $R32$ (155); [2] $R3m$ (160); [2] $R3c$ (161); [4] $P23$ (195); [4] $F23$ (196); [4] $I23$ (197); [4] $P2_13$ (198); [4] $I2_13$ (199)

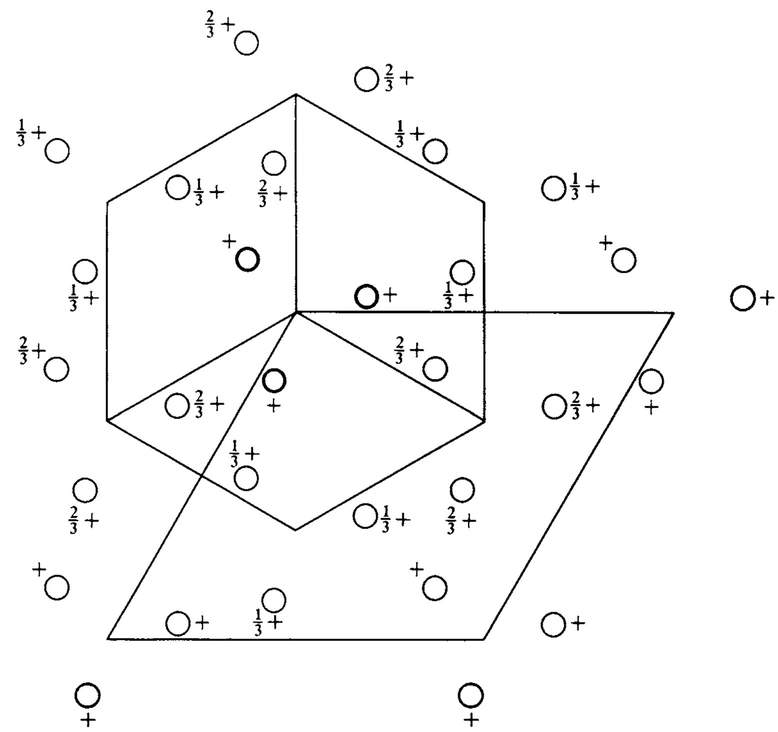
II [3] $P3$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b}),\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (143)

$R3$ | C_3^4 | 3 | Trigonal

No. 146 | $R3$ | Patterson symmetry $R\bar{3}$

RHOMBOHEDRAL AXES





Heights refer to hexagonal axes

Origin on 3

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le 1$; $z \le \min(x, y)$

Vertices 0,0,0 1,0,0 1,1,0 0,1,0 1,1,1

Symmetry operations

(1) 1 (2) 3^{+} x,x,x (3) 3^{-} x,x,x

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
3	b	1	(1) x,y,z	(2) z,x,y	(3) y,z,x	no conditions
						Special: no extra conditions
1	a	3 .	x,x,x			

Symmetry of special projections

Along [111] $p3$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along $[1\bar{1}0]$ $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\bar{x},0$

Along $[2\bar{1}\bar{1}]$ $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

Maximal non-isomorphic subgroups

I [3] $R1$ ($P1$, 1) 1

IIa none

IIb [3] $P3_2$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{b}-\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (145); [3] $P3_1$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{b}-\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (144); [3] $P3$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{b}-\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (143)

Maximal isomorphic subgroups of lowest index

IIc [2] $R3$ ($\mathbf{a}'=\mathbf{b}+\mathbf{c},\mathbf{b}'=\mathbf{a}+\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}$) (146); [4] $R3$ ($\mathbf{a}'=-\mathbf{a}+\mathbf{b}+\mathbf{c},\mathbf{b}'=\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}-\mathbf{c}$) (146)

Minimal non-isomorphic supergroups

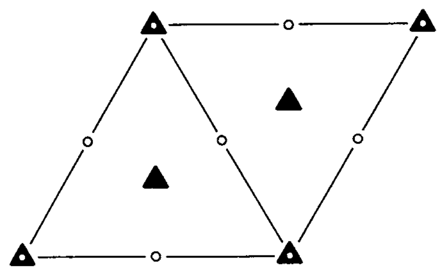
I [2] $R\bar{3}$ (148); [2] $R32$ (155); [2] $R3m$ (160); [2] $R3c$ (161); [4] $P23$ (195); [4] $F23$ (196); [4] $I23$ (197); [4] $P2_13$ (198); [4] $I2_13$ (199)

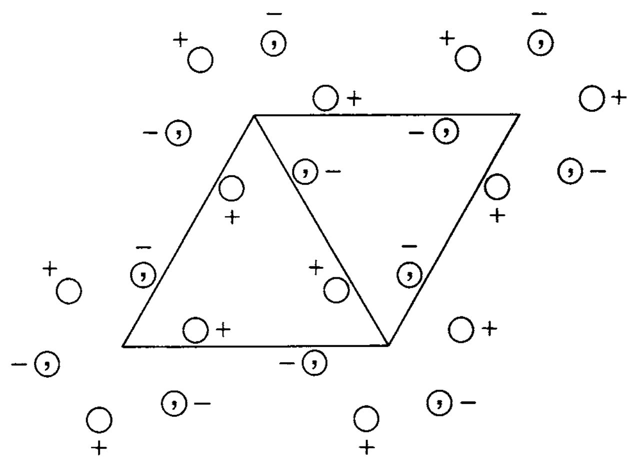
II [3] $P3$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}),\mathbf{c}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$) (143)

International Tables for Crystallography (2006). Vol. A, Space group 147, pp. 498–499.

$P\bar{3}$ $\quad C_{3i}^{1}$ $\quad \bar{3}$ $\quad$ Trigonal

No. 147 $\quad P\bar{3}$ $\quad$ Patterson symmetry $P\bar{3}$





Origin at centre ($\bar{3}$)

Asymmetric unit $\quad 0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{2}{3};\quad 0 \le z \le \frac{1}{2};\quad x \le (1+y)/2;\quad y \le \min(1-x,(1+x)/2)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0 \quad 0,\frac{1}{2},0$

$\quad 0,0,\frac{1}{2} \quad \frac{1}{2},0,\frac{1}{2} \quad \frac{2}{3},\frac{1}{3},\frac{1}{2} \quad \frac{1}{3},\frac{2}{3},\frac{1}{2} \quad 0,\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) $3^{+}\ 0,0,z$	(3) $3^{-}\ 0,0,z$
(4) $\bar{1}\ \ 0,0,0$	(5) $\bar{3}^{+}\ 0,0,z;\ 0,0,0$	(6) $\bar{3}^{-}\ 0,0,z;\ 0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	g	1	(1) x,y,z (4) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,\bar{z}$	no conditions
						Special: no extra conditions
3	f	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	
3	e	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	
2	d	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2	c	$3\,.\,.$	$0,0,z$	$0,0,\bar{z}$		
1	b	$\bar{3}\,.\,.$	$0,0,\frac{1}{2}$			
1	a	$\bar{3}\,.\,.$	$0,0,0$			

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P3$ (143) 1; 2; 3
[3] $P\bar{1}$ (2) 1; 4

IIa none

IIb [3] $R\bar{3}$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{a}+2\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (148); [3] $R\bar{3}$ ($\mathbf{a}'=2\mathbf{a}+\mathbf{b},\mathbf{b}'=-\mathbf{a}+\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (148)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{3}$ ($\mathbf{c}'=2\mathbf{c}$) (147); [3] $H\bar{3}$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P\bar{3}$, 147)

Minimal non-isomorphic supergroups

I [2] $P\bar{3}1m$ (162); [2] $P\bar{3}1c$ (163); [2] $P\bar{3}m1$ (164); [2] $P\bar{3}c1$ (165); [2] $P6/m$ (175); [2] $P6_3/m$ (176)

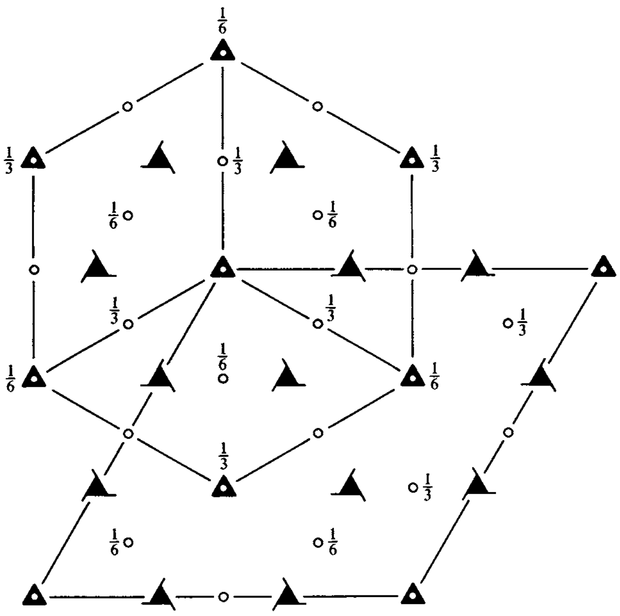
II [3] $R\bar{3}$ (obverse) (148); [3] $R\bar{3}$ (reverse) (148)

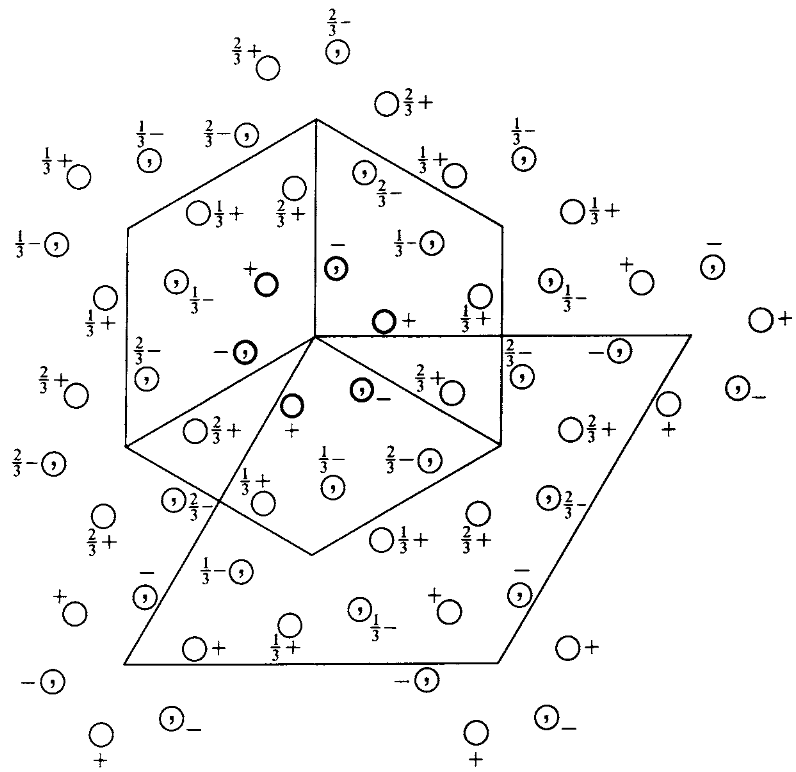
International Tables for Crystallography (2006). Vol. A, Space group 148, pp. 500–503.

$R\bar{3}$ $\quad C_{3i}^2$ $\quad \bar{3}$ $\quad$ Trigonal

No. 148 $\quad R\bar{3}$ $\quad$ Patterson symmetry $R\bar{3}$

HEXAGONAL AXES





Origin at centre ($\bar{3}$)

Asymmetric unit $\quad 0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{2}{3};\quad 0 \le z \le \frac{1}{6};\quad x \le (1+y)/2;\quad y \le \min(1-x,(1+x)/2)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0 \quad 0,\frac{1}{2},0$

$0,0,\frac{1}{6} \quad \frac{1}{2},0,\frac{1}{6} \quad \frac{2}{3},\frac{1}{3},\frac{1}{6} \quad \frac{1}{3},\frac{2}{3},\frac{1}{6} \quad 0,\frac{1}{2},\frac{1}{6}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $3^+\ 0,0,z$	(3) $3^-\ 0,0,z$
(4) $\bar{1}\ \ 0,0,0$	(5) $\bar{3}^+\ 0,0,z;\ \ 0,0,0$	(6) $\bar{3}^-\ 0,0,z;\ \ 0,0,0$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	(2) $3^+(0,0,\frac{1}{3})\ \ \frac{1}{3},\frac{1}{3},z$	(3) $3^-(0,0,\frac{1}{3})\ \ \frac{1}{3},0,z$
(4) $\bar{1}\ \ \frac{1}{3},\frac{1}{6},\frac{1}{6}$	(5) $\bar{3}^+\ \frac{1}{3},-\frac{1}{3},z;\ \ \frac{1}{3},-\frac{1}{3},\frac{1}{6}$	(6) $\bar{3}^-\ \frac{1}{3},\frac{2}{3},z;\ \ \frac{1}{3},\frac{2}{3},\frac{1}{6}$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$	(2) $3^+(0,0,\frac{2}{3})\ \ 0,\frac{1}{3},z$	(3) $3^-(0,0,\frac{2}{3})\ \ \frac{1}{3},\frac{1}{3},z$
(4) $\bar{1}\ \ \frac{1}{6},\frac{1}{3},\frac{1}{3}$	(5) $\bar{3}^+\ \frac{2}{3},\frac{1}{3},z;\ \ \frac{2}{3},\frac{1}{3},\frac{1}{3}$	(6) $\bar{3}^-\ -\frac{1}{3},\frac{1}{3},z;\ \ -\frac{1}{3},\frac{1}{3},\frac{1}{3}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
			$(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$	General:
18	*f*	1	(1) x,y,z (4) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,\bar{z}$	$hkil$: $-h+k+l=3n$ $hki0$: $-h+k=3n$ $hh\overline{2h}l$: $l=3n$ $h\bar{h}0l$: $h+l=3n$ $000l$: $l=3n$ $h\bar{h}00$: $h=3n$ Special: no extra conditions
9	*e*	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	
9	*d*	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	
6	*c*	3 .	$0,0,z$	$0,0,\bar{z}$		
3	*b*	$\bar{3}$.	$0,0,\frac{1}{2}$			
3	*a*	$\bar{3}$.	$0,0,0$			

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

Along [210] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $R3$ (146) (1; 2; 3)+
[3] $R\bar{1}$ ($P\bar{1}$, 2) (1; 4)+

IIa [3] $P\bar{3}$ (147) 1; 2; 3; 4; 5; 6
[3] $P\bar{3}$ (147) 1; 2; 3; (4; 5; 6) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$
[3] $P\bar{3}$ (147) 1; 2; 3; (4; 5; 6) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $R\bar{3}$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (148); [4] $R\bar{3}$ ($\mathbf{a}'=-2\mathbf{a},\mathbf{b}'=-2\mathbf{b}$) (148)

Minimal non-isomorphic supergroups

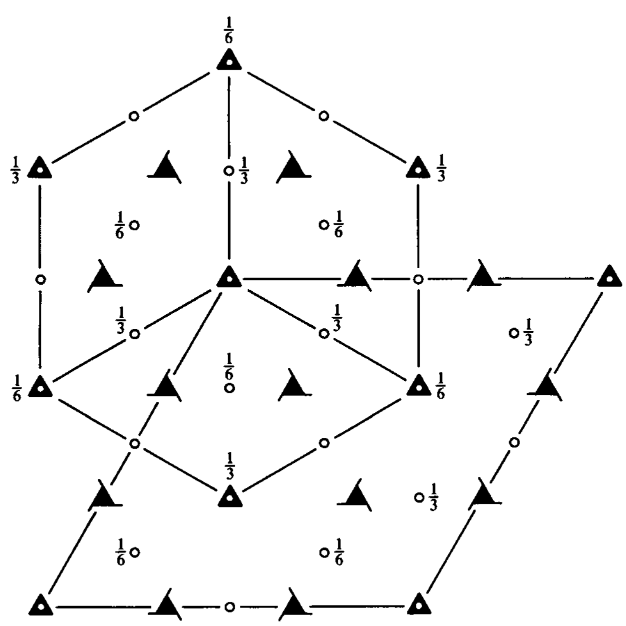
I [2] $R\bar{3}m$ (166); [2] $R\bar{3}c$ (167); [4] $Pm\bar{3}$ (200); [4] $Pn\bar{3}$ (201); [4] $Fm\bar{3}$ (202); [4] $Fd\bar{3}$ (203); [4] $Im\bar{3}$ (204); [4] $Pa\bar{3}$ (205); [4] $Ia\bar{3}$ (206)

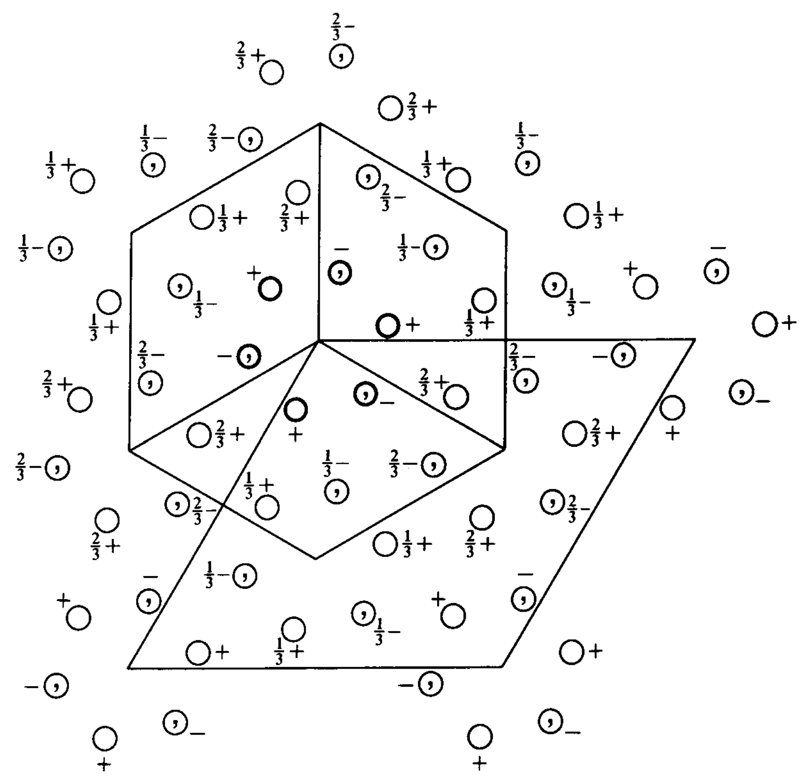
II [3] $P\bar{3}$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b}),\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (147)

$R\bar{3}$ C_{3i}^2 $\bar{3}$ Trigonal

No. 148 $R\bar{3}$ Patterson symmetry $R\bar{3}$

RHOMBOHEDRAL AXES





Heights refer to hexagonal axes

Origin at centre ($\bar{3}$)

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le \frac{1}{2}$; $z \le \min(x, y, 1-x, 1-y)$

Vertices $0,0,0$ $1,0,0$ $1,1,0$ $0,1,0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^+ x,x,x	(3) 3^- x,x,x
(4) $\bar{1}$ $0,0,0$	(5) $\bar{3}^+$ x,x,x; $0,0,0$	(6) $\bar{3}^-$ x,x,x; $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	f	1	(1) x,y,z	(2) z,x,y	(3) y,z,x	no conditions
			(4) $\bar{x},\bar{y},\bar{z}$	(5) $\bar{z},\bar{x},\bar{y}$	(6) $\bar{y},\bar{z},\bar{x}$	
						Special: no extra conditions
3	e	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	
3	d	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$	
2	c	$3\,.$	x,x,x	$\bar{x},\bar{x},\bar{x}$		
1	b	$\bar{3}\,.$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			
1	a	$\bar{3}\,.$	$0,0,0$			

Symmetry of special projections

Along [111] $p6$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along $[1\bar{1}0]$ $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\bar{x},0$

Along $[2\bar{1}\bar{1}]$ $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

Maximal non-isomorphic subgroups

I [2] $R3$ (146) 1; 2; 3
[3] $R\bar{1}$ ($P\bar{1}$, 2) 1; 4

IIa none

IIb [3] $P\bar{3}$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b}, \mathbf{b}'=\mathbf{b}-\mathbf{c}, \mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (147)

Maximal isomorphic subgroups of lowest index

IIc [2] $R\bar{3}$ ($\mathbf{a}'=\mathbf{b}+\mathbf{c}, \mathbf{b}'=\mathbf{a}+\mathbf{c}, \mathbf{c}'=\mathbf{a}+\mathbf{b}$) (148); [4] $R\bar{3}$ ($\mathbf{a}'=-\mathbf{a}+\mathbf{b}+\mathbf{c}, \mathbf{b}'=\mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{c}'=\mathbf{a}+\mathbf{b}-\mathbf{c}$) (148)

Minimal non-isomorphic supergroups

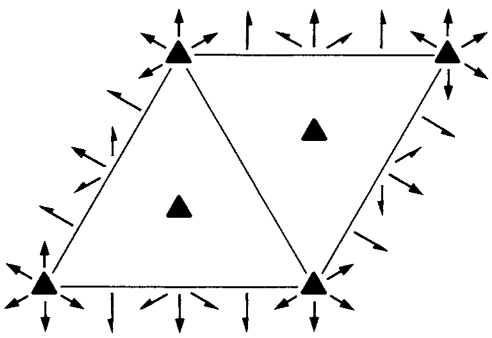
I [2] $R\bar{3}m$ (166); [2] $R\bar{3}c$ (167); [4] $Pm\bar{3}$ (200); [4] $Pn\bar{3}$ (201); [4] $Fm\bar{3}$ (202); [4] $Fd\bar{3}$ (203); [4] $Im\bar{3}$ (204); [4] $Pa\bar{3}$ (205); [4] $Ia\bar{3}$ (206)

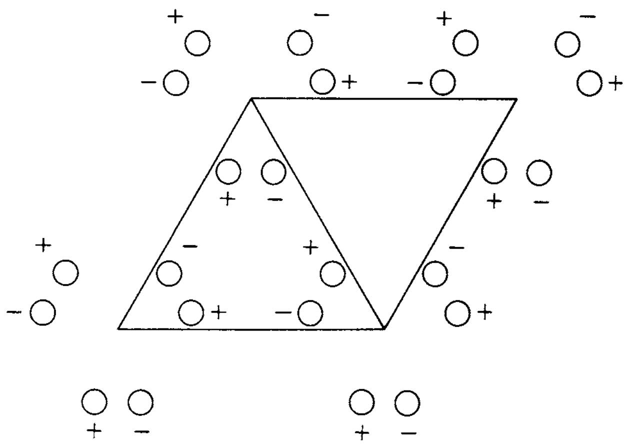
II [3] $P\bar{3}$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}), \mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}), \mathbf{c}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$) (147)

International Tables for Crystallography (2006). Vol. A, Space group 149, pp. 504–505.

$P312$ D_3^1 312 Trigonal

No. 149 $P312$ Patterson symmetry $P\bar{3}1m$





Origin at 312

Asymmetric unit $0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{2}{3};\quad 0 \le z \le \frac{1}{2};\quad x \le (1+y)/2;\quad y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0 \quad 0,\frac{1}{2},0$

$0,0,\frac{1}{2} \quad \frac{1}{2},0,\frac{1}{2} \quad \frac{2}{3},\frac{1}{3},\frac{1}{2} \quad \frac{1}{3},\frac{2}{3},\frac{1}{2} \quad 0,\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) $3^+\ 0,0,z$	(3) $3^-\ 0,0,z$
(4) $2\quad x,\bar{x},0$	(5) $2\quad x,2x,0$	(6) $2\quad 2x,x,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $\bar{y},\bar{x},\bar{z}$	(5) $\bar{x}+y,y,\bar{z}$	(6) $x,x-y,\bar{z}$	
						Special: no extra conditions
3	k	. . 2	$x,\bar{x},\frac{1}{2}$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	
3	j	. . 2	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	
2	i	3 . .	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2	h	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$		
2	g	3 . .	$0,0,z$	$0,0,\bar{z}$		
1	f	3 . 2	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$			
1	e	3 . 2	$\frac{2}{3},\frac{1}{3},0$			
1	d	3 . 2	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$			
1	c	3 . 2	$\frac{1}{3},\frac{2}{3},0$			
1	b	3 . 2	$0,0,\frac{1}{2}$			
1	a	3 . 2	$0,0,0$			

Symmetry of special projections

Along [001] $p3m1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p11m$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P311$ ($P3$, 143) 1; 2; 3
[3] $P112$ ($C2$, 5) 1; 4
[3] $P112$ ($C2$, 5) 1; 5
[3] $P112$ ($C2$, 5) 1; 6

IIa none

IIb [3] $P3_2 12$ ($\mathbf{c}'=3\mathbf{c}$) (153); [3] $P3_1 12$ ($\mathbf{c}'=3\mathbf{c}$) (151); [3] $H312$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P321$, 150);
[3] $R32$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{a}+2\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (155); [3] $R32$ ($\mathbf{a}'=2\mathbf{a}+\mathbf{b},\mathbf{b}'=-\mathbf{a}+\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (155)

Maximal isomorphic subgroups of lowest index

IIc [2] $P312$ ($\mathbf{c}'=2\mathbf{c}$) (149); [4] $P312$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (149)

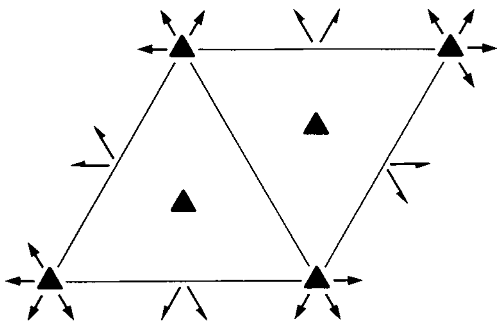
Minimal non-isomorphic supergroups

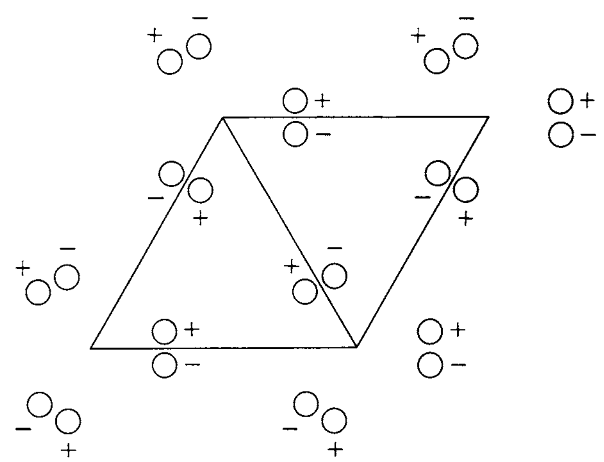
I [2] $P\bar{3}1m$ (162); [2] $P\bar{3}1c$ (163); [2] $P622$ (177); [2] $P6_3 22$ (182); [2] $P\bar{6}m2$ (187); [2] $P\bar{6}c2$ (188)

II [3] $H312$ ($P321$, 150)

$P\,3\,2\,1$ $\qquad D_3^2$ $\qquad 3\,2\,1$ $\qquad$ Trigonal

No. 150 $\qquad P\,3\,2\,1$ $\qquad$ Patterson symmetry $P\bar{3}m1$





Origin at $3\,2\,1$

Asymmetric unit $\quad 0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{2}{3};\quad 0 \le z \le \frac{1}{2};\quad x \le (1+y)/2;\quad y \le \min(1-x,(1+x)/2)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0 \quad 0,\frac{1}{2},0$

$0,0,\frac{1}{2} \quad \frac{1}{2},0,\frac{1}{2} \quad \frac{2}{3},\frac{1}{3},\frac{1}{2} \quad \frac{1}{3},\frac{2}{3},\frac{1}{2} \quad 0,\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) $3^+\ 0,0,z$	(3) $3^-\ 0,0,z$
(4) $2\quad x,x,0$	(5) $2\quad x,0,0$	(6) $2\quad 0,y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	g	1	(1) x,y,z (4) $y,x,\bar{z}$	(2) $\bar{y},x-y,z$ (5) $x-y,\bar{y},\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x},\bar{x}+y,\bar{z}$	no conditions
						Special: no extra conditions
3	f	. 2 .	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	
3	e	. 2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	
2	d	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2	c	3 . .	$0,0,z$	$0,0,\bar{z}$		
1	b	3 2 .	$0,0,\frac{1}{2}$			
1	a	3 2 .	$0,0,0$			

Symmetry of special projections

Along [001] $p31m$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P311$ ($P3$, 143) 1; 2; 3
$\begin{cases} \text{[3] } P121\ (C2, 5) & 1;\ 4 \\ \text{[3] } P121\ (C2, 5) & 1;\ 5 \\ \text{[3] } P121\ (C2, 5) & 1;\ 6 \end{cases}$

IIa none

IIb [3] $P3_221$ ($\mathbf{c}'=3\mathbf{c}$) (154); [3] $P3_121$ ($\mathbf{c}'=3\mathbf{c}$) (152); [3] $H321$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P312$, 149)

Maximal isomorphic subgroups of lowest index

IIc [2] $P321$ ($\mathbf{c}'=2\mathbf{c}$) (150); [4] $P321$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (150)

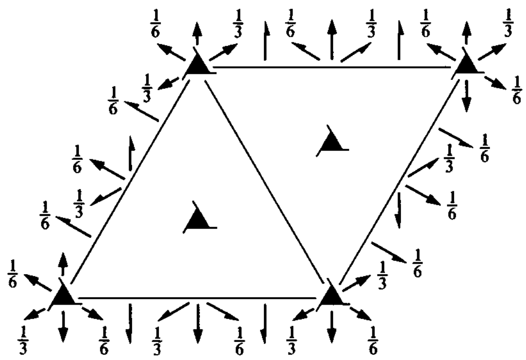
Minimal non-isomorphic supergroups

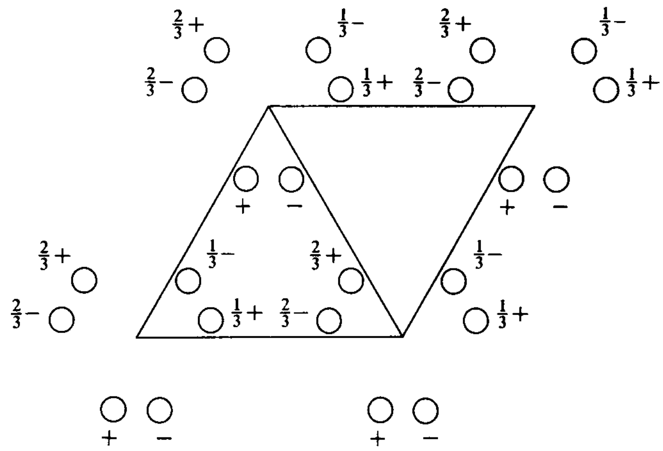
I [2] $P\bar{3}m1$ (164); [2] $P\bar{3}c1$ (165); [2] $P622$ (177); [2] $P6_322$ (182); [2] $P\bar{6}2m$ (189); [2] $P\bar{6}2c$ (190)

II [3] $H321$ ($P312$, 149); [3] $R32$ (obverse) (155); [3] $R32$ (reverse) (155)

$P3_112$ D_3^3 312 Trigonal

No. 151 $P3_112$ Patterson symmetry $P\bar{3}1m$





Origin on $2[2\,1\,0]$ at $3_1\,1\,(1,1,2)$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{6}$

Vertices $0,0,0\quad 1,0,0\quad 1,1,0\quad 0,1,0$

$0,0,\frac{1}{6}\quad 1,0,\frac{1}{6}\quad 1,1,\frac{1}{6}\quad 0,1,\frac{1}{6}$

Symmetry operations

(1) 1	(2) $3^+(0,0,\frac{1}{3})\quad 0,0,z$	(3) $3^-(0,0,\frac{2}{3})\quad 0,0,z$
(4) $2\quad x,\bar{x},\frac{1}{3}$	(5) $2\quad x,2x,\frac{1}{6}$	(6) $2\quad 2x,x,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	c	1	(1) x,y,z (4) $\bar{y},\bar{x},\bar{z}+\frac{2}{3}$	(2) $\bar{y},x-y,z+\frac{1}{3}$ (5) $\bar{x}+y,y,\bar{z}+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$ (6) $x,x-y,\bar{z}$	$000l$: $l=3n$
						Special: no extra conditions
3	b	$..2$	$x,\bar{x},\frac{5}{6}$	$x,2x,\frac{1}{6}$	$2\bar{x},\bar{x},\frac{1}{2}$	
3	a	$..2$	$x,\bar{x},\frac{1}{3}$	$x,2x,\frac{2}{3}$	$2\bar{x},\bar{x},0$	

Symmetry of special projections

Along [001] $p3m1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p11m$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,\frac{1}{6}$

Along [210] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P3_111$ ($P3_1$, 144) 1; 2; 3
[3] $P112$ ($C2$, 5) 1; 4
[3] $P112$ ($C2$, 5) 1; 5
[3] $P112$ ($C2$, 5) 1; 6

IIa none

IIb [3] $H3_112$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P3_121$, 152)

Maximal isomorphic subgroups of lowest index

IIc [2] $P3_212$ ($\mathbf{c}'=2\mathbf{c}$) (153); [4] $P3_112$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (151); [7] $P3_112$ ($\mathbf{c}'=7\mathbf{c}$) (151)

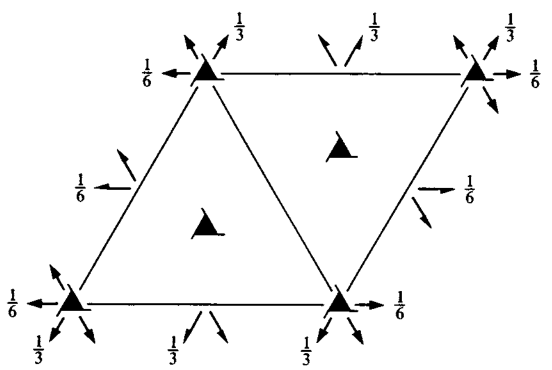
Minimal non-isomorphic supergroups

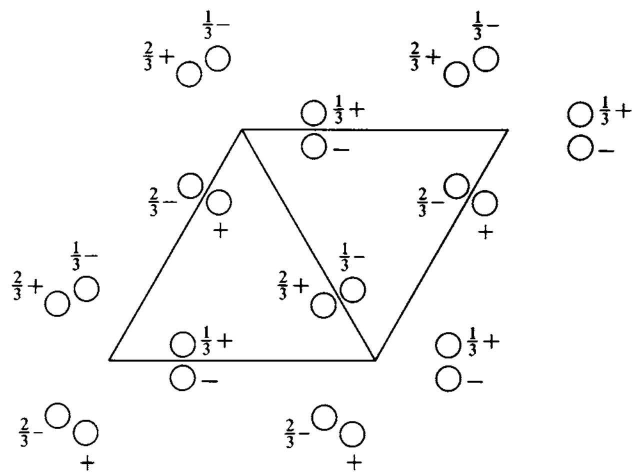
I [2] $P6_122$ (178); [2] $P6_422$ (181)

II [3] $H3_112$ ($P3_121$, 152); [3] $P312$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (149)

$P3_121$ D_3^4 321 Trigonal

No. 152 $P3_121$ Patterson symmetry $P\bar{3}m1$





Origin on $2[1\,1\,0]$ at $3_1\,(1,1,2)\,1$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{6}$

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$

$0,0,\frac{1}{6} \quad 1,0,\frac{1}{6} \quad 1,1,\frac{1}{6} \quad 0,1,\frac{1}{6}$

Symmetry operations

(1) 1	(2) $3^+(0,0,\frac{1}{3})\quad 0,0,z$	(3) $3^-(0,0,\frac{2}{3})\quad 0,0,z$
(4) $2\quad x,x,0$	(5) $2\quad x,0,\frac{1}{3}$	(6) $2\quad 0,y,\frac{1}{6}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	c	1	(1) x,y,z (4) $y,x,\bar{z}$	(2) $\bar{y},x-y,z+\frac{1}{3}$ (5) $x-y,\bar{y},\bar{z}+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$ (6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{3}$	$000l$: $l=3n$
						Special: no extra conditions
3	b	$.2.$	$x,0,\frac{5}{6}$	$0,x,\frac{1}{6}$	$\bar{x},\bar{x},\frac{1}{2}$	
3	a	$.2.$	$x,0,\frac{1}{3}$	$0,x,\frac{2}{3}$	$\bar{x},\bar{x},0$	

Symmetry of special projections

Along [001] $p31m$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,\frac{1}{3}$

Along [210] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{6}$

Maximal non-isomorphic subgroups

I [2] $P3_111$ ($P3_1$, 144) 1; 2; 3
{ [3] $P121$ ($C2$, 5) 1; 4
{ [3] $P121$ ($C2$, 5) 1; 5
{ [3] $P121$ ($C2$, 5) 1; 6

IIa none

IIb [3] $H3_121$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P3_112$, 151)

Maximal isomorphic subgroups of lowest index

IIc [2] $P3_221$ ($\mathbf{c}'=2\mathbf{c}$) (154); [4] $P3_121$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (152); [7] $P3_121$ ($\mathbf{c}'=7\mathbf{c}$) (152)

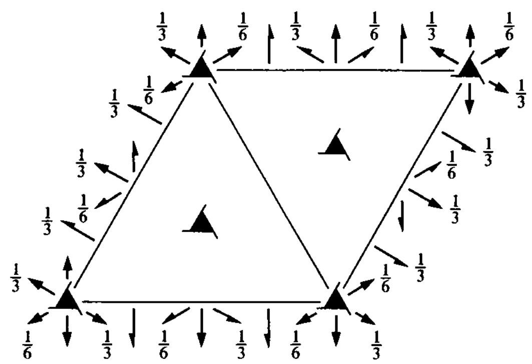
Minimal non-isomorphic supergroups

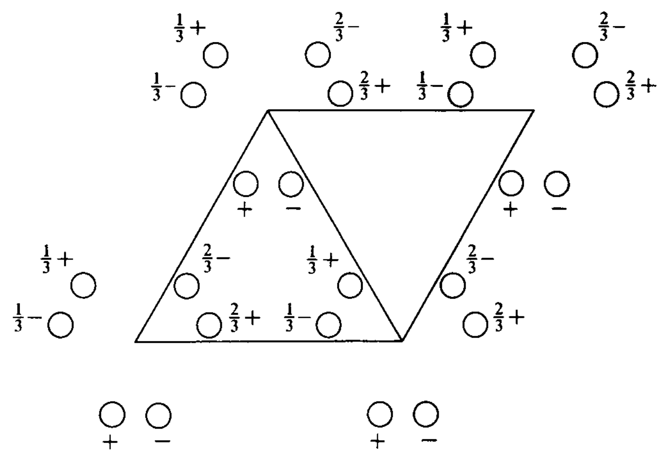
I [2] $P6_122$ (178); [2] $P6_422$ (181)

II [3] $H3_121$ ($P3_112$, 151); [3] $R32$ (obverse) (155); [3] $R32$ (reverse) (155); [3] $P321$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (150)

$P\,3_2\,1\,2$ $\quad D_3^5$ $\quad 3\,1\,2$ $\quad$ Trigonal

No. 153 $\quad P\,3_2\,1\,2$ $\quad$ Patterson symmetry $P\,\bar{3}\,1\,m$





Origin on $2[2\,1\,0]$ at $3_2\,1\,(1,1,2)$

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{6}$

Vertices $\quad 0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$

$0,0,\frac{1}{6} \quad 1,0,\frac{1}{6} \quad 1,1,\frac{1}{6} \quad 0,1,\frac{1}{6}$

Symmetry operations

(1) 1	(2) $3^+(0,0,\frac{2}{3})\quad 0,0,z$	(3) $3^-(0,0,\frac{1}{3})\quad 0,0,z$
(4) $2\quad x,\bar{x},\frac{1}{6}$	(5) $2\quad x,2x,\frac{1}{3}$	(6) $2\quad 2x,x,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	c	1	(1) x,y,z (4) $\bar{y},\bar{x},\bar{z}+\frac{1}{3}$	(2) $\bar{y},x-y,z+\frac{2}{3}$ (5) $\bar{x}+y,y,\bar{z}+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$ (6) $x,x-y,\bar{z}$	$000l$: $l=3n$
						Special: no extra conditions
3	b	. . 2	$x,\bar{x},\frac{1}{6}$	$x,2x,\frac{5}{6}$	$2\bar{x},\bar{x},\frac{1}{2}$	
3	a	. . 2	$x,\bar{x},\frac{2}{3}$	$x,2x,\frac{1}{3}$	$2\bar{x},\bar{x},0$	

Symmetry of special projections

Along [001] $p3m1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p11m$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,\frac{1}{3}$

Along [210] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P3_211$ ($P3_2$, 145) 1; 2; 3
$\left\{\begin{array}{ll} [3]\ P112\ (C2, 5) & 1;\ 4 \\ [3]\ P112\ (C2, 5) & 1;\ 5 \\ [3]\ P112\ (C2, 5) & 1;\ 6 \end{array}\right.$

IIa none

IIb [3] $H3_212$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P3_221$, 154)

Maximal isomorphic subgroups of lowest index

IIc [2] $P3_112$ ($\mathbf{c}'=2\mathbf{c}$) (151); [4] $P3_212$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (153); [7] $P3_212$ ($\mathbf{c}'=7\mathbf{c}$) (153)

Minimal non-isomorphic supergroups

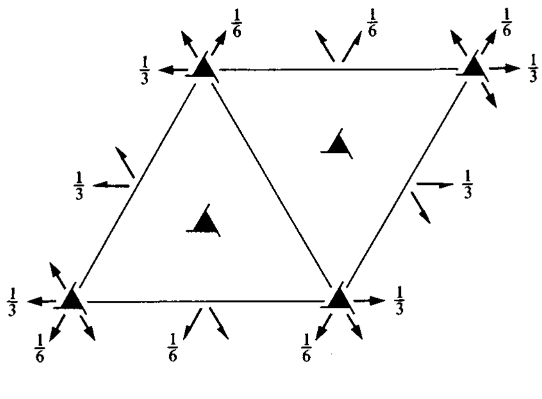
I [2] $P6_522$ (179); [2] $P6_222$ (180)

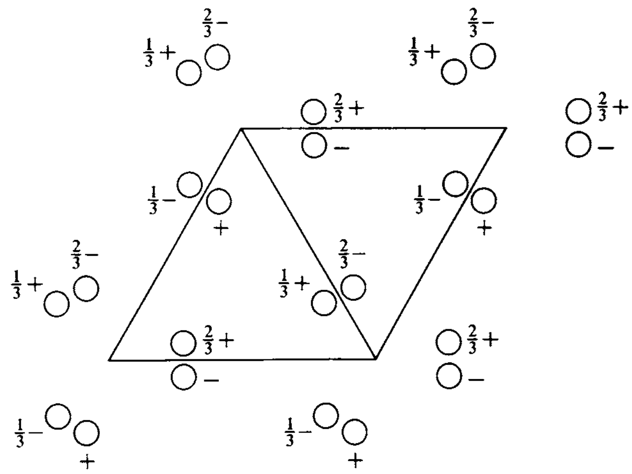
II [3] $H3_212$ ($P3_221$, 154); [3] $P312$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (149)

International Tables for Crystallography (2006). Vol. A, Space group 154, pp. 514–515.

$P\,3_2\,2\,1$ $\quad$ D_3^6 $\quad$ $3\,2\,1$ $\quad$ Trigonal

No. 154 $\quad$ $P\,3_2\,2\,1$ $\quad$ Patterson symmetry $P\,\bar{3}\,m\,1$





Origin on $2[1\,1\,0]$ at $3_2\,(1,1,2)\,1$

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{6}$

Vertices $\quad 0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$

$\quad 0,0,\frac{1}{6} \quad 1,0,\frac{1}{6} \quad 1,1,\frac{1}{6} \quad 0,1,\frac{1}{6}$

Symmetry operations

(1) 1	(2) $3^+(0,0,\frac{2}{3})\quad 0,0,z$	(3) $3^-(0,0,\frac{1}{3})\quad 0,0,z$
(4) $2\quad x,x,0$	(5) $2\quad x,0,\frac{1}{6}$	(6) $2\quad 0,y,\frac{1}{3}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	*c*	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$	$000l$: $l=3n$
			(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}+\frac{1}{3}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{2}{3}$	
						Special: no extra conditions
3	*b*	. 2 .	$x,0,\frac{1}{6}$	$0,x,\frac{5}{6}$	$\bar{x},\bar{x},\frac{1}{2}$	
3	*a*	. 2 .	$x,0,\frac{2}{3}$	$0,x,\frac{1}{3}$	$\bar{x},\bar{x},0$	

Symmetry of special projections

Along [001] $p31m$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,\frac{1}{6}$

Along [210] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{3}$

Maximal non-isomorphic subgroups

I [2] $P3_211$ ($P3_2$, 145) 1; 2; 3
[3] $P121$ ($C2$, 5) 1; 4
[3] $P121$ ($C2$, 5) 1; 5
[3] $P121$ ($C2$, 5) 1; 6

IIa none

IIb [3] $H3_221$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P3_212$, 153)

Maximal isomorphic subgroups of lowest index

IIc [2] $P3_121$ ($\mathbf{c}'=2\mathbf{c}$) (152); [4] $P3_221$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (154); [7] $P3_221$ ($\mathbf{c}'=7\mathbf{c}$) (154)

Minimal non-isomorphic supergroups

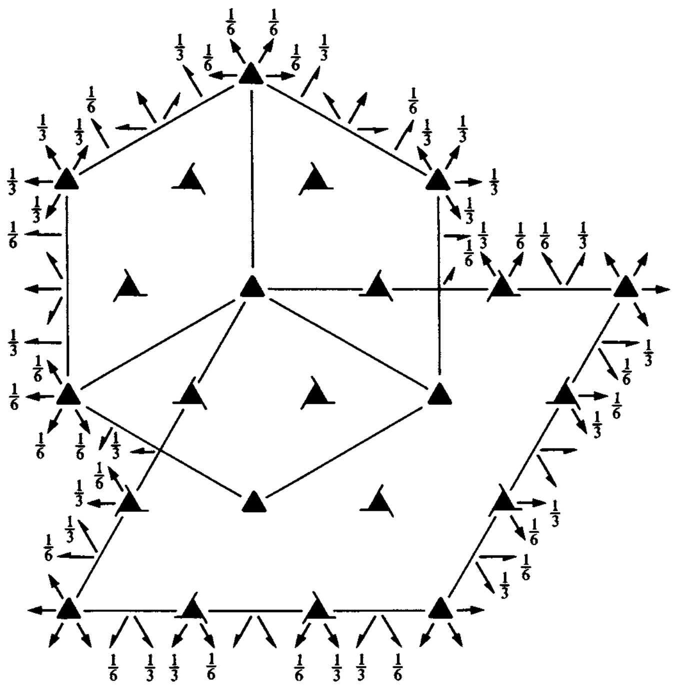
I [2] $P6_522$ (179); [2] $P6_222$ (180)

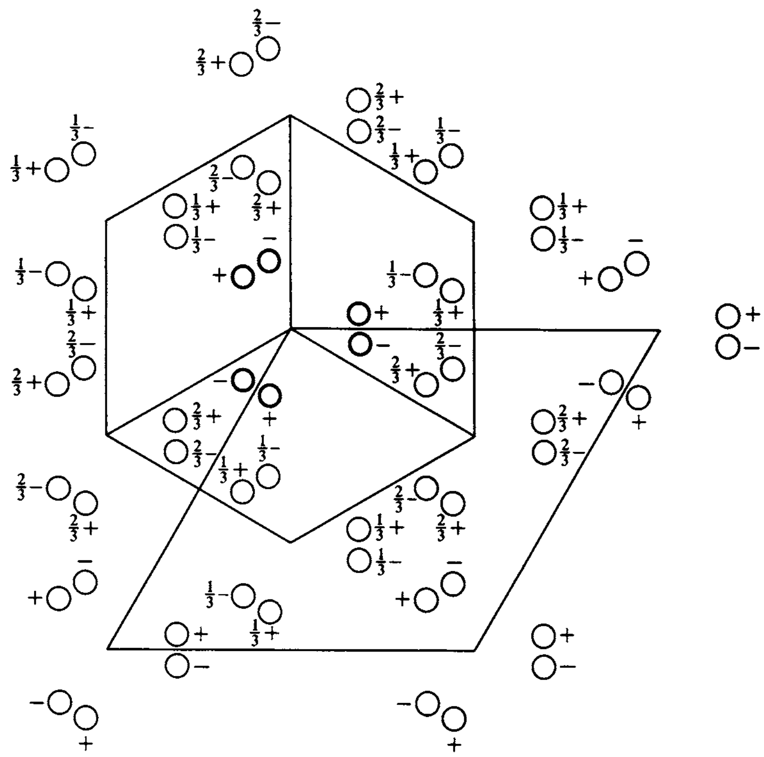
II [3] $H3_221$ ($P3_212$, 153); [3] $R32$ (obverse) (155); [3] $R32$ (reverse) (155); [3] $P321$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (150)

$R32$ D_3^7 32 Trigonal

No. 155 $R32$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





Origin at 32

Asymmetric unit $0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{2}{3};\quad 0 \le z \le \frac{1}{6};\quad x \le (1+y)/2;\quad y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0\quad \frac{1}{2},0,0\quad \frac{2}{3},\frac{1}{3},0\quad \frac{1}{3},\frac{2}{3},0\quad 0,\frac{1}{2},0$

$0,0,\frac{1}{6}\quad \frac{1}{2},0,\frac{1}{6}\quad \frac{2}{3},\frac{1}{3},\frac{1}{6}\quad \frac{1}{3},\frac{2}{3},\frac{1}{6}\quad 0,\frac{1}{2},\frac{1}{6}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $3^+\ 0,0,z$	(3) $3^-\ 0,0,z$
(4) $2\ \ x,x,0$	(5) $2\ \ x,0,0$	(6) $2\ \ 0,y,0$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	(2) $3^+(0,0,\frac{1}{3})\ \ \frac{1}{3},\frac{1}{3},z$	(3) $3^-(0,0,\frac{1}{3})\ \ \frac{1}{3},0,z$
(4) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x-\frac{1}{6},\frac{1}{6}$	(5) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{6},\frac{1}{6}$	(6) $2\ \ \frac{1}{3},y,\frac{1}{6}$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$	(2) $3^+(0,0,\frac{2}{3})\ \ 0,\frac{1}{3},z$	(3) $3^-(0,0,\frac{2}{3})\ \ \frac{1}{3},\frac{1}{3},z$
(4) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x+\frac{1}{6},\frac{1}{3}$	(5) $2\ \ x,\frac{1}{3},\frac{1}{3}$	(6) $2(0,\frac{1}{2},0)\ \ \frac{1}{6},y,\frac{1}{3}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
			$(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$	General:
18	*f*	1	(1) x,y,z (4) $y,x,\bar{z}$	(2) $\bar{y},x-y,z$ (5) $x-y,\bar{y},\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x},\bar{x}+y,\bar{z}$	$hkil$: $-h+k+l=3n$ $hki0$: $-h+k=3n$ $hh\overline{2h}l$: $l=3n$ $h\bar{h}0l$: $h+l=3n$ $000l$: $l=3n$ $h\bar{h}00$: $h=3n$ Special: no extra conditions
9	*e*	. 2	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	
9	*d*	. 2	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	
6	*c*	3 .	$0,0,z$	$0,0,\bar{z}$		
3	*b*	3 2	$0,0,\frac{1}{2}$			
3	*a*	3 2	$0,0,0$			

Symmetry of special projections

Along [001] $p3m1$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

Along [210] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I	[2] $R31$ ($R3$, 146)	(1; 2; 3)+
	[3] $R12$ ($C2$, 5)	(1; 4)+
	[3] $R12$ ($C2$, 5)	(1; 5)+
	[3] $R12$ ($C2$, 5)	(1; 6)+
IIa	[3] $P3_221$ (154)	1; 4; (2; 6) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$; (3; 5) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$
	[3] $P3_221$ (154)	1; 5; (2; 4) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$; (3; 6) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$
	[3] $P3_221$ (154)	1; 6; (2; 5) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$; (3; 4) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$
	[3] $P3_121$ (152)	1; 4; (2; 6) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (3; 5) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$
	[3] $P3_121$ (152)	1; 5; (2; 4) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (3; 6) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$
	[3] $P3_121$ (152)	1; 6; (2; 5) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (3; 4) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$
	[3] $P321$ (150)	1; 2; 3; 4; 5; 6
	[3] $P321$ (150)	1; 2; 3; (4; 5; 6) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$
	[3] $P321$ (150)	1; 2; 3; (4; 5; 6) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [2] $R32$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (155); [4] $R32$ ($\mathbf{a}'=-2\mathbf{a},\mathbf{b}'=-2\mathbf{b}$) (155)

Minimal non-isomorphic supergroups

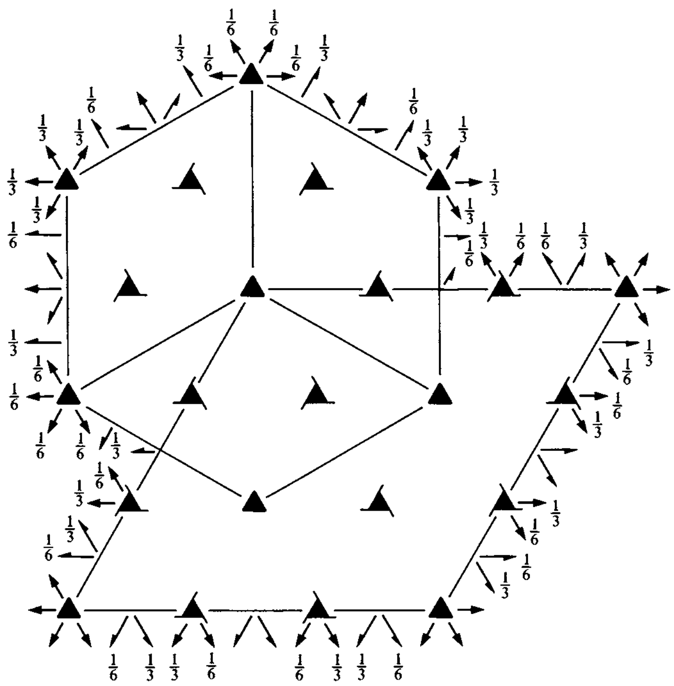
I [2] $R\bar{3}m$ (166); [2] $R\bar{3}c$ (167); [4] $P432$ (207); [4] $P4_232$ (208); [4] $F432$ (209); [4] $F4_132$ (210); [4] $I432$ (211); [4] $P4_332$ (212); [4] $P4_132$ (213); [4] $I4_132$ (214)

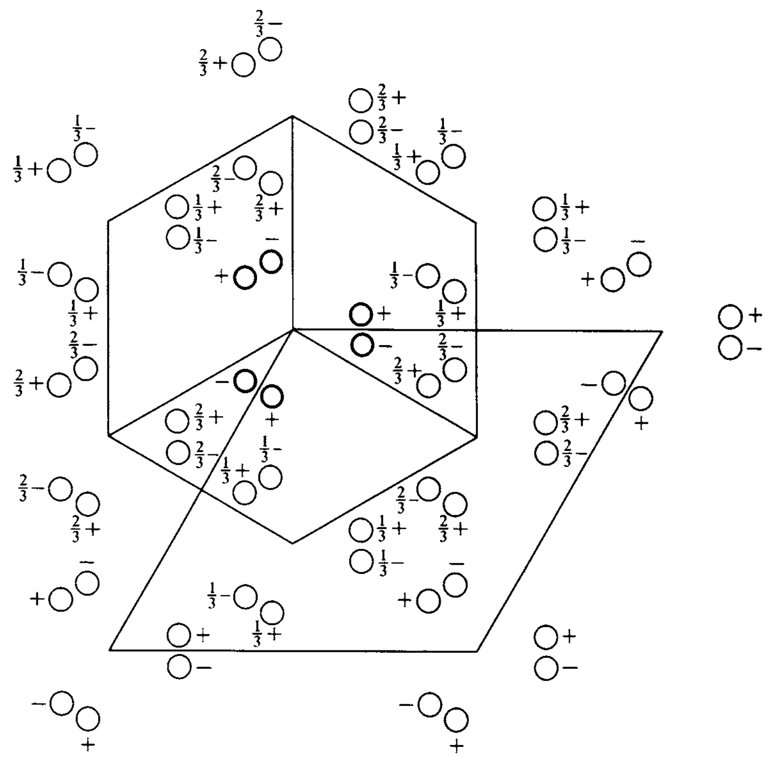
II [3] $P312$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b}),\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (149)

$R32$ $\qquad D_3^7$ $\qquad 32$ $\qquad$ Trigonal

No. 155 $\qquad R32$ $\qquad$ Patterson symmetry $R\bar{3}m$

RHOMBOHEDRAL AXES





Heights refer to hexagonal axes

Origin at 32

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}; \quad z \le \min(x, y, 1-x, 1-y)$

Vertices $\quad 0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0 \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^+ x,x,x	(3) 3^- x,x,x
(4) 2 $\bar{x},0,x$	(5) 2 $x,\bar{x},0$	(6) 2 $0,y,\bar{y}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	f	1	(1) x,y,z (4) $\bar{z},\bar{y},\bar{x}$	(2) z,x,y (5) $\bar{y},\bar{x},\bar{z}$	(3) y,z,x (6) $\bar{x},\bar{z},\bar{y}$	no conditions
						Special: no extra conditions
3	e	. 2	$\frac{1}{2},y,\bar{y}$	$\bar{y},\frac{1}{2},y$	$y,\bar{y},\frac{1}{2}$	
3	d	. 2	$0,y,\bar{y}$	$\bar{y},0,y$	$y,\bar{y},0$	
2	c	3 .	x,x,x	$\bar{x},\bar{x},\bar{x}$		
1	b	3 2	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			
1	a	3 2	$0,0,0$			

Symmetry of special projections

Along [111] $p3m1$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [$1\bar{1}0$] $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\bar{x},0$

Along [$2\bar{1}\bar{1}$] $p11m$
$\mathbf{a}' = \frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

Maximal non-isomorphic subgroups

I [2] $R31$ ($R3$, 146) 1; 2; 3
[3] $R12$ ($C2$, 5) 1; 4
[3] $R12$ ($C2$, 5) 1; 5
[3] $R12$ ($C2$, 5) 1; 6

IIa none

IIb [3] $P321$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{b}-\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (150); [3] $P3_121$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{b}-\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (152); [3] $P3_221$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{b}-\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (154)

Maximal isomorphic subgroups of lowest index

IIc [2] $R32$ ($\mathbf{a}'=\mathbf{b}+\mathbf{c},\mathbf{b}'=\mathbf{a}+\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}$) (155); [4] $R32$ ($\mathbf{a}'=-\mathbf{a}+\mathbf{b}+\mathbf{c},\mathbf{b}'=\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}-\mathbf{c}$) (155)

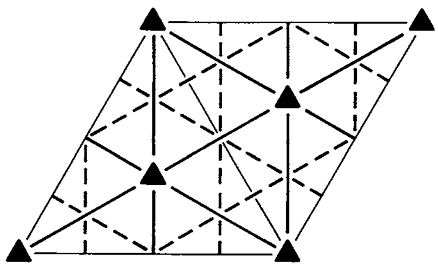
Minimal non-isomorphic supergroups

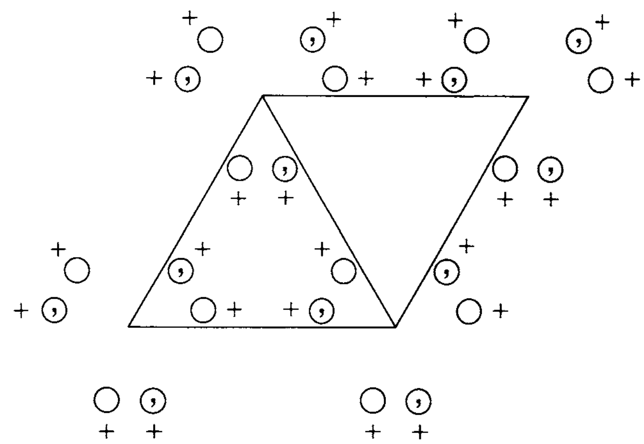
I [2] $R\bar{3}m$ (166); [2] $R\bar{3}c$ (167); [4] $P432$ (207); [4] $P4_232$ (208); [4] $F432$ (209); [4] $F4_132$ (210); [4] $I432$ (211); [4] $P4_332$ (212); [4] $P4_132$ (213); [4] $I4_132$ (214)

II [3] $P312$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}),\mathbf{c}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$) (149)

$P3m1$ C_{3v}^1 $3m1$ Trigonal

No. 156 $P3m1$ Patterson symmetry $P\bar{3}m1$





Origin on $3m1$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le 1$; $x \le 2y$; $y \le \min(1-x, 2x)$

Vertices $0,0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$

$0,0,1$ $\frac{2}{3},\frac{1}{3},1$ $\frac{1}{3},\frac{2}{3},1$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) m $x,\bar{x},z$	(5) m $x,2x,z$	(6) m $2x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	e	1	(1) x,y,z (4) $\bar{y},\bar{x},z$	(2) $\bar{y},x-y,z$ (5) $\bar{x}+y,y,z$	(3) $\bar{x}+y,\bar{x},z$ (6) $x,x-y,z$	no conditions
						Special: no extra conditions
3	d	$.m.$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	
1	c	$3m.$	$\frac{2}{3},\frac{1}{3},z$			
1	b	$3m.$	$\frac{1}{3},\frac{2}{3},z$			
1	a	$3m.$	$0,0,z$			

Symmetry of special projections

Along [001] $p3m1$
$\mathbf{a}' = \mathbf{a}$ $\quad \mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\quad \mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\quad \mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P311$ ($P3$, 143) 1; 2; 3
[3] $P1m1$ (Cm, 8) 1; 4
[3] $P1m1$ (Cm, 8) 1; 5
[3] $P1m1$ (Cm, 8) 1; 6

IIa none

IIb [2] $P3c1$ ($\mathbf{c}' = 2\mathbf{c}$) (158); [3] $H3m1$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P31m$, 157)

Maximal isomorphic subgroups of lowest index

IIc [2] $P3m1$ ($\mathbf{c}' = 2\mathbf{c}$) (156); [4] $P3m1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (156)

Minimal non-isomorphic supergroups

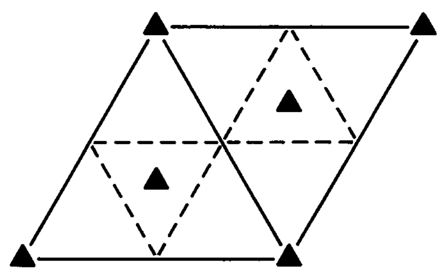
I [2] $P\bar{3}m1$ (164); [2] $P6mm$ (183); [2] $P6_3mc$ (186); [2] $P\bar{6}m2$ (187)

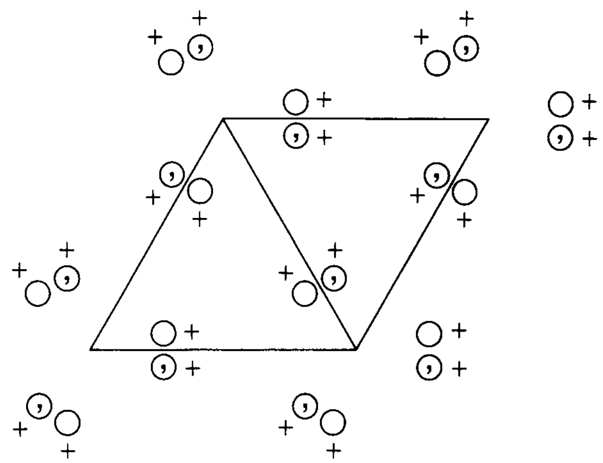
II [3] $H3m1$ ($P31m$, 157); [3] $R3m$ (obverse) (160); [3] $R3m$ (reverse) (160)

International Tables for Crystallography (2006). Vol. A, Space group 157, pp. 522–523.

$P\,3\,1\,m$ $\qquad C_{3v}^{2}$ $\qquad 3\,1\,m$ $\qquad$ Trigonal

No. 157 $\qquad P\,3\,1\,m$ $\qquad$ Patterson symmetry $P\,\bar{3}\,1\,m$





Origin on $3\,1\,m$

Asymmetric unit $\quad 0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le 1;\quad x \le (y+1)/2;\quad y \le \min(1-x, x)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{2},\frac{1}{2},0$

$0,0,1 \quad \frac{1}{2},0,1 \quad \frac{2}{3},\frac{1}{3},1 \quad \frac{1}{2},\frac{1}{2},1$

Symmetry operations

(1) 1	(2) $3^{+}\ 0,0,z$	(3) $3^{-}\ 0,0,z$
(4) $m\ \ x,x,z$	(5) $m\ \ x,0,z$	(6) $m\ \ 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	d	1	(1) x,y,z (4) y,x,z	(2) $\bar{y},x-y,z$ (5) $x-y,\bar{y},z$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x},\bar{x}+y,z$	no conditions
						Special: no extra conditions
3	c	$..m$	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	
2	b	$3..$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$		
1	a	$3.m$	$0,0,z$			

Symmetry of special projections

Along [001] $p31m$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P311$ ($P3$, 143) 1; 2; 3
$\left\{\begin{array}{ll} [3]\ P11m\ (Cm, 8) & 1;\ 4 \\ [3]\ P11m\ (Cm, 8) & 1;\ 5 \\ [3]\ P11m\ (Cm, 8) & 1;\ 6 \end{array}\right.$

IIa none

IIb [2] $P31c$ ($\mathbf{c}' = 2\mathbf{c}$) (159); [3] $H31m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P3m1$, 156); [3] $R3m$ ($\mathbf{a}' = \mathbf{a}-\mathbf{b}, \mathbf{b}' = \mathbf{a}+2\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (160); [3] $R3m$ ($\mathbf{a}' = 2\mathbf{a}+\mathbf{b}, \mathbf{b}' = -\mathbf{a}+\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (160)

Maximal isomorphic subgroups of lowest index

IIc [2] $P31m$ ($\mathbf{c}' = 2\mathbf{c}$) (157); [4] $P31m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (157)

Minimal non-isomorphic supergroups

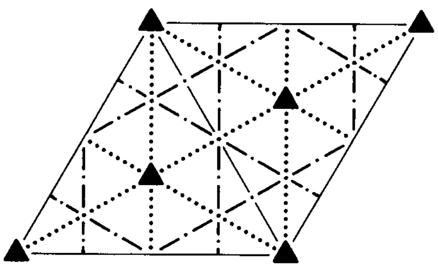
I [2] $P\bar{3}1m$ (162); [2] $P6mm$ (183); [2] $P6_3cm$ (185); [2] $P\bar{6}2m$ (189)

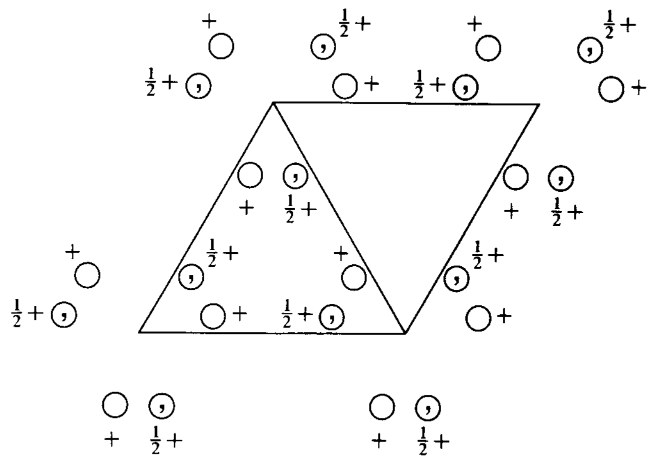
II [3] $H31m$ ($P3m1$, 156)

International Tables for Crystallography (2006). Vol. A, Space group 158, pp. 524–525.

$P3c1$ C_{3v}^3 $3m1$ Trigonal

No. 158 $P3c1$ Patterson symmetry $P\bar{3}m1$





Origin on $3c1$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$

$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) c $x,\bar{x},z$	(5) c $x,2x,z$	(6) c $2x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$h\bar{h}0l$: $l=2n$
			(4) $\bar{y},\bar{x},z+\frac{1}{2}$	(5) $\bar{x}+y,y,z+\frac{1}{2}$	(6) $x,x-y,z+\frac{1}{2}$	$000l$: $l=2n$
						Special: as above, plus
2	c	$3\,.\,.$	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$		$hkil$: $l=2n$
2	b	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},z+\frac{1}{2}$		$hkil$: $l=2n$
2	a	$3\,.\,.$	$0,0,z$	$0,0,z+\frac{1}{2}$		$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p3m1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1g1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P311$ ($P3$, 143) 1; 2; 3
[3] $P1c1$ (Cc, 9) 1; 4
[3] $P1c1$ (Cc, 9) 1; 5
[3] $P1c1$ (Cc, 9) 1; 6

IIa none

IIb [3] $H3c1$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P31c$, 159)

Maximal isomorphic subgroups of lowest index

IIc [3] $P3c1$ ($\mathbf{c}'=3\mathbf{c}$) (158); [4] $P3c1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (158)

Minimal non-isomorphic supergroups

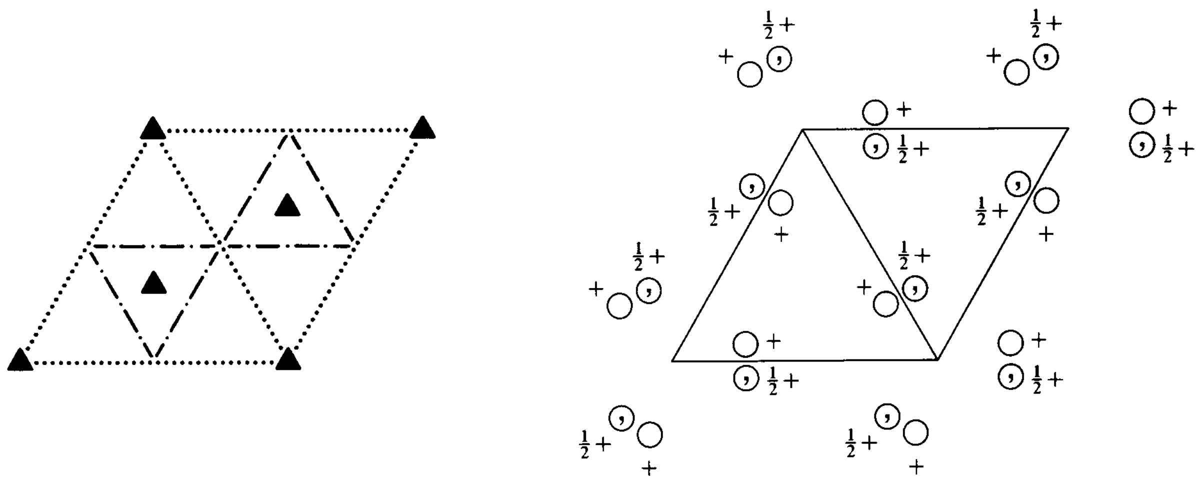
I [2] $P\bar{3}c1$ (165); [2] $P6cc$ (184); [2] $P6_3cm$ (185); [2] $P\bar{6}c2$ (188)

II [3] $H3c1$ ($P31c$, 159); [3] $R3c$ (obverse) (161); [3] $R3c$ (reverse) (161); [2] $P3m1$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (156)

International Tables for Crystallography (2006). Vol. A, Space group 159, pp. 526–527.

$P31c$ C_{3v}^4 $31m$ Trigonal

No. 159 $P31c$ Patterson symmetry $P\bar{3}1m$



Origin on $31c$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$

$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^{+} $0,0,z$	(3) 3^{-} $0,0,z$
(4) c x,x,z	(5) c $x,0,z$	(6) c $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	c	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$hh\overline{2h}l$: $l=2n$
			(4) $y,x,z+\frac{1}{2}$	(5) $x-y,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},\bar{x}+y,z+\frac{1}{2}$	$000l$: $l=2n$
						Special: as above, plus
2	b	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$		$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	a	$3\,.\,.$	$0,0,z$	$0,0,z+\frac{1}{2}$		$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p31m$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P311$ ($P3$, 143) 1; 2; 3
[3] $P11c$ (Cc, 9) 1; 4
[3] $P11c$ (Cc, 9) 1; 5
[3] $P11c$ (Cc, 9) 1; 6

IIa none

IIb [3] $H31c$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P3c1$, 158); [3] $R3c$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{a}+2\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (161);
[3] $R3c$ ($\mathbf{a}'=2\mathbf{a}+\mathbf{b},\mathbf{b}'=-\mathbf{a}+\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (161)

Maximal isomorphic subgroups of lowest index

IIc [3] $P31c$ ($\mathbf{c}'=3\mathbf{c}$) (159); [4] $P31c$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (159)

Minimal non-isomorphic supergroups

I [2] $P\bar{3}1c$ (163); [2] $P6cc$ (184); [2] $P6_3mc$ (186); [2] $P\bar{6}2c$ (190)

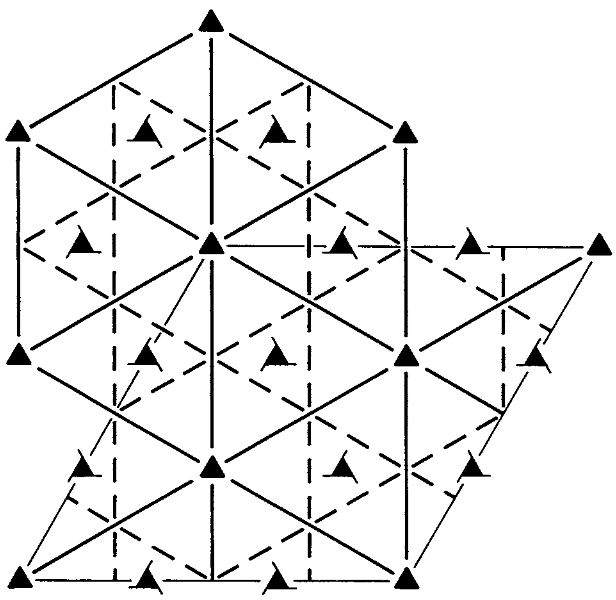
II [3] $H31c$ ($P3c1$, 158); [2] $P31m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (157)

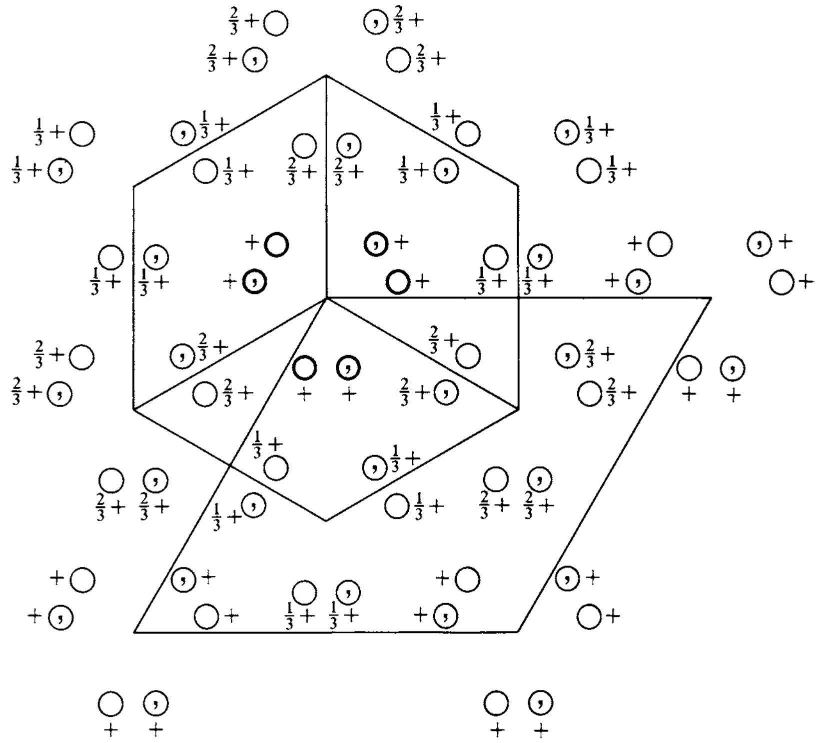
International Tables for Crystallography (2006). Vol. A, Space group 160, pp. 528–531.

$R3m$ $\quad C_{3v}^5$ $\quad 3m$ $\quad$ Trigonal

No. 160 $\quad R3m$ $\quad$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





Origin on $3m$

Asymmetric unit $\quad 0 \le x \le \frac{2}{3}$; $\quad 0 \le y \le \frac{2}{3}$; $\quad 0 \le z \le \frac{1}{3}$; $\quad x \le 2y$; $\quad y \le \min(1-x, 2x)$

Vertices $\quad 0,0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0$

$0,0,\frac{1}{3} \quad \frac{2}{3},\frac{1}{3},\frac{1}{3} \quad \frac{1}{3},\frac{2}{3},\frac{1}{3}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $3^+ \; 0,0,z$	(3) $3^- \; 0,0,z$
(4) $m \; x,\bar{x},z$	(5) $m \; x,2x,z$	(6) $m \; 2x,x,z$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	(2) $3^+(0,0,\frac{1}{3}) \; \frac{1}{3},\frac{1}{3},z$	(3) $3^-(0,0,\frac{1}{3}) \; \frac{1}{3},0,z$
(4) $g(\frac{1}{6},-\frac{1}{6},\frac{1}{3}) \; x+\frac{1}{2},\bar{x},z$	(5) $g(\frac{1}{6},\frac{1}{3},\frac{1}{3}) \; x+\frac{1}{4},2x,z$	(6) $g(\frac{2}{3},\frac{1}{3},\frac{1}{3}) \; 2x,x,z$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$	(2) $3^+(0,0,\frac{2}{3}) \; 0,\frac{1}{3},z$	(3) $3^-(0,0,\frac{2}{3}) \; \frac{1}{3},\frac{1}{3},z$
(4) $g(-\frac{1}{6},\frac{1}{6},\frac{2}{3}) \; x+\frac{1}{2},\bar{x},z$	(5) $g(\frac{1}{3},\frac{2}{3},\frac{2}{3}) \; x,2x,z$	(6) $g(\frac{1}{3},\frac{1}{6},\frac{2}{3}) \; 2x-\frac{1}{2},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
			$(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$	General:
18	c	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$hkil$: $-h+k+l=3n$
			(4) $\bar{y},\bar{x},z$	(5) $\bar{x}+y,y,z$	(6) $x,x-y,z$	$hki0$: $-h+k=3n$
						$hh\overline{2h}l$: $l=3n$
						$h\bar{h}0l$: $h+l=3n$
						$000l$: $l=3n$
						$h\bar{h}00$: $h=3n$
						Special: no extra conditions
9	b	$.m$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	
3	a	$3m$	$0,0,z$			

Symmetry of special projections

Along [001] $p31m$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $R31$ ($R3$, 146) (1; 2; 3)+
$\left\{\begin{array}{ll} [3]\ R1m\,(Cm, 8) & (1;\ 4)+ \\ [3]\ R1m\,(Cm, 8) & (1;\ 5)+ \\ [3]\ R1m\,(Cm, 8) & (1;\ 6)+ \end{array}\right.$

IIa [3] $P3m1$ (156) 1; 2; 3; 4; 5; 6

IIb [2] $R3c$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (161)

Maximal isomorphic subgroups of lowest index

IIc [2] $R3m$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (160); [4] $R3m$ ($\mathbf{a}'=-2\mathbf{a},\mathbf{b}'=-2\mathbf{b}$) (160)

Minimal non-isomorphic supergroups

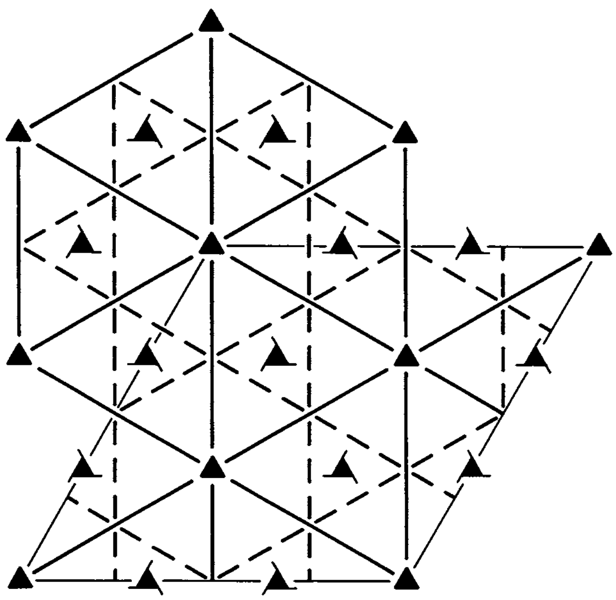
I [2] $R\bar{3}m$ (166); [4] $P\bar{4}3m$ (215); [4] $F\bar{4}3m$ (216); [4] $I\bar{4}3m$ (217)

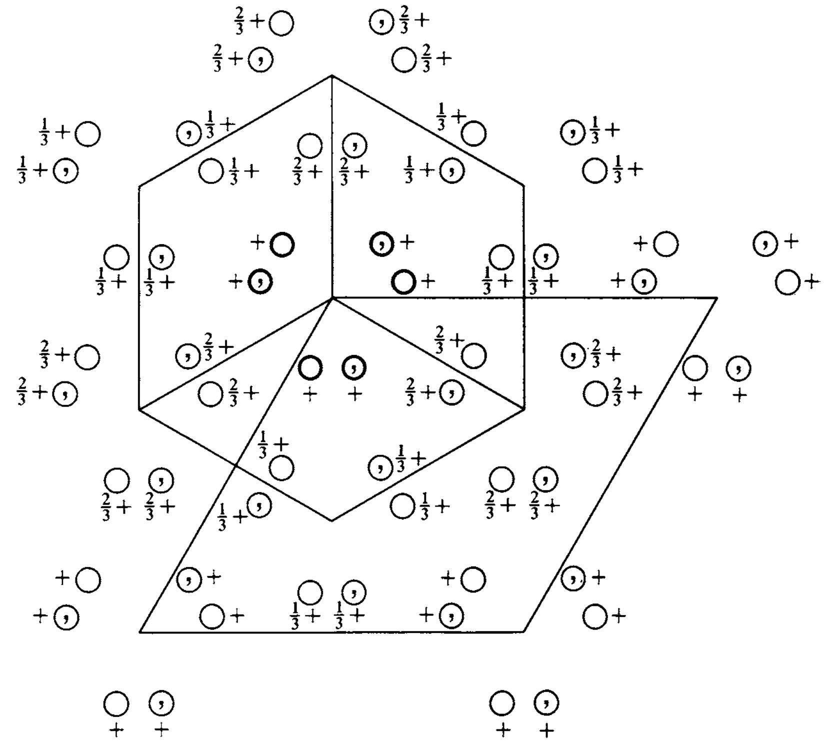
II [3] $P31m$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b}),\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (157)

$R3m$ C_{3v}^5 $3m$ Trigonal

No. 160 $R3m$ Patterson symmetry $R\bar{3}m$

RHOMBOHEDRAL AXES





Heights refer to hexagonal axes

Origin on $3m$

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le 1$; $y \le x$; $z \le y$

Vertices 0,0,0 1,0,0 1,1,0 1,1,1

Symmetry operations

(1) 1	(2) 3^+ x,x,x	(3) 3^- x,x,x
(4) m x,y,x	(5) m x,x,z	(6) m x,y,y

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	c	1	(1) x,y,z (4) z,y,x	(2) z,x,y (5) y,x,z	(3) y,z,x (6) x,z,y	no conditions
						Special: no extra conditions
3	b	$.m$	x,x,z	z,x,x	x,z,x	
1	a	$3m$	x,x,x			

Symmetry of special projections

Along [111] $p31m$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along $[1\bar{1}0]$ $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\bar{x},0$

Along $[2\bar{1}\bar{1}]$ $p1m1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

Maximal non-isomorphic subgroups

I [2] $R31$ ($R3$, 146) 1; 2; 3
[3] $R1m$ (Cm, 8) 1; 4
[3] $R1m$ (Cm, 8) 1; 5
[3] $R1m$ (Cm, 8) 1; 6

IIa none

IIb [2] $F3c$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($R3c$, 161); [3] $P3m1$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{b}-\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (156)

Maximal isomorphic subgroups of lowest index

IIc [2] $R3m$ ($\mathbf{a}'=\mathbf{b}+\mathbf{c},\mathbf{b}'=\mathbf{a}+\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}$) (160); [4] $R3m$ ($\mathbf{a}'=-\mathbf{a}+\mathbf{b}+\mathbf{c},\mathbf{b}'=\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}-\mathbf{c}$) (160)

Minimal non-isomorphic supergroups

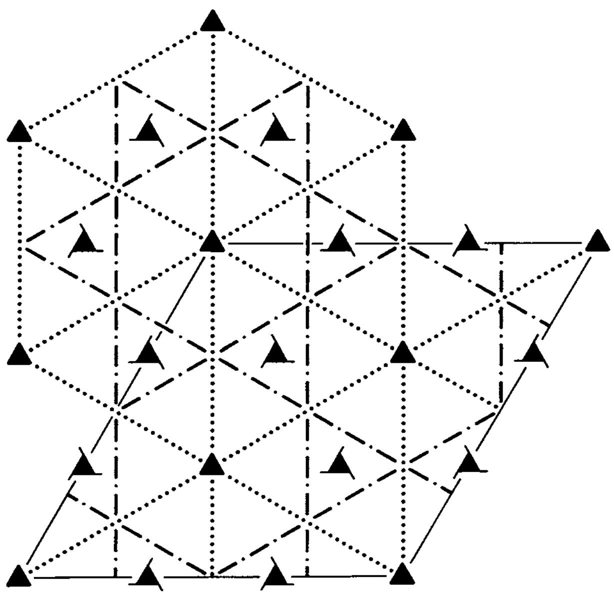
I [2] $R\bar{3}m$ (166); [4] $P\bar{4}3m$ (215); [4] $F\bar{4}3m$ (216); [4] $I\bar{4}3m$ (217)

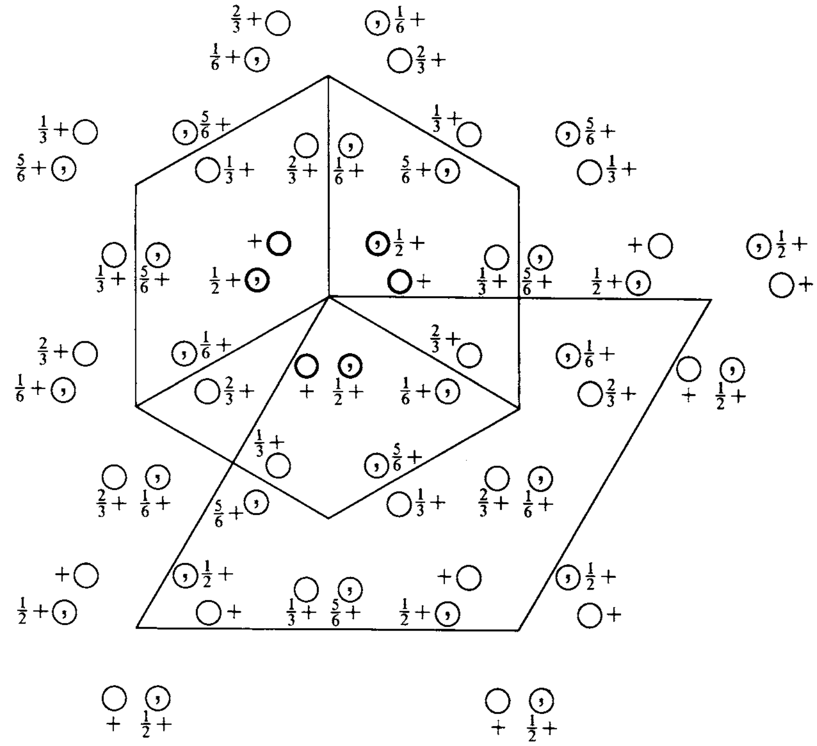
II [3] $P31m$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}),\mathbf{c}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$) (157)

$R3c$ $\quad C_{3v}^{6}$ $\quad 3m$ $\quad$ Trigonal

No. 161 $\quad R3c$ $\quad$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





Origin on $3c$

Asymmetric unit $\quad 0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{2}{3};\quad 0 \le z \le \frac{1}{6};\quad x \le (1+y)/2;\quad y \le \min(1-x,(1+x)/2)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0 \quad 0,\frac{1}{2},0$

$0,0,\frac{1}{6} \quad \frac{1}{2},0,\frac{1}{6} \quad \frac{2}{3},\frac{1}{3},\frac{1}{6} \quad \frac{1}{3},\frac{2}{3},\frac{1}{6} \quad 0,\frac{1}{2},\frac{1}{6}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $3^{+}\ 0,0,z$	(3) $3^{-}\ 0,0,z$
(4) $c\quad x,\bar{x},z$	(5) $c\quad x,2x,z$	(6) $c\quad 2x,x,z$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	(2) $3^{+}(0,0,\frac{1}{3})\quad \frac{1}{3},\frac{1}{3},z$	(3) $3^{-}(0,0,\frac{1}{3})\quad \frac{1}{3},0,z$
(4) $g(\frac{1}{6},-\frac{1}{6},\frac{5}{6})\quad x+\frac{1}{2},\bar{x},z$	(5) $g(\frac{1}{6},\frac{1}{3},\frac{5}{6})\quad x+\frac{1}{4},2x,z$	(6) $g(\frac{2}{3},\frac{1}{3},\frac{5}{6})\quad 2x,x,z$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$	(2) $3^{+}(0,0,\frac{2}{3})\quad 0,\frac{1}{3},z$	(3) $3^{-}(0,0,\frac{2}{3})\quad \frac{1}{3},\frac{1}{3},z$
(4) $g(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\quad x+\frac{1}{2},\bar{x},z$	(5) $g(\frac{1}{3},\frac{2}{3},\frac{1}{6})\quad x,2x,z$	(6) $g(\frac{1}{3},\frac{1}{6},\frac{1}{6})\quad 2x-\frac{1}{2},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
			$(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$	General:
18	b	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$hkil$: $-h+k+l=3n$
			(4) $\bar{y},\bar{x},z+\frac{1}{2}$	(5) $\bar{x}+y,y,z+\frac{1}{2}$	(6) $x,x-y,z+\frac{1}{2}$	$hki0$: $-h+k=3n$
						$hh\overline{2h}l$: $l=3n$
						$h\bar{h}0l$: $h+l=3n$, $l=2n$
						$000l$: $l=6n$
						$h\bar{h}00$: $h=3n$
						Special: as above, plus
6	a	$3.$	$0,0,z$	$0,0,z+\frac{1}{2}$		$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p31m$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}'=\frac{1}{6}(2\mathbf{a}+4\mathbf{b}+\mathbf{c})$ $\mathbf{b}'=\frac{1}{6}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

Along [210] $p1g1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $R31$ ($R3$, 146) (1; 2; 3)+
{ [3] $R1c$ (Cc, 9) (1; 4)+
[3] $R1c$ (Cc, 9) (1; 5)+
[3] $R1c$ (Cc, 9) (1; 6)+

IIa [3] $P3c1$ (158) 1; 2; 3; 4; 5; 6

IIb none

Maximal isomorphic subgroups of lowest index

IIc [4] $R3c$ ($\mathbf{a}'=-2\mathbf{a},\mathbf{b}'=-2\mathbf{b}$) (161); [5] $R3c$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=5c$) (161)

Minimal non-isomorphic supergroups

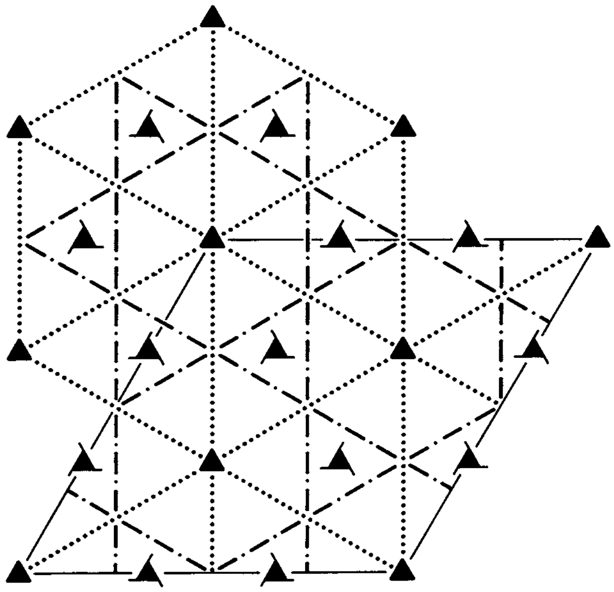
I [2] $R\bar{3}c$ (167); [4] $P\bar{4}3n$ (218); [4] $F\bar{4}3c$ (219); [4] $I\bar{4}3d$ (220)

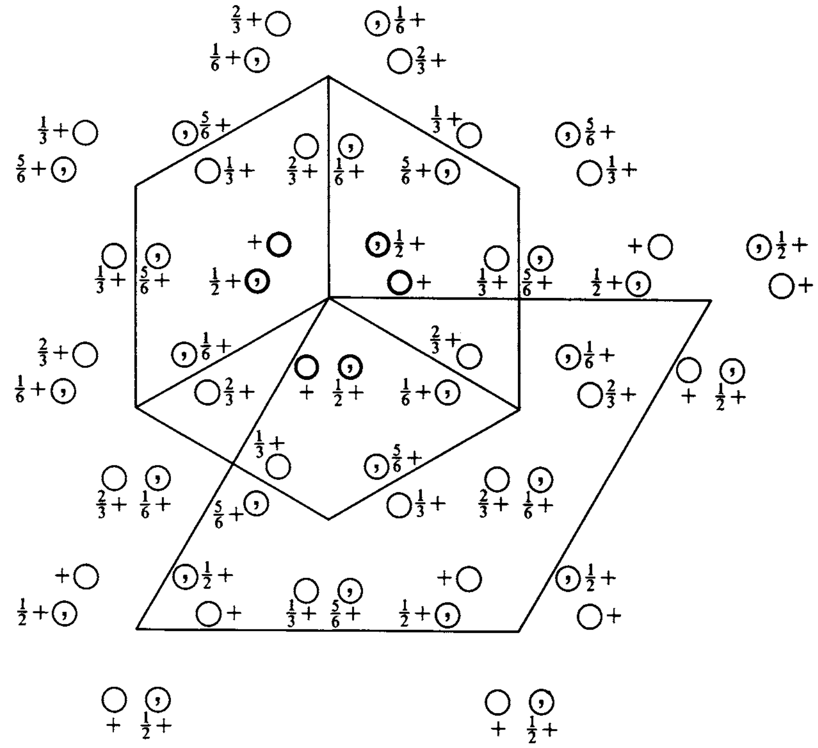
II [2] $R3m$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (160); [3] $P31c$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b}),\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (159)

$R3c$ $\quad C_{3v}^{6}$ $\quad 3m$ $\quad$ Trigonal

No. 161 $\quad R3c$ $\quad$ Patterson symmetry $R\bar{3}m$

RHOMBOHEDRAL AXES





Heights refer to hexagonal axes

Origin on $3c$

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le 1; \quad y \le x; \quad z \le y$

Vertices $\quad 0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 1,1,1$

Symmetry operations

(1) 1	(2) $3^{+}\ x,x,x$	(3) $3^{-}\ x,x,x$
(4) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,y,x$	(5) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,z$	(6) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,y,y$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	b	1	(1) x,y,z	(2) z,x,y	(3) y,z,x	hhl : $l=2n$
			(4) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(5) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(6) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	hhh : $h=2n$
						Special: as above, plus
2	a	3 .	x,x,x	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$		hkl : $h+k+l=2n$

Symmetry of special projections

Along [111] $p31m$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along $[1\bar{1}0]$ $p1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\bar{x},0$

Along $[2\bar{1}\bar{1}]$ $p1g1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

Maximal non-isomorphic subgroups

I [2] $R31$ ($R3$, 146) 1; 2; 3
[3] $R1c$ (Cc, 9) 1; 4
[3] $R1c$ (Cc, 9) 1; 5
[3] $R1c$ (Cc, 9) 1; 6

IIa none

IIb [3] $P3c1$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{b}-\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (158)

Maximal isomorphic subgroups of lowest index

IIc [4] $R3c$ ($\mathbf{a}'=-\mathbf{a}+\mathbf{b}+\mathbf{c},\mathbf{b}'=\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}-\mathbf{c}$) (161); [5] $R3c$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b}+2\mathbf{c},\mathbf{b}'=2\mathbf{a}+\mathbf{b}+2\mathbf{c},\mathbf{c}'=2\mathbf{a}+2\mathbf{b}+\mathbf{c}$) (161)

Minimal non-isomorphic supergroups

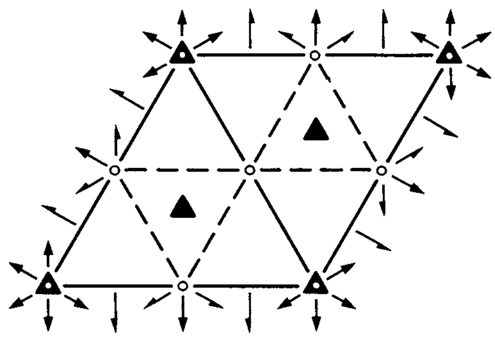
I [2] $R\bar{3}c$ (167); [4] $P\bar{4}3n$ (218); [4] $F\bar{4}3c$ (219); [4] $I\bar{4}3d$ (220)

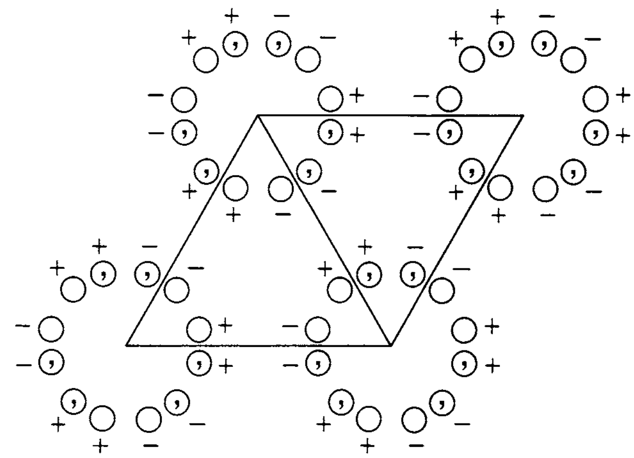
II [2] $R3m$ ($\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}),\mathbf{b}'=\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c}),\mathbf{c}'=\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$) (160);
[3] $P31c$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}),\mathbf{c}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$) (159)

International Tables for Crystallography (2006). Vol. A, Space group 162, pp. 536–537.

$P\bar{3}1m$ D_{3d}^1 $\bar{3}1m$ Trigonal

No. 162 $P\bar{3}12/m$ Patterson symmetry $P\bar{3}1m$





Origin at centre ($\bar{3}1m$)

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x, x)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{2},\frac{1}{2},0$

$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) 2 $x,\bar{x},0$	(5) 2 $x,2x,0$	(6) 2 $2x,x,0$
(7) $\bar{1}$ $0,0,0$	(8) $\bar{3}^+$ $0,0,z$; $0,0,0$	(9) $\bar{3}^-$ $0,0,z$; $0,0,0$
(10) m x,x,z	(11) m $x,0,z$	(12) m $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	l	1	(1) x,y,z (4) $\bar{y},\bar{x},\bar{z}$ (7) $\bar{x},\bar{y},\bar{z}$ (10) y,x,z	(2) $\bar{y},x-y,z$ (5) $\bar{x}+y,y,\bar{z}$ (8) $y,\bar{x}+y,\bar{z}$ (11) $x-y,\bar{y},z$	(3) $\bar{x}+y,\bar{x},z$ (6) $x,x-y,\bar{z}$ (9) $x-y,x,\bar{z}$ (12) $\bar{x},\bar{x}+y,z$				no conditions
									Special: no extra conditions
6	k	$..m$	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$0,\bar{x},\bar{z}$	$\bar{x},0,\bar{z}$	$x,x,\bar{z}$	
6	j	$..2$	$x,\bar{x},\frac{1}{2}$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{1}{2}$	
6	i	$..2$	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	$\bar{x},x,0$	$\bar{x},2\bar{x},0$	$2x,x,0$	
4	h	$3..$	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},z$			
3	g	$..2/m$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
3	f	$..2/m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$				
2	e	$3.m$	$0,0,z$	$0,0,\bar{z}$					
2	d	3.2	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$					
2	c	3.2	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$					
1	b	$\bar{3}.m$	$0,0,\frac{1}{2}$						
1	a	$\bar{3}.m$	$0,0,0$						

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I
- [2] $P31m$ (157) 1; 2; 3; 10; 11; 12
- [2] $P312$ (149) 1; 2; 3; 4; 5; 6
- [2] $P\bar{3}11$ ($P\bar{3}$, 147) 1; 2; 3; 7; 8; 9
- { [3] $P112/m$ ($C2/m$, 12) 1; 4; 7; 10
- [3] $P112/m$ ($C2/m$, 12) 1; 5; 7; 11
- [3] $P112/m$ ($C2/m$, 12) 1; 6; 7; 12

IIa none

IIb [2] $P\bar{3}1c$ ($\mathbf{c}'=2\mathbf{c}$) (163); [3] $H\bar{3}1m$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P\bar{3}m1$, 164); [3] $R\bar{3}m$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{a}+2\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (166); [3] $R\bar{3}m$ ($\mathbf{a}'=2\mathbf{a}+\mathbf{b},\mathbf{b}'=-\mathbf{a}+\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (166)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{3}1m$ ($\mathbf{c}'=2\mathbf{c}$) (162); [4] $P\bar{3}1m$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (162)

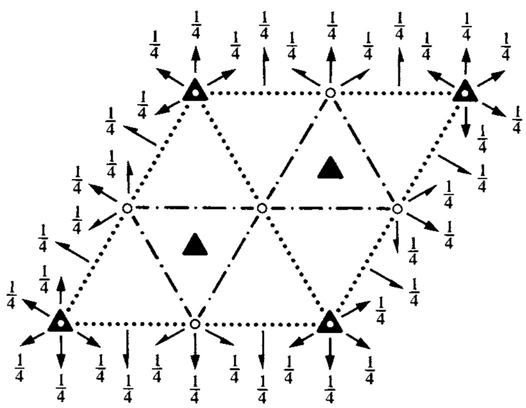
Minimal non-isomorphic supergroups

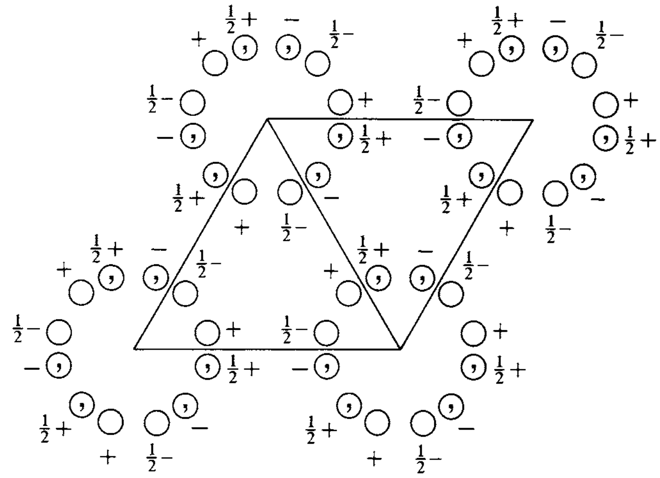
I [2] $P6/mmm$ (191); [2] $P6_3/mcm$ (193)

II [3] $H\bar{3}1m$ ($P\bar{3}m1$, 164)

$P\bar{3}1c$ $\quad D_{3d}^{2}$ $\quad \bar{3}1m$ $\quad$ Trigonal

No. 163 $\quad P\bar{3}12/c$ $\quad$ Patterson symmetry $P\bar{3}1m$





Origin at centre ($\bar{3}$) at $\bar{3}1c$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $\quad 0 \le y \le \frac{2}{3}$; $\quad 0 \le z \le \frac{1}{4}$; $\quad x \le (1+y)/2$; $\quad y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0 \quad 0,\frac{1}{2},0$

$0,0,\frac{1}{4} \quad \frac{1}{2},0,\frac{1}{4} \quad \frac{2}{3},\frac{1}{3},\frac{1}{4} \quad \frac{1}{3},\frac{2}{3},\frac{1}{4} \quad 0,\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1	(2) $3^{+}\ 0,0,z$	(3) $3^{-}\ 0,0,z$
(4) $2\quad x,\bar{x},\frac{1}{4}$	(5) $2\quad x,2x,\frac{1}{4}$	(6) $2\quad 2x,x,\frac{1}{4}$
(7) $\bar{1}\quad 0,0,0$	(8) $\bar{3}^{+}\ 0,0,z;\ 0,0,0$	(9) $\bar{3}^{-}\ 0,0,z;\ 0,0,0$
(10) $c\quad x,x,z$	(11) $c\quad x,0,z$	(12) $c\quad 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	Reflection conditions
				General:
12	*i*	1	(1) x,y,z (2) $\bar{y},x-y,z$ (3) $\bar{x}+y,\bar{x},z$ (4) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$ (5) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$ (6) $x,x-y,\bar{z}+\frac{1}{2}$ (7) $\bar{x},\bar{y},\bar{z}$ (8) $y,\bar{x}+y,\bar{z}$ (9) $x-y,x,\bar{z}$ (10) $y,x,z+\frac{1}{2}$ (11) $x-y,\bar{y},z+\frac{1}{2}$ (12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$	$hh\overline{2h}l$: $l=2n$; $000l$: $l=2n$
				Special: as above, plus
6	*h*	. . 2	$x,\bar{x},\frac{1}{4}$ $x,2x,\frac{1}{4}$ $2\bar{x},\bar{x},\frac{1}{4}$ $\bar{x},x,\frac{3}{4}$ $\bar{x},2\bar{x},\frac{3}{4}$ $2x,x,\frac{3}{4}$	no extra conditions
6	*g*	$\bar{1}$	$\frac{1}{2},0,0$ $0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
4	*f*	3 . .	$\frac{1}{3},\frac{2}{3},z$ $\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\bar{z}$ $\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
4	*e*	3 . .	$0,0,z$ $0,0,\bar{z}+\frac{1}{2}$ $0,0,\bar{z}$ $0,0,z+\frac{1}{2}$	$hkil$: $l=2n$
2	*d*	3 . 2	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\frac{1}{3},\frac{2}{3},\frac{3}{4}$	$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	*c*	3 . 2	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{3}{4}$	$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	*b*	$\bar{3}$ . .	$0,0,0$ $0,0,\frac{1}{2}$	$hkil$: $l=2n$
2	*a*	3 . 2	$0,0,\frac{1}{4}$ $0,0,\frac{3}{4}$	$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I
- [2] $P31c$ (159) 1; 2; 3; 10; 11; 12
- [2] $P312$ (149) 1; 2; 3; 4; 5; 6
- [2] $P\bar{3}11$ ($P\bar{3}$, 147) 1; 2; 3; 7; 8; 9
- { [3] $P112/c$ ($C2/c$, 15) 1; 4; 7; 10
- [3] $P112/c$ ($C2/c$, 15) 1; 5; 7; 11
- [3] $P112/c$ ($C2/c$, 15) 1; 6; 7; 12

IIa none

IIb [3] $H\bar{3}1c$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P\bar{3}c1$, 165); [3] $R\bar{3}c$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{a}+2\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (167); [3] $R\bar{3}c$ ($\mathbf{a}'=2\mathbf{a}+\mathbf{b},\mathbf{b}'=-\mathbf{a}+\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (167)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{3}1c$ ($\mathbf{c}'=3\mathbf{c}$) (163); [4] $P\bar{3}1c$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (163)

Minimal non-isomorphic supergroups

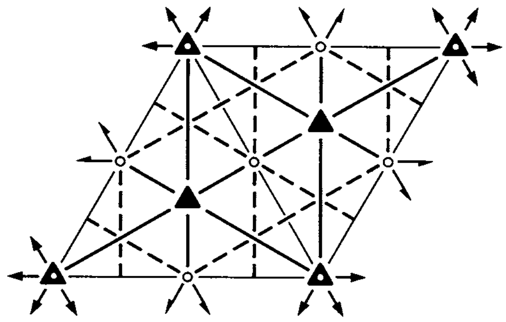
I [2] $P6/mcc$ (192); [2] $P6_3/mmc$ (194)

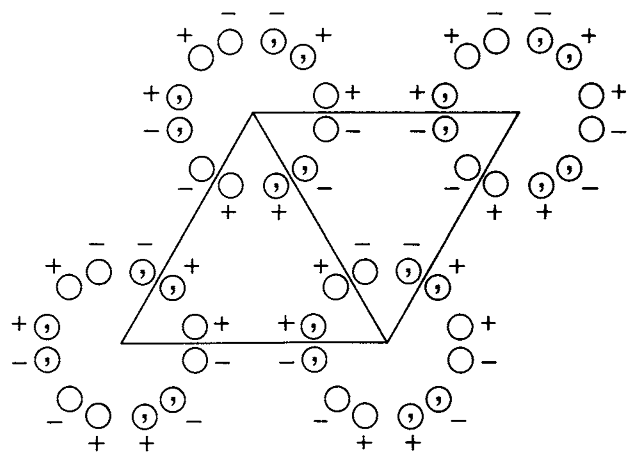
II [3] $H\bar{3}1c$ ($P\bar{3}c1$, 165); [2] $P\bar{3}1m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (162)

International Tables for Crystallography (2006). Vol. A, Space group 164, pp. 540–541.

$P\bar{3}m1$ D_{3d}^{3} $\bar{3}m1$ Trigonal

No. 164 $P\bar{3}2/m1$ Patterson symmetry $P\bar{3}m1$





Origin at centre ($\bar{3}m1$)

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{3}$; $0 \le z \le 1$; $x \le (1+y)/2$; $y \le x/2$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$

$0,0,1$ $\frac{1}{2},0,1$ $\frac{2}{3},\frac{1}{3},1$

Symmetry operations

(1) 1	(2) 3^{+} $0,0,z$	(3) 3^{-} $0,0,z$
(4) 2 $x,x,0$	(5) 2 $x,0,0$	(6) 2 $0,y,0$
(7) $\bar{1}$ $0,0,0$	(8) $\bar{3}^{+}$ $0,0,z$; $0,0,0$	(9) $\bar{3}^{-}$ $0,0,z$; $0,0,0$
(10) m $x,\bar{x},z$	(11) m $x,2x,z$	(12) m $2x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	j	1	(1) x,y,z (4) $y,x,\bar{z}$ (7) $\bar{x},\bar{y},\bar{z}$ (10) $\bar{y},\bar{x},z$	(2) $\bar{y},x-y,z$ (5) $x-y,\bar{y},\bar{z}$ (8) $y,\bar{x}+y,\bar{z}$ (11) $\bar{x}+y,y,z$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x},\bar{x}+y,\bar{z}$ (9) $x-y,x,\bar{z}$ (12) $x,x-y,z$				no conditions
									Special: no extra conditions
6	i	$.m.$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$2x,x,\bar{z}$	$\bar{x},2\bar{x},\bar{z}$	
6	h	$.2.$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	
6	g	$.2.$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	
3	f	$.2/m.$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
3	e	$.2/m.$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$				
2	d	$3m.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$					
2	c	$3m.$	$0,0,z$	$0,0,\bar{z}$					
1	b	$\bar{3}m.$	$0,0,\frac{1}{2}$						
1	a	$\bar{3}m.$	$0,0,0$						

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P3m1$ (156) 1; 2; 3; 10; 11; 12
[2] $P321$ (150) 1; 2; 3; 4; 5; 6
[2] $P\bar{3}11$ ($P\bar{3}$, 147) 1; 2; 3; 7; 8; 9
$\left\{\begin{array}{l}\text{[3] } P12/m1\ (C2/m,\ 12)\quad 1;\ 4;\ 7;\ 10\\ \text{[3] } P12/m1\ (C2/m,\ 12)\quad 1;\ 5;\ 7;\ 11\\ \text{[3] } P12/m1\ (C2/m,\ 12)\quad 1;\ 6;\ 7;\ 12\end{array}\right.$

IIa none

IIb [2] $P\bar{3}c1$ ($\mathbf{c}'=2\mathbf{c}$) (165); [3] $H\bar{3}m1$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P\bar{3}1m$, 162)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{3}m1$ ($\mathbf{c}'=2\mathbf{c}$) (164); [4] $P\bar{3}m1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (164)

Minimal non-isomorphic supergroups

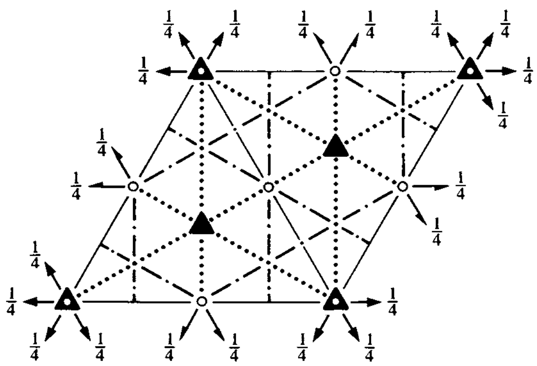
I [2] $P6/mmm$ (191); [2] $P6_3/mmc$ (194)

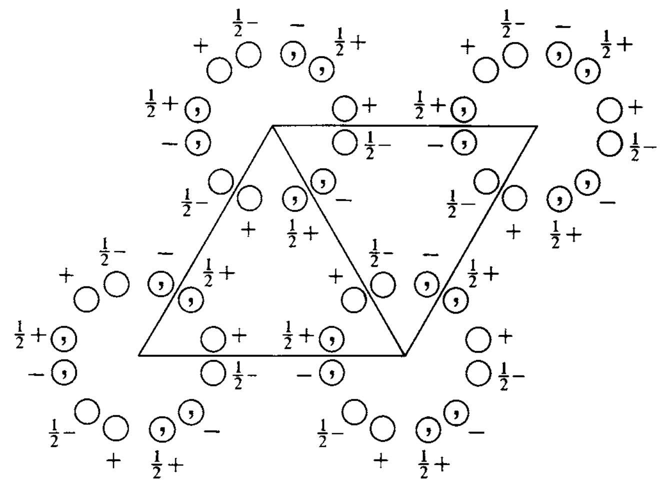
II [3] $H\bar{3}m1$ ($P\bar{3}1m$, 162); [3] $R\bar{3}m$ (obverse) (166); [3] $R\bar{3}m$ (reverse) (166)

International Tables for Crystallography (2006). Vol. A, Space group 165, pp. 542–543.

$P\bar{3}c1$ $\quad D_{3d}^{4}$ $\quad \bar{3}m1$ $\quad$ Trigonal

No. 165 $\quad P\bar{3}2/c1$ $\quad$ Patterson symmetry $P\bar{3}m1$





Origin at centre ($\bar{3}$) at $\bar{3}c1$

Asymmetric unit $\quad 0 \le x \le \frac{2}{3}$; $\quad 0 \le y \le \frac{2}{3}$; $\quad 0 \le z \le \frac{1}{4}$; $\quad x \le (1+y)/2$; $\quad y \le \min(1-x,(1+x)/2)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0 \quad 0,\frac{1}{2},0$

$0,0,\frac{1}{4} \quad \frac{1}{2},0,\frac{1}{4} \quad \frac{2}{3},\frac{1}{3},\frac{1}{4} \quad \frac{1}{3},\frac{2}{3},\frac{1}{4} \quad 0,\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1	(2) $3^{+}\ 0,0,z$	(3) $3^{-}\ 0,0,z$
(4) $2\ \ x,x,\frac{1}{4}$	(5) $2\ \ x,0,\frac{1}{4}$	(6) $2\ \ 0,y,\frac{1}{4}$
(7) $\bar{1}\ \ 0,0,0$	(8) $\bar{3}^{+}\ 0,0,z;\ \ 0,0,0$	(9) $\bar{3}^{-}\ 0,0,z;\ \ 0,0,0$
(10) $c\ \ x,\bar{x},z$	(11) $c\ \ x,2x,z$	(12) $c\ \ 2x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	g	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$h\bar{h}0l$: $l=2n$
			(4) $y,x,\bar{z}+\frac{1}{2}$	(5) $x-y,\bar{y},\bar{z}+\frac{1}{2}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$				$000l$: $l=2n$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$				
			(10) $\bar{y},\bar{x},z+\frac{1}{2}$	(11) $\bar{x}+y,y,z+\frac{1}{2}$	(12) $x,x-y,z+\frac{1}{2}$				
									Special: as above, plus
6	f	. 2 .	$x,0,\frac{1}{4}$	$0,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$0,\bar{x},\frac{3}{4}$	$x,x,\frac{3}{4}$	no extra conditions
6	e	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
4	d	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},z+\frac{1}{2}$			$hkil$: $l=2n$
4	c	3 . .	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$			$hkil$: $l=2n$
2	b	$\bar{3}$ . .	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$
2	a	3 2 .	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P3c1$ (158) 1; 2; 3; 10; 11; 12
[2] $P321$ (150) 1; 2; 3; 4; 5; 6
[2] $P\bar{3}11$ ($P\bar{3}$, 147) 1; 2; 3; 7; 8; 9
$\left\{\begin{array}{l}\text{[3] } P12/c1\ (C2/c,\ 15)\quad 1;\ 4;\ 7;\ 10\\ \text{[3] } P12/c1\ (C2/c,\ 15)\quad 1;\ 5;\ 7;\ 11\\ \text{[3] } P12/c1\ (C2/c,\ 15)\quad 1;\ 6;\ 7;\ 12\end{array}\right.$

IIa none

IIb [3] $H\bar{3}c1$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P\bar{3}1c$, 163)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{3}c1$ ($\mathbf{c}'=3\mathbf{c}$) (165); [4] $P\bar{3}c1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (165)

Minimal non-isomorphic supergroups

I [2] $P6/mcc$ (192); [2] $P6_3/mcm$ (193)

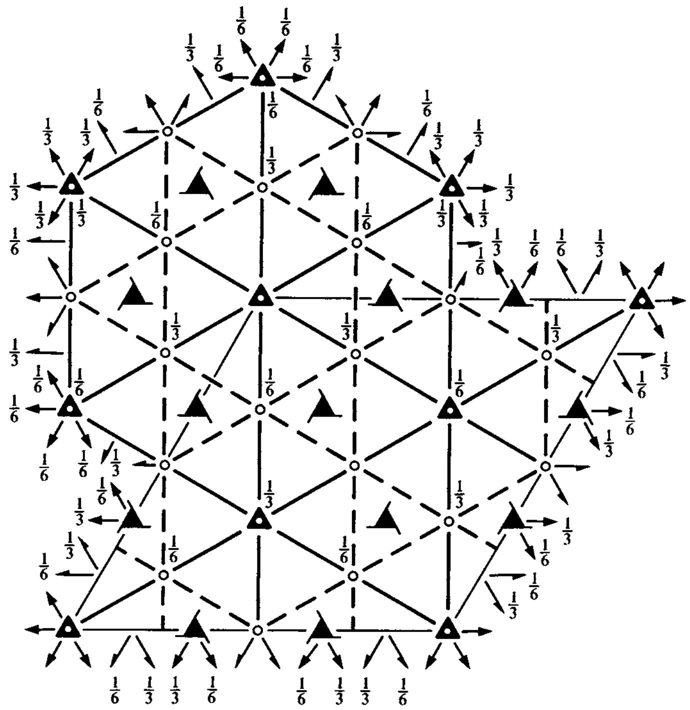
II [3] $H\bar{3}c1$ ($P\bar{3}1c$, 163); [3] $R\bar{3}c$ (obverse) (167); [3] $R\bar{3}c$ (reverse) (167); [2] $P\bar{3}m1$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (164)

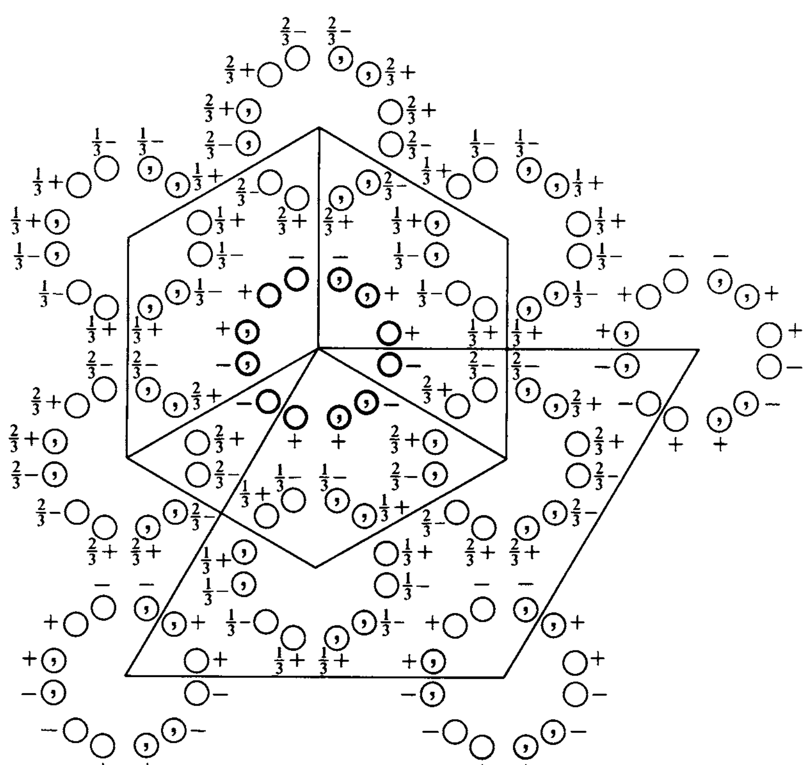
International Tables for Crystallography (2006). Vol. A, Space group 166, pp. 544–547.

$R\bar{3}m$ D_{3d}^{5} $\bar{3}m$ Trigonal

No. 166 $R\bar{3}2/m$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





Origin at centre ($\bar{3}m$)

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{6}$; $x \le 2y$; $y \le \min(1-x, 2x)$

Vertices $0,0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$

$0,0,\frac{1}{6}$ $\frac{2}{3},\frac{1}{3},\frac{1}{6}$ $\frac{1}{3},\frac{2}{3},\frac{1}{6}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $3^{+}\ 0,0,z$	(3) $3^{-}\ 0,0,z$
(4) $2\ \ x,x,0$	(5) $2\ \ x,0,0$	(6) $2\ \ 0,y,0$
(7) $\bar{1}\ \ 0,0,0$	(8) $\bar{3}^{+}\ 0,0,z;\ 0,0,0$	(9) $\bar{3}^{-}\ 0,0,z;\ 0,0,0$
(10) $m\ \ x,\bar{x},z$	(11) $m\ \ x,2x,z$	(12) $m\ \ 2x,x,z$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	(2) $3^{+}(0,0,\frac{1}{3})\ \ \frac{1}{3},\frac{1}{3},z$	(3) $3^{-}(0,0,\frac{1}{3})\ \ \frac{1}{3},0,z$
(4) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x-\frac{1}{6},\frac{1}{6}$	(5) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{6},\frac{1}{6}$	(6) $2\ \ \frac{1}{3},y,\frac{1}{6}$
(7) $\bar{1}\ \ \frac{1}{3},\frac{1}{6},\frac{1}{6}$	(8) $\bar{3}^{+}\ \frac{1}{3},-\frac{1}{3},z;\ \ \frac{1}{3},-\frac{1}{3},\frac{1}{6}$	(9) $\bar{3}^{-}\ \frac{1}{3},\frac{2}{3},z;\ \ \frac{1}{3},\frac{2}{3},\frac{1}{6}$
(10) $g(\frac{1}{6},-\frac{1}{6},\frac{1}{3})\ \ x+\frac{1}{2},\bar{x},z$	(11) $g(\frac{1}{6},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{4},2x,z$	(12) $g(\frac{2}{3},\frac{1}{3},\frac{1}{3})\ \ 2x,x,z$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$	(2) $3^{+}(0,0,\frac{2}{3})\ \ 0,\frac{1}{3},z$	(3) $3^{-}(0,0,\frac{2}{3})\ \ \frac{1}{3},\frac{1}{3},z$
(4) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x+\frac{1}{6},\frac{1}{3}$	(5) $2\ \ x,\frac{1}{3},\frac{1}{3}$	(6) $2(0,\frac{1}{2},0)\ \ \frac{1}{6},y,\frac{1}{3}$
(7) $\bar{1}\ \ \frac{1}{6},\frac{1}{3},\frac{1}{3}$	(8) $\bar{3}^{+}\ \frac{2}{3},\frac{1}{3},z;\ \ \frac{2}{3},\frac{1}{3},\frac{1}{3}$	(9) $\bar{3}^{-}\ -\frac{1}{3},\frac{1}{3},z;\ \ -\frac{1}{3},\frac{1}{3},\frac{1}{3}$
(10) $g(-\frac{1}{6},\frac{1}{6},\frac{2}{3})\ \ x+\frac{1}{2},\bar{x},z$	(11) $g(\frac{1}{3},\frac{2}{3},\frac{2}{3})\ \ x,2x,z$	(12) $g(\frac{1}{3},\frac{1}{6},\frac{2}{3})\ \ 2x-\frac{1}{2},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates: $(0,0,0)+\quad(\frac{2}{3},\frac{1}{3},\frac{1}{3})+\quad(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ — Reflection conditions

									Reflection conditions
36	i	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				General:
			(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}$	(6) $\bar{x},\bar{x}+y,\bar{z}$				$hkil$: $-h+k+l=3n$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$				$hki0$: $-h+k=3n$
			(10) $\bar{y},\bar{x},z$	(11) $\bar{x}+y,y,z$	(12) $x,x-y,z$				$hh\overline{2h}l$: $l=3n$
									$h\bar{h}0l$: $h+l=3n$
									$000l$: $l=3n$
									$h\bar{h}00$: $h=3n$
									Special: no extra conditions
18	h	$.m$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$2x,x,\bar{z}$	$\bar{x},2\bar{x},\bar{z}$	
18	g	$.2$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	
18	f	$.2$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	
9	e	$.2/m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$				
9	d	$.2/m$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
6	c	$3m$	$0,0,z$	$0,0,\bar{z}$					
3	b	$\bar{3}m$	$0,0,\frac{1}{2}$						
3	a	$\bar{3}m$	$0,0,0$						

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})\qquad \mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})\qquad \mathbf{b}'=\frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}\qquad \mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

HEXAGONAL AXES

Maximal non-isomorphic subgroups

I	[2] $R3m$ (160)	(1; 2; 3; 10; 11; 12)+
	[2] $R32$ (155)	(1; 2; 3; 4; 5; 6)+
	[2] $R\bar{3}1$ ($R\bar{3}$, 148)	(1; 2; 3; 7; 8; 9)+
	{ [3] $R12/m$ ($C2/m$, 12)	(1; 4; 7; 10)+
	{ [3] $R12/m$ ($C2/m$, 12)	(1; 5; 7; 11)+
	{ [3] $R12/m$ ($C2/m$, 12)	(1; 6; 7; 12)+
IIa	{ [3] $P\bar{3}m1$ (164)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	{ [3] $P\bar{3}m1$ (164)	1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$
	{ [3] $P\bar{3}m1$ (164)	1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$
IIb	[2] $R\bar{3}c$ ($\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (167)	

Maximal isomorphic subgroups of lowest index

IIc [2] $R\bar{3}m$ ($\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (166); [4] $R\bar{3}m$ ($\mathbf{a}' = -2\mathbf{a}, \mathbf{b}' = -2\mathbf{b}$) (166)

Minimal non-isomorphic supergroups

I [4] $Pm\bar{3}m$ (221); [4] $Pn\bar{3}m$ (224); [4] $Fm\bar{3}m$ (225); [4] $Fd\bar{3}m$ (227); [4] $Im\bar{3}m$ (229)

II [3] $P\bar{3}1m$ ($\mathbf{a}' = \frac{1}{3}(2\mathbf{a}+\mathbf{b}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a}+\mathbf{b}), \mathbf{c}' = \frac{1}{3}\mathbf{c}$) (162)

RHOMBOHEDRAL AXES

Maximal non-isomorphic subgroups

I	[2] $R3m$ (160)	1; 2; 3; 10; 11; 12
	[2] $R32$ (155)	1; 2; 3; 4; 5; 6
	[2] $R\bar{3}1$ ($R\bar{3}$, 148)	1; 2; 3; 7; 8; 9
	{ [3] $R12/m$ ($C2/m$, 12)	1; 4; 7; 10
	{ [3] $R12/m$ ($C2/m$, 12)	1; 5; 7; 11
	{ [3] $R12/m$ ($C2/m$, 12)	1; 6; 7; 12
IIa	none	

IIb [2] $F\bar{3}c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($R\bar{3}c$, 167); [3] $P\bar{3}m1$ ($\mathbf{a}' = \mathbf{a}-\mathbf{b}, \mathbf{b}' = \mathbf{b}-\mathbf{c}, \mathbf{c}' = \mathbf{a}+\mathbf{b}+\mathbf{c}$) (164)

Maximal isomorphic subgroups of lowest index

IIc [2] $R\bar{3}m$ ($\mathbf{a}' = \mathbf{b}+\mathbf{c}, \mathbf{b}' = \mathbf{a}+\mathbf{c}, \mathbf{c}' = \mathbf{a}+\mathbf{b}$) (166); [4] $R\bar{3}m$ ($\mathbf{a}' = -\mathbf{a}+\mathbf{b}+\mathbf{c}, \mathbf{b}' = \mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{c}' = \mathbf{a}+\mathbf{b}-\mathbf{c}$) (166)

Minimal non-isomorphic supergroups

I [4] $Pm\bar{3}m$ (221); [4] $Pn\bar{3}m$ (224); [4] $Fm\bar{3}m$ (225); [4] $Fd\bar{3}m$ (227); [4] $Im\bar{3}m$ (229)

II [3] $P\bar{3}1m$ ($\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}), \mathbf{c}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$) (162)

Trigonal	$\bar{3}m$	D_{3d}^5	$R\bar{3}m$
Patterson symmetry $R\bar{3}m$		$R\bar{3}2/m$	No. 166

RHOMBOHEDRAL AXES
(For drawings see hexagonal axes)

Origin at centre ($\bar{3}m$)

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le \frac{1}{2}$; $y \le x$; $z \le \min(y, 1-x)$

Vertices $0,0,0$ $1,0,0$ $1,1,0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^+ x,x,x	(3) 3^- x,x,x
(4) 2 $\bar{x},0,x$	(5) 2 $x,\bar{x},0$	(6) 2 $0,y,\bar{y}$
(7) $\bar{1}$ $0,0,0$	(8) $\bar{3}^+$ x,x,x; $0,0,0$	(9) $\bar{3}^-$ x,x,x; $0,0,0$
(10) m x,y,x	(11) m x,x,z	(12) m x,y,y

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	i	1	(1) x,y,z	(2) z,x,y	(3) y,z,x				no conditions
			(4) $\bar{z},\bar{y},\bar{x}$	(5) $\bar{y},\bar{x},\bar{z}$	(6) $\bar{x},\bar{z},\bar{y}$				
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $\bar{z},\bar{x},\bar{y}$	(9) $\bar{y},\bar{z},\bar{x}$				
			(10) z,y,x	(11) y,x,z	(12) x,z,y				
									Special: no extra conditions
6	h	$.m$	x,x,z	z,x,x	x,z,x	$\bar{z},\bar{x},\bar{x}$	$\bar{x},\bar{x},\bar{z}$	$\bar{x},\bar{z},\bar{x}$	
6	g	$.2$	$x,\bar{x},\frac{1}{2}$	$\frac{1}{2},x,\bar{x}$	$\bar{x},\frac{1}{2},x$	$\bar{x},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},x$	$x,\frac{1}{2},\bar{x}$	
6	f	$.2$	$x,\bar{x},0$	$0,x,\bar{x}$	$\bar{x},0,x$	$\bar{x},x,0$	$0,\bar{x},x$	$x,0,\bar{x}$	
3	e	$.2/m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$				
3	d	$.2/m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$				
2	c	$3m$	x,x,x	$\bar{x},\bar{x},\bar{x}$					
1	b	$\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						
1	a	$\bar{3}m$	$0,0,0$						

Symmetry of special projections

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along $[1\bar{1}0]$ $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\bar{x},0$

Along $[2\bar{1}\bar{1}]$ $p2mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

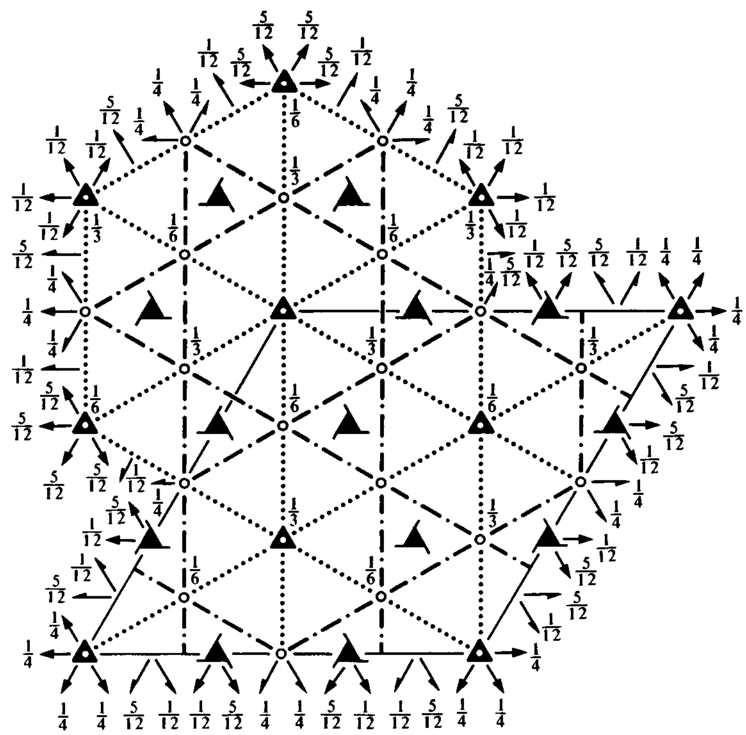
(*Continued on preceding page*)

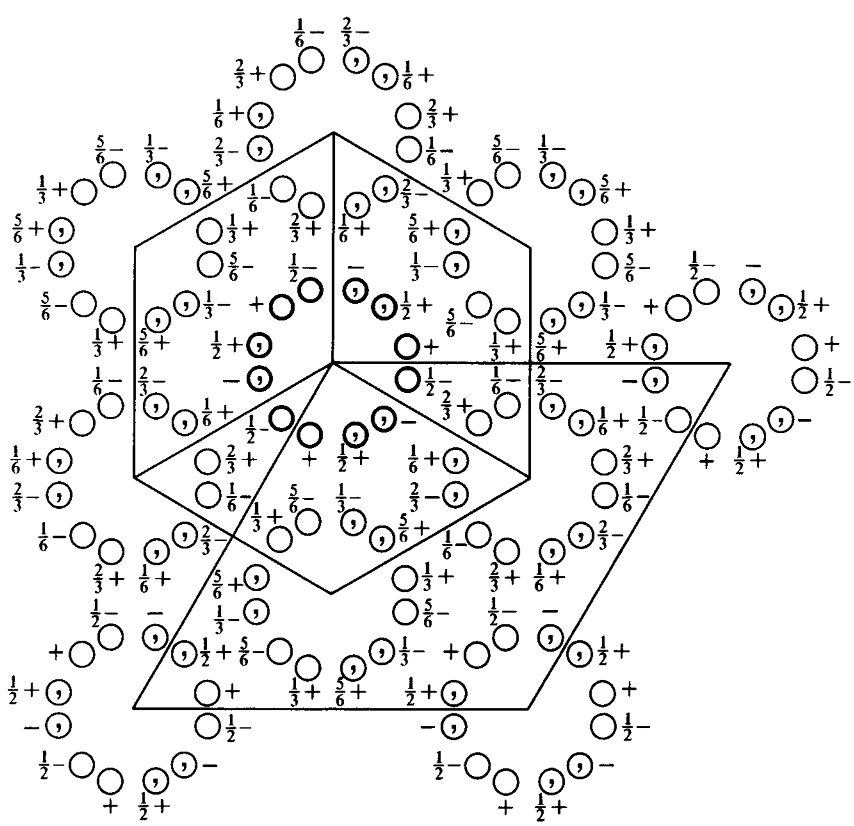
International Tables for Crystallography (2006). Vol. A, Space group 167, pp. 548–551.

$R\bar{3}c$ $\quad$ D_{3d}^{6} $\quad$ $\bar{3}m$ $\quad$ Trigonal

No. 167 $\quad$ $R\bar{3}2/c$ $\quad$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





Origin at centre ($\bar{3}$) at $\bar{3}c$

Asymmetric unit $\quad 0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{2}{3};\quad 0 \le z \le \frac{1}{12};\quad x \le (1+y)/2;\quad y \le \min(1-x,(1+x)/2)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0 \quad 0,\frac{1}{2},0$

$0,0,\frac{1}{12} \quad \frac{1}{2},0,\frac{1}{12} \quad \frac{2}{3},\frac{1}{3},\frac{1}{12} \quad \frac{1}{3},\frac{2}{3},\frac{1}{12} \quad 0,\frac{1}{2},\frac{1}{12}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $3^{+}\ 0,0,z$	(3) $3^{-}\ 0,0,z$
(4) $2\ \ x,x,\frac{1}{4}$	(5) $2\ \ x,0,\frac{1}{4}$	(6) $2\ \ 0,y,\frac{1}{4}$
(7) $\bar{1}\ \ 0,0,0$	(8) $\bar{3}^{+}\ 0,0,z;\ \ 0,0,0$	(9) $\bar{3}^{-}\ 0,0,z;\ \ 0,0,0$
(10) $c\ \ x,\bar{x},z$	(11) $c\ \ x,2x,z$	(12) $c\ \ 2x,x,z$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	(2) $3^{+}(0,0,\frac{1}{3})\ \ \frac{1}{3},\frac{1}{3},z$	(3) $3^{-}(0,0,\frac{1}{3})\ \ \frac{1}{3},0,z$
(4) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x-\frac{1}{6},\frac{5}{12}$	(5) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{6},\frac{5}{12}$	(6) $2\ \ \frac{1}{3},y,\frac{5}{12}$
(7) $\bar{1}\ \ \frac{1}{3},\frac{1}{6},\frac{1}{6}$	(8) $\bar{3}^{+}\ \frac{1}{3},-\frac{1}{3},z;\ \ \frac{1}{3},-\frac{1}{3},\frac{1}{6}$	(9) $\bar{3}^{-}\ \frac{1}{3},\frac{2}{3},z;\ \ \frac{1}{3},\frac{2}{3},\frac{1}{6}$
(10) $g(\frac{1}{6},-\frac{1}{6},\frac{5}{6})\ \ x+\frac{1}{2},\bar{x},z$	(11) $g(\frac{1}{6},\frac{1}{3},\frac{5}{6})\ \ x+\frac{1}{4},2x,z$	(12) $g(\frac{2}{3},\frac{1}{3},\frac{5}{6})\ \ 2x,x,z$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$	(2) $3^{+}(0,0,\frac{2}{3})\ \ 0,\frac{1}{3},z$	(3) $3^{-}(0,0,\frac{2}{3})\ \ \frac{1}{3},\frac{1}{3},z$
(4) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x+\frac{1}{6},\frac{1}{12}$	(5) $2\ \ x,\frac{1}{3},\frac{1}{12}$	(6) $2(0,\frac{1}{2},0)\ \ \frac{1}{6},y,\frac{1}{12}$
(7) $\bar{1}\ \ \frac{1}{6},\frac{1}{3},\frac{1}{3}$	(8) $\bar{3}^{+}\ \frac{2}{3},\frac{1}{3},z;\ \ \frac{2}{3},\frac{1}{3},\frac{1}{3}$	(9) $\bar{3}^{-}\ -\frac{1}{3},\frac{1}{3},z;\ \ -\frac{1}{3},\frac{1}{3},\frac{1}{3}$
(10) $g(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\ \ x+\frac{1}{2},\bar{x},z$	(11) $g(\frac{1}{3},\frac{2}{3},\frac{1}{6})\ \ x,2x,z$	(12) $g(\frac{1}{3},\frac{1}{6},\frac{1}{6})\ \ 2x-\frac{1}{2},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\ \ (\frac{2}{3},\frac{1}{3},\frac{1}{3})+\ \ (\frac{1}{3},\frac{2}{3},\frac{2}{3})+$						Reflection conditions
									General:
36	f	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$hkil$: $-h+k+l=3n$
			(4) $y,x,\bar{z}+\frac{1}{2}$	(5) $x-y,\bar{y},\bar{z}+\frac{1}{2}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$				$hki0$: $-h+k=3n$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$				$hh\overline{2h}l$: $l=3n$
			(10) $\bar{y},\bar{x},z+\frac{1}{2}$	(11) $\bar{x}+y,y,z+\frac{1}{2}$	(12) $x,x-y,z+\frac{1}{2}$				$h\bar{h}0l$: $h+l=3n,\ l=2n$
									$000l$: $l=6n$
									$h\bar{h}00$: $h=3n$
									Special: as above, plus
18	e	$.2$	$x,0,\frac{1}{4}$	$0,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$0,\bar{x},\frac{3}{4}$	$x,x,\frac{3}{4}$	no extra conditions
18	d	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
12	c	$3.$	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$			$hkil$: $l=2n$
6	b	$\bar{3}.$	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$
6	a	32	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}'=\frac{1}{6}(2\mathbf{a}+4\mathbf{b}+\mathbf{c})$ $\mathbf{b}'=\frac{1}{6}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

Along [210] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

HEXAGONAL AXES

Maximal non-isomorphic subgroups

I	[2] $R3c$ (161)	(1; 2; 3; 10; 11; 12)+
	[2] $R32$ (155)	(1; 2; 3; 4; 5; 6)+
	[2] $R\bar{3}1$ ($R\bar{3}$, 148)	(1; 2; 3; 7; 8; 9)+
	{ [3] $R12/c$ ($C2/c$, 15)	(1; 4; 7; 10)+
	{ [3] $R12/c$ ($C2/c$, 15)	(1; 5; 7; 11)+
	{ [3] $R12/c$ ($C2/c$, 15)	(1; 6; 7; 12)+
IIa	{ [3] $P\bar{3}c1$ (165)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	{ [3] $P\bar{3}c1$ (165)	1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$
	{ [3] $P\bar{3}c1$ (165)	1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [4] $R\bar{3}c$ ($\mathbf{a}'=-2\mathbf{a},\mathbf{b}'=-2\mathbf{b}$) (167); [5] $R\bar{3}c$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=5\mathbf{c}$) (167)

Minimal non-isomorphic supergroups

I [4] $Pn\bar{3}n$ (222); [4] $Pm\bar{3}n$ (223); [4] $Fm\bar{3}c$ (226); [4] $Fd\bar{3}c$ (228); [4] $Ia\bar{3}d$ (230)

II [2] $R\bar{3}m$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (166); [3] $P\bar{3}1c$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b}),\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (163)

RHOMBOHEDRAL AXES

Maximal non-isomorphic subgroups

I	[2] $R3c$ (161)	1; 2; 3; 10; 11; 12
	[2] $R32$ (155)	1; 2; 3; 4; 5; 6
	[2] $R\bar{3}1$ ($R\bar{3}$, 148)	1; 2; 3; 7; 8; 9
	{ [3] $R12/c$ ($C2/c$, 15)	1; 4; 7; 10
	{ [3] $R12/c$ ($C2/c$, 15)	1; 5; 7; 11
	{ [3] $R12/c$ ($C2/c$, 15)	1; 6; 7; 12
IIa	none	
IIb	[3] $P\bar{3}c1$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{b}-\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (165)	

Maximal isomorphic subgroups of lowest index

IIc [4] $R\bar{3}c$ ($\mathbf{a}'=-\mathbf{a}+\mathbf{b}+\mathbf{c},\mathbf{b}'=\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}-\mathbf{c}$) (167); [5] $R\bar{3}c$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b}+2\mathbf{c},\mathbf{b}'=2\mathbf{a}+\mathbf{b}+2\mathbf{c},\mathbf{c}'=2\mathbf{a}+2\mathbf{b}+\mathbf{c}$) (167)

Minimal non-isomorphic supergroups

I [4] $Pn\bar{3}n$ (222); [4] $Pm\bar{3}n$ (223); [4] $Fm\bar{3}c$ (226); [4] $Fd\bar{3}c$ (228); [4] $Ia\bar{3}d$ (230)

II [2] $R\bar{3}m$ ($\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}),\mathbf{b}'=\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c}),\mathbf{c}'=\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$) (166);
[3] $P\bar{3}1c$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}),\mathbf{c}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$) (163)

RHOMBOHEDRAL AXES
(For drawings see hexagonal axes)

Origin at centre ($\bar{3}$) at $\bar{3}c$

Asymmetric unit $\frac{1}{4} \le x \le \frac{5}{4}$; $\frac{1}{4} \le y \le \frac{5}{4}$; $\frac{1}{4} \le z \le \frac{3}{4}$; $y \le x$; $z \le \min(y, \frac{3}{2} - x)$

Vertices $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{5}{4},\frac{1}{4},\frac{1}{4}$ $\frac{5}{4},\frac{5}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$

Symmetry operations

(1) 1	(2) 3^+ x,x,x	(3) 3^- x,x,x
(4) 2 $\bar{x}+\frac{1}{2},\frac{1}{4},x$	(5) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$	(6) 2 $\frac{1}{4},y+\frac{1}{2},\bar{y}$
(7) $\bar{1}$ 0,0,0	(8) $\bar{3}^+$ x,x,x; 0,0,0	(9) $\bar{3}^-$ x,x,x; 0,0,0
(10) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x	(11) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z	(12) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	f	1	(1) x,y,z	(2) z,x,y	(3) y,z,x	hhl : $l=2n$
			(4) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(5) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	hhh : $h=2n$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $\bar{z},\bar{x},\bar{y}$	(9) $\bar{y},\bar{z},\bar{x}$	
			(10) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(11) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(12) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	
						Special: as above, plus
6	e	.2	$x,\bar{x}+\frac{1}{2},\frac{1}{4}$ $\frac{1}{4},x,\bar{x}+\frac{1}{2}$ $\bar{x}+\frac{1}{2},\frac{1}{4},x$			no extra conditions
			$\bar{x},x+\frac{1}{2},\frac{3}{4}$ $\frac{3}{4},\bar{x},x+\frac{1}{2}$ $x+\frac{1}{2},\frac{3}{4},\bar{x}$			
6	d	$\bar{1}$	$\frac{1}{2},0,0$ $0,\frac{1}{2},0$ $0,0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},0,\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$			hkl : $h+k+l=2n$
4	c	3 .	x,x,x $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$ $\bar{x},\bar{x},\bar{x}$ $x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$			hkl : $h+k+l=2n$
2	b	$\bar{3}$.	$0,0,0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k+l=2n$
2	a	3 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along $[1\bar{1}0]$ $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,\bar{x},0$

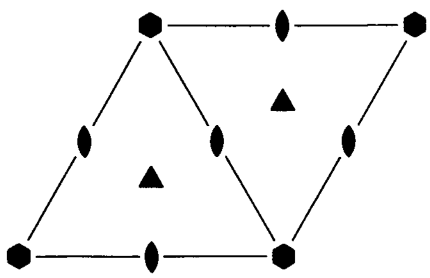
Along $[2\bar{1}\bar{1}]$ $p2gm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

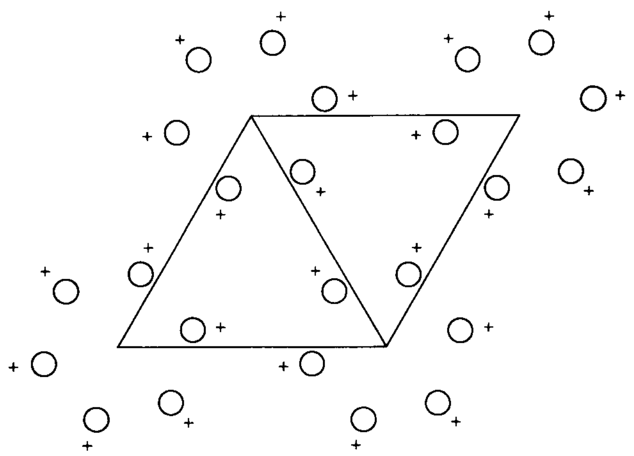
(*Continued on preceding page*)

International Tables for Crystallography (2006). Vol. A, Space group 168, pp. 552–553.

$P6$ $\quad C_6^1$ $\quad 6$ $\quad$ Hexagonal

No. 168 $\quad P6$ $\quad$ Patterson symmetry $P6/m$





Origin on 6

Asymmetric unit $\quad 0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le 1;\quad x \le (1+y)/2;\quad y \le \min(1-x, x)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{2},\frac{1}{2},0$

$0,0,1 \quad \frac{1}{2},0,1 \quad \frac{2}{3},\frac{1}{3},1 \quad \frac{1}{2},\frac{1}{2},1$

Symmetry operations

(1) 1	(2) 3^{+} $0,0,z$	(3) 3^{-} $0,0,z$
(4) 2 $\quad 0,0,z$	(5) 6^{-} $0,0,z$	(6) 6^{+} $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$	
						Special: no extra conditions
3	c	$2\,.\,.$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$	
2	b	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$		
1	a	$6\,.\,.$	$0,0,z$			

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P3$ (143) 1; 2; 3
[3] $P2$ (3) 1; 4

IIa none

IIb [2] $P6_3$ ($\mathbf{c}'=2\mathbf{c}$) (173); [3] $P6_4$ ($\mathbf{c}'=3\mathbf{c}$) (172); [3] $P6_2$ ($\mathbf{c}'=3\mathbf{c}$) (171)

Maximal isomorphic subgroups of lowest index

IIc [2] $P6$ ($\mathbf{c}'=2\mathbf{c}$) (168); [3] $H6$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6$, 168)

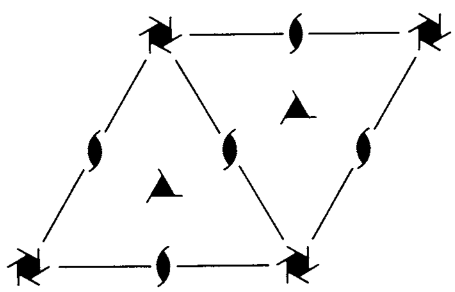
Minimal non-isomorphic supergroups

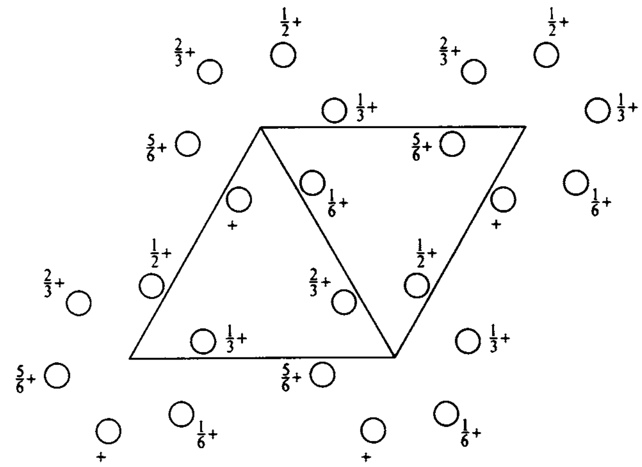
I [2] $P6/m$ (175); [2] $P622$ (177); [2] $P6mm$ (183); [2] $P6cc$ (184)

II none

$P6_1$ $\quad C_6^2$ $\quad 6$ $\quad$ Hexagonal

No. 169 $\quad P6_1$ $\quad$ Patterson symmetry $P6/m$





Origin on 6_1

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{6}$

Vertices $\quad 0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$

$0,0,\frac{1}{6} \quad 1,0,\frac{1}{6} \quad 1,1,\frac{1}{6} \quad 0,1,\frac{1}{6}$

Symmetry operations

(1) 1	(2) $3^{+}(0,0,\frac{1}{3})\quad 0,0,z$	(3) $3^{-}(0,0,\frac{2}{3})\quad 0,0,z$
(4) $2(0,0,\frac{1}{2})\quad 0,0,z$	(5) $6^{-}(0,0,\frac{5}{6})\quad 0,0,z$	(6) $6^{+}(0,0,\frac{1}{6})\quad 0,0,z$

Generators selected $\quad$ (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 $\quad a \quad 1$	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	$000l$: $l=6n$
	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{5}{6}$	(6) $x-y,x,z+\frac{1}{6}$	

Symmetry of special projections

Along [001] $p6$	Along [100] $p1g1$	Along [210] $p1g1$
$\mathbf{a}'=\mathbf{a} \quad \mathbf{b}'=\mathbf{b}$	$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b}) \quad \mathbf{b}'=\mathbf{c}$	$\mathbf{a}'=\frac{1}{2}\mathbf{b} \quad \mathbf{b}'=\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I $\quad$ [2] $P3_1$ (144) $\quad$ 1; 2; 3

[3] $P2_1$ (4) $\quad$ 1; 4

IIa $\quad$ none

IIb $\quad$ none

Maximal isomorphic subgroups of lowest index

IIc $\quad$ [3] $H6_1$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6_1$, 169); [5] $P6_5$ ($\mathbf{c}'=5\mathbf{c}$) (170); [7] $P6_1$ ($\mathbf{c}'=7\mathbf{c}$) (169)

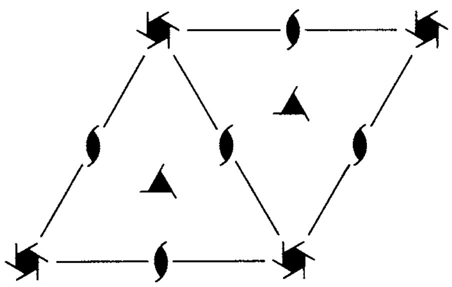
Minimal non-isomorphic supergroups

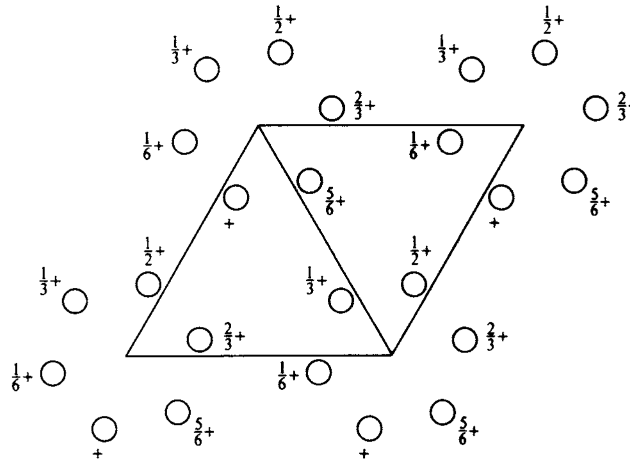
I $\quad$ [2] $P6_122$ (178)

II $\quad$ [2] $P6_2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (171); [3] $P6_3$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (173)

Hexagonal 6 C_6^3 $P6_5$

Patterson symmetry $P6/m$ $P6_5$ No. 170





Origin on 6_5

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le \frac{1}{6}$

Vertices $0,0,0$ $1,0,0$ $1,1,0$ $0,1,0$

$0,0,\frac{1}{6}$ $1,0,\frac{1}{6}$ $1,1,\frac{1}{6}$ $0,1,\frac{1}{6}$

Symmetry operations

(1) 1	(2) $3^+(0,0,\frac{2}{3})$ $0,0,z$	(3) $3^-(0,0,\frac{1}{3})$ $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$	(5) $6^-(0,0,\frac{1}{6})$ $0,0,z$	(6) $6^+(0,0,\frac{5}{6})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

General:

6 *a* 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$	$000l$: $l=6n$
	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{6}$	(6) $x-y,x,z+\frac{5}{6}$	

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1g1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P3_2$ (145) 1; 2; 3
[3] $P2_1$ (4) 1; 4

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $H6_5$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6_5$, 170); [5] $P6_1$ ($\mathbf{c}'=5\mathbf{c}$) (169); [7] $P6_5$ ($\mathbf{c}'=7\mathbf{c}$) (170)

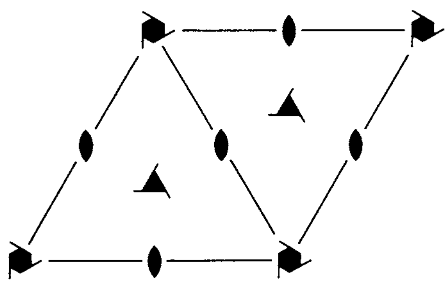
Minimal non-isomorphic supergroups

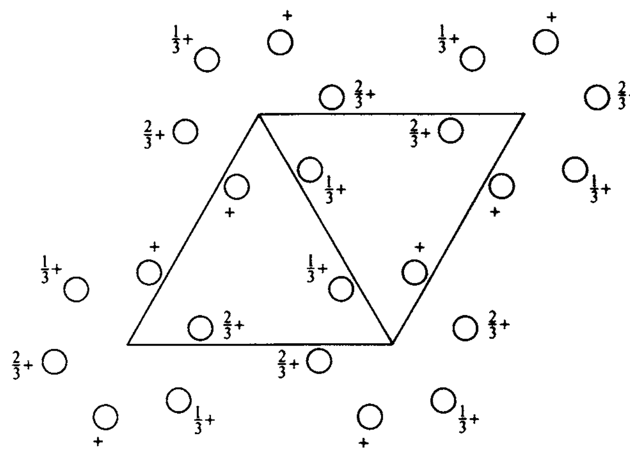
I [2] $P6_522$ (179)

II [2] $P6_4$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (172); [3] $P6_3$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (173)

$P6_2$ C_6^4 6   Hexagonal

No. 171 $P6_2$ Patterson symmetry $P6/m$





Origin on 2 on 6_2

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le \frac{1}{3}$; $y \le x$

Vertices $0,0,0$ $1,0,0$ $1,1,0$

$0,0,\frac{1}{3}$ $1,0,\frac{1}{3}$ $1,1,\frac{1}{3}$

Symmetry operations

(1) 1	(2) $3^+(0,0,\frac{2}{3})$ $0,0,z$	(3) $3^-(0,0,\frac{1}{3})$ $0,0,z$
(4) 2 $0,0,z$	(5) $6^-(0,0,\frac{2}{3})$ $0,0,z$	(6) $6^+(0,0,\frac{1}{3})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	*c*	1	(1) x,y,z (4) $\bar{x},\bar{y},z$	(2) $\bar{y},x-y,z+\frac{2}{3}$ (5) $y,\bar{x}+y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$ (6) $x-y,x,z+\frac{1}{3}$	$000l$: $l=3n$
						Special: as above, plus
3	*b*	2 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{2}{3}$	$0,\frac{1}{2},z+\frac{1}{3}$	$hkil$: $h=2n+1$ or $k=2n+1$ or $l=3n$
3	*a*	2 . .	$0,0,z$	$0,0,z+\frac{2}{3}$	$0,0,z+\frac{1}{3}$	$hkil$: $l=3n$

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P3_2$ (145) 1; 2; 3
[3] $P2$ (3) 1; 4

IIa none

IIb [2] $P6_1$ ($\mathbf{c}'=2\mathbf{c}$) (169)

Maximal isomorphic subgroups of lowest index

IIc [2] $P6_4$ ($\mathbf{c}'=2\mathbf{c}$) (172); [3] $H6_2$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6_2$, 171); [7] $P6_2$ ($\mathbf{c}'=7\mathbf{c}$) (171)

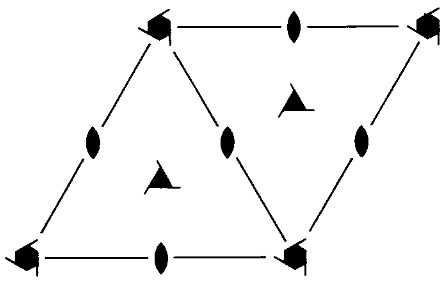
Minimal non-isomorphic supergroups

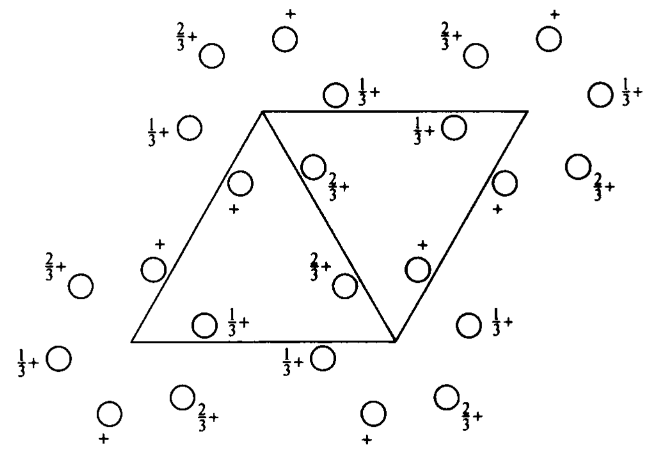
I [2] $P6_222$ (180)

II [3] $P6$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (168)

Hexagonal | 6 | C_6^5 | $P6_4$

Patterson symmetry $P6/m$ | $P6_4$ | No. 172





Origin on 2 on 6_4

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le \frac{1}{3}$; $y \le x$

Vertices $0,0,0$ $1,0,0$ $1,1,0$

$0,0,\frac{1}{3}$ $1,0,\frac{1}{3}$ $1,1,\frac{1}{3}$

Symmetry operations

(1) 1	(2) $3^+(0,0,\frac{1}{3})$ $0,0,z$	(3) $3^-(0,0,\frac{2}{3})$ $0,0,z$
(4) 2 $0,0,z$	(5) $6^-(0,0,\frac{1}{3})$ $0,0,z$	(6) $6^+(0,0,\frac{2}{3})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	c	1	(1) x,y,z (4) $\bar{x},\bar{y},z$	(2) $\bar{y},x-y,z+\frac{1}{3}$ (5) $y,\bar{x}+y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$ (6) $x-y,x,z+\frac{2}{3}$	$000l$: $l=3n$
						Special: as above, plus
3	b	2 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{3}$	$0,\frac{1}{2},z+\frac{2}{3}$	$hkil$: $h=2n+1$ or $k=2n+1$ or $l=3n$
3	a	2 . .	$0,0,z$	$0,0,z+\frac{1}{3}$	$0,0,z+\frac{2}{3}$	$hkil$: $l=3n$

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P3_1$ (144) 1; 2; 3
[3] $P2$ (3) 1; 4

IIa none

IIb [2] $P6_5$ ($\mathbf{c}'=2\mathbf{c}$) (170)

Maximal isomorphic subgroups of lowest index

IIc [2] $P6_2$ ($\mathbf{c}'=2\mathbf{c}$) (171); [3] $H6_4$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6_4$, 172); [7] $P6_4$ ($\mathbf{c}'=7\mathbf{c}$) (172)

Minimal non-isomorphic supergroups

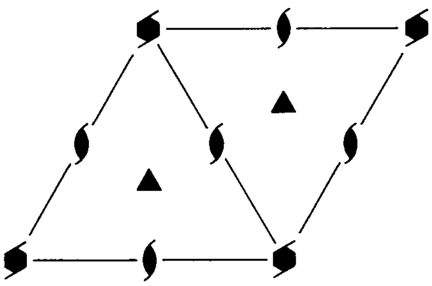
I [2] $P6_422$ (181)

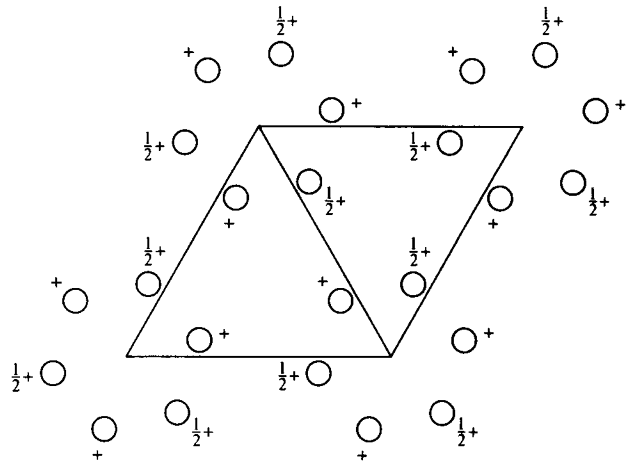
II [3] $P6$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (168)

International Tables for Crystallography (2006). Vol. A, Space group 173, pp. 558–559.

$P6_3$ $\quad C_6^6$ $\quad 6$ $\quad$ Hexagonal

No. 173 $\quad P6_3$ $\quad$ Patterson symmetry $P6/m$





Origin on 3 on 6_3

Asymmetric unit $\quad 0 \le x \le \frac{2}{3}$; $\quad 0 \le y \le \frac{2}{3}$; $\quad 0 \le z \le \frac{1}{2}$; $\quad x \le (1+y)/2$; $\quad y \le \min(1-x, (1+x)/2)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0 \quad 0,\frac{1}{2},0$

$0,0,\frac{1}{2} \quad \frac{1}{2},0,\frac{1}{2} \quad \frac{2}{3},\frac{1}{3},\frac{1}{2} \quad \frac{1}{3},\frac{2}{3},\frac{1}{2} \quad 0,\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) $3^{+}\ 0,0,z$	(3) $3^{-}\ 0,0,z$
(4) $2(0,0,\frac{1}{2})\ \ 0,0,z$	(5) $6^{-}(0,0,\frac{1}{2})\ \ 0,0,z$	(6) $6^{+}(0,0,\frac{1}{2})\ \ 0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	c	1	(1) x,y,z (4) $\bar{x},\bar{y},z+\frac{1}{2}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,z+\frac{1}{2}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,z+\frac{1}{2}$	$000l$: $l=2n$
						Special: as above, plus
2	b	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$		$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	a	$3\,.\,.$	$0,0,z$	$0,0,z+\frac{1}{2}$		$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1g1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P3$ (143) 1; 2; 3
[3] $P2_1$ (4) 1; 4

IIa none

IIb [3] $P6_5$ ($\mathbf{c}'=3\mathbf{c}$) (170); [3] $P6_1$ ($\mathbf{c}'=3\mathbf{c}$) (169)

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_3$ ($\mathbf{c}'=3\mathbf{c}$) (173); [3] $H6_3$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6_3$, 173)

Minimal non-isomorphic supergroups

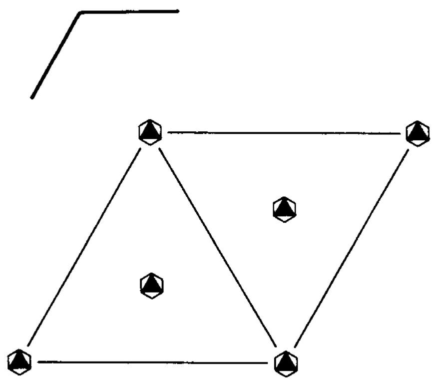
I [2] $P6_3/m$ (176); [2] $P6_322$ (182); [2] $P6_3cm$ (185); [2] $P6_3mc$ (186)

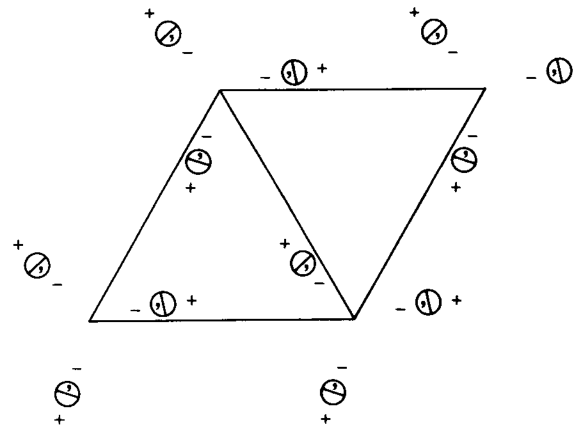
II [2] $P6$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (168)

International Tables for Crystallography (2006). Vol. A, Space group 174, pp. 560–561.

$P\bar{6}$ $\quad$ C_{3h}^1 $\quad$ $\bar{6}$ $\quad$ Hexagonal

No. 174 $\quad$ $P\bar{6}$ $\quad$ Patterson symmetry $P6/m$





Origin at $\bar{6}$

Asymmetric unit $\quad 0 \le x \le \frac{2}{3}; \quad 0 \le y \le \frac{2}{3}; \quad 0 \le z \le \frac{1}{2}; \quad x \le (1+y)/2; \quad y \le \min(1-x, (1+x)/2)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0 \quad 0,\frac{1}{2},0$

$0,0,\frac{1}{2} \quad \frac{1}{2},0,\frac{1}{2} \quad \frac{2}{3},\frac{1}{3},\frac{1}{2} \quad \frac{1}{3},\frac{2}{3},\frac{1}{2} \quad 0,\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) $3^+ \;\; 0,0,z$	(3) $3^- \;\; 0,0,z$
(4) $m \;\; x,y,0$	(5) $\bar{6}^- \;\; 0,0,z; \;\; 0,0,0$	(6) $\bar{6}^+ \;\; 0,0,z; \;\; 0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	*l*	1	(1) x,y,z (4) $x,y,\bar{z}$	(2) $\bar{y},x-y,z$ (5) $\bar{y},x-y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x}+y,\bar{x},\bar{z}$	no conditions
						Special: no extra conditions
3	*k*	$m\,.\,.$	$x,y,\frac{1}{2}$	$\bar{y},x-y,\frac{1}{2}$	$\bar{x}+y,\bar{x},\frac{1}{2}$	
3	*j*	$m\,.\,.$	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	
2	*i*	$3\,.\,.$	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2	*h*	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$		
2	*g*	$3\,.\,.$	$0,0,z$	$0,0,\bar{z}$		
1	*f*	$\bar{6}\,.\,.$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$			
1	*e*	$\bar{6}\,.\,.$	$\frac{2}{3},\frac{1}{3},0$			
1	*d*	$\bar{6}\,.\,.$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$			
1	*c*	$\bar{6}\,.\,.$	$\frac{1}{3},\frac{2}{3},0$			
1	*b*	$\bar{6}\,.\,.$	$0,0,\frac{1}{2}$			
1	*a*	$\bar{6}\,.\,.$	$0,0,0$			

Symmetry of special projections

Along [001] $p3$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p11m$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P3$ (143) 1; 2; 3
[3] Pm (6) 1; 4

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{6}$ ($\mathbf{c}'=2\mathbf{c}$) (174); [3] $H\bar{6}$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P\bar{6}$, 174)

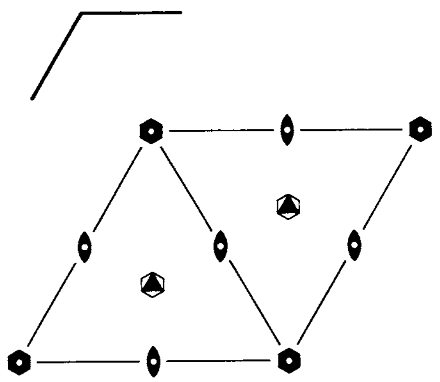
Minimal non-isomorphic supergroups

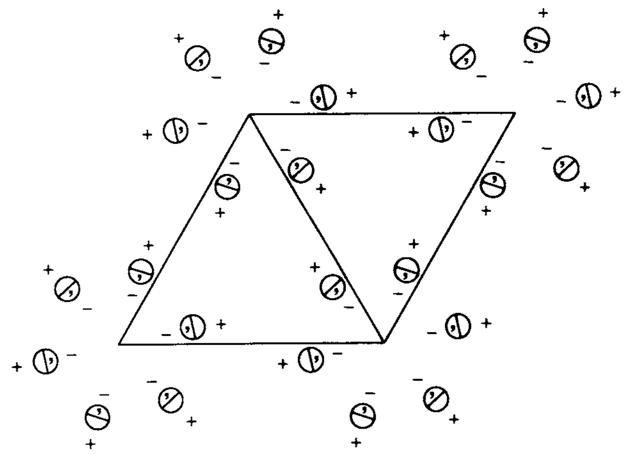
I [2] $P6/m$ (175); [2] $P6_3/m$ (176); [2] $P\bar{6}m2$ (187); [2] $P\bar{6}c2$ (188); [2] $P\bar{6}2m$ (189); [2] $P\bar{6}2c$ (190)

II none

$P6/m$ $\quad C_{6h}^{1}$ $\quad 6/m$ $\quad$ Hexagonal

No. 175 $\quad P6/m$ $\quad$ Patterson symmetry $P6/m$





Origin at centre $(6/m)$

Asymmetric unit $\quad 0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2};\quad x \le (1+y)/2;\quad y \le \min(1-x,x)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{2},\frac{1}{2},0$

$0,0,\frac{1}{2} \quad \frac{1}{2},0,\frac{1}{2} \quad \frac{2}{3},\frac{1}{3},\frac{1}{2} \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) $3^{+}\ 0,0,z$	(3) $3^{-}\ 0,0,z$
(4) $2\ \ 0,0,z$	(5) $6^{-}\ 0,0,z$	(6) $6^{+}\ 0,0,z$
(7) $\bar{1}\ \ 0,0,0$	(8) $\bar{3}^{+}\ 0,0,z;\ 0,0,0$	(9) $\bar{3}^{-}\ 0,0,z;\ 0,0,0$
(10) $m\ \ x,y,0$	(11) $\bar{6}^{-}\ 0,0,z;\ 0,0,0$	(12) $\bar{6}^{+}\ 0,0,z;\ 0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	l	1	(1) x,y,z (4) $\bar{x},\bar{y},z$ (7) $\bar{x},\bar{y},\bar{z}$ (10) $x,y,\bar{z}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,z$ (8) $y,\bar{x}+y,\bar{z}$ (11) $\bar{y},x-y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,z$ (9) $x-y,x,\bar{z}$ (12) $\bar{x}+y,\bar{x},\bar{z}$				no conditions
									Special: no extra conditions
6	k	$m\,.\,.$	$x,y,\frac{1}{2}$	$\bar{y},x-y,\frac{1}{2}$	$\bar{x}+y,\bar{x},\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$y,\bar{x}+y,\frac{1}{2}$	$x-y,x,\frac{1}{2}$	
6	j	$m\,.\,.$	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$\bar{x},\bar{y},0$	$y,\bar{x}+y,0$	$x-y,x,0$	
6	i	$2\,.\,.$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	
4	h	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}$			
3	g	$2/m\,.\,.$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
3	f	$2/m\,.\,.$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$				
2	e	$6\,.\,.$	$0,0,z$	$0,0,\bar{z}$					
2	d	$\bar{6}\,.\,.$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$					
2	c	$\bar{6}\,.\,.$	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$					
1	b	$6/m\,.\,.$	$0,0,\frac{1}{2}$						
1	a	$6/m\,.\,.$	$0,0,0$						

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{6}$ (174) 1; 2; 3; 10; 11; 12
[2] $P6$ (168) 1; 2; 3; 4; 5; 6
[2] $P\bar{3}$ (147) 1; 2; 3; 7; 8; 9
[3] $P2/m$ (10) 1; 4; 7; 10

IIa none

IIb [2] $P6_3/m$ ($\mathbf{c}'=2\mathbf{c}$) (176)

Maximal isomorphic subgroups of lowest index

IIc [2] $P6/m$ ($\mathbf{c}'=2\mathbf{c}$) (175); [3] $H6/m$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6/m$, 175)

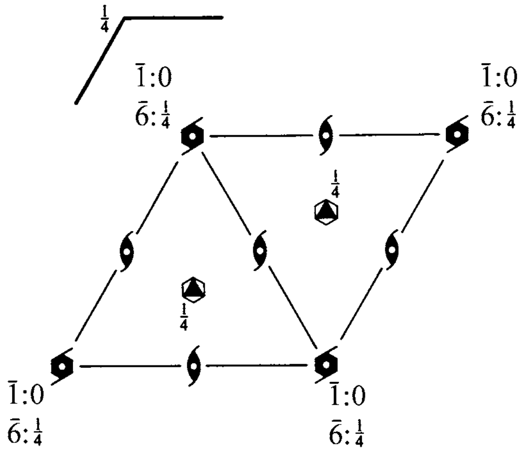
Minimal non-isomorphic supergroups

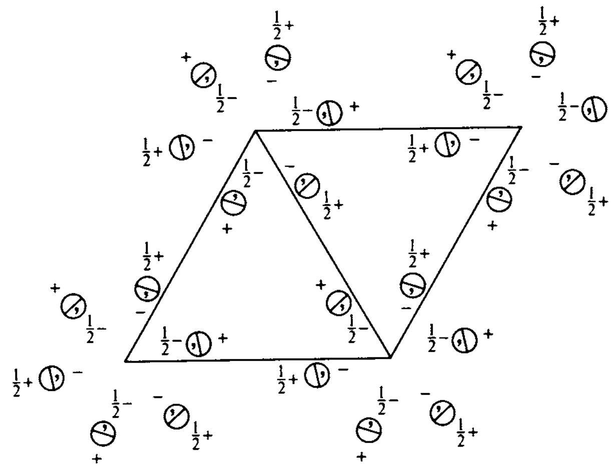
I [2] $P6/mmm$ (191); [2] $P6/mcc$ (192)

II none

$P6_3/m$ $\quad$ C_{6h}^2 $\quad$ $6/m$ $\quad$ Hexagonal

No. 176 $\quad$ $P6_3/m$ $\quad$ Patterson symmetry $P6/m$





Origin at centre ($\bar{3}$) on 6_3

Asymmetric unit $\quad 0 \le x \le \frac{2}{3}$; $\quad 0 \le y \le \frac{2}{3}$; $\quad 0 \le z \le \frac{1}{4}$; $\quad x \le (1+y)/2$; $\quad y \le \min(1-x,(1+x)/2)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0 \quad 0,\frac{1}{2},0$

$0,0,\frac{1}{4} \quad \frac{1}{2},0,\frac{1}{4} \quad \frac{2}{3},\frac{1}{3},\frac{1}{4} \quad \frac{1}{3},\frac{2}{3},\frac{1}{4} \quad 0,\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1	(2) $3^+ \ 0,0,z$	(3) $3^- \ 0,0,z$
(4) $2(0,0,\frac{1}{2}) \ \ 0,0,z$	(5) $6^-(0,0,\frac{1}{2}) \ \ 0,0,z$	(6) $6^+(0,0,\frac{1}{2}) \ \ 0,0,z$
(7) $\bar{1} \ \ 0,0,0$	(8) $\bar{3}^+ \ 0,0,z; \ 0,0,0$	(9) $\bar{3}^- \ 0,0,z; \ 0,0,0$
(10) $m \ \ x,y,\frac{1}{4}$	(11) $\bar{6}^- \ 0,0,z; \ 0,0,\frac{1}{4}$	(12) $\bar{6}^+ \ 0,0,z; \ 0,0,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	i	1	(1) x,y,z (4) $\bar{x},\bar{y},z+\frac{1}{2}$ (7) $\bar{x},\bar{y},\bar{z}$ (10) $x,y,\bar{z}+\frac{1}{2}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,z+\frac{1}{2}$ (8) $y,\bar{x}+y,\bar{z}$ (11) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,z+\frac{1}{2}$ (9) $x-y,x,\bar{z}$ (12) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$				$000l$: $l=2n$
									Special: as above, plus
6	h	$m\,.\,.$	$x,y,\frac{1}{4}$	$\bar{y},x-y,\frac{1}{4}$	$\bar{x}+y,\bar{x},\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$y,\bar{x}+y,\frac{3}{4}$	$x-y,x,\frac{3}{4}$	no extra conditions
6	g	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
4	f	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$			$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
4	e	$3\,.\,.$	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$			$hkil$: $l=2n$
2	d	$\bar{6}\,.\,.$	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	c	$\bar{6}\,.\,.$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	b	$\bar{3}\,.\,.$	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$
2	a	$\bar{6}\,.\,.$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P\bar{6}$ (174) 1; 2; 3; 10; 11; 12
[2] $P6_3$ (173) 1; 2; 3; 4; 5; 6
[2] $P\bar{3}$ (147) 1; 2; 3; 7; 8; 9
[3] $P2_1/m$ (11) 1; 4; 7; 10

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_3/m$ ($\mathbf{c}'=3\mathbf{c}$) (176); [3] $H6_3/m$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6_3/m$, 176)

Minimal non-isomorphic supergroups

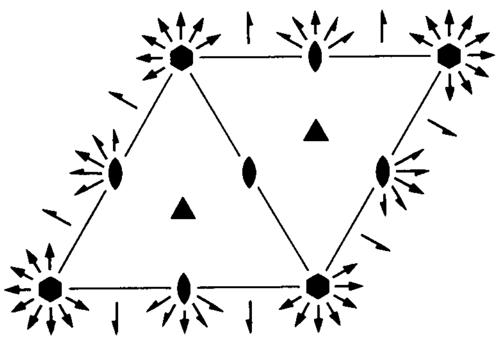
I [2] $P6_3/mcm$ (193); [2] $P6_3/mmc$ (194)

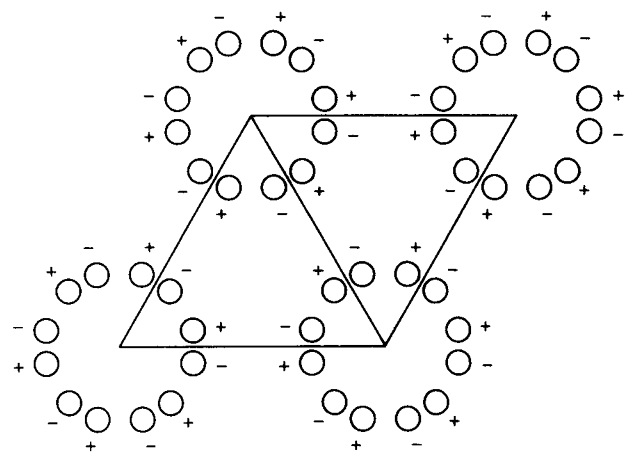
II [2] $P6/m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (175)

International Tables for Crystallography (2006). Vol. A, Space group 177, pp. 566–567.

$P622$ D_6^1 622 Hexagonal

No. 177 $P622$ Patterson symmetry $P6/mmm$





Origin at 622

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x, x)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{2},\frac{1}{2},0$

$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) 2 $0,0,z$	(5) 6^- $0,0,z$	(6) 6^+ $0,0,z$
(7) 2 $x,x,0$	(8) 2 $x,0,0$	(9) 2 $0,y,0$
(10) 2 $x,\bar{x},0$	(11) 2 $x,2x,0$	(12) 2 $2x,x,0$

Maximal isomorphic subgroups of lowest index

IIc [2] $P622$ ($\mathbf{c}' = 2\mathbf{c}$) (177); [3] $H622$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P622$, 177)

Minimal non-isomorphic supergroups

I [2] $P6/mmm$ (191); [2] $P6/mcc$ (192)

II none

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	n	1	(1) x,y,z (4) $\bar{x},\bar{y},z$ (7) $y,x,\bar{z}$ (10) $\bar{y},\bar{x},\bar{z}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,z$ (8) $x-y,\bar{y},\bar{z}$ (11) $\bar{x}+y,y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,z$ (9) $\bar{x},\bar{x}+y,\bar{z}$ (12) $x,x-y,\bar{z}$				no conditions
									Special: no extra conditions
6	m	. . 2	$x,\bar{x},\frac{1}{2}$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{1}{2}$	
6	l	. . 2	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	$\bar{x},x,0$	$\bar{x},2\bar{x},0$	$2x,x,0$	
6	k	. 2 .	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	
6	j	. 2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	
6	i	2 . .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	
4	h	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}$			
3	g	2 2 2	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
3	f	2 2 2	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$				
2	e	6 . .	$0,0,z$	$0,0,\bar{z}$					
2	d	3 . 2	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$					
2	c	3 . 2	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$					
1	b	6 2 2	$0,0,\frac{1}{2}$						
1	a	6 2 2	$0,0,0$						

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I
- [2] $P611$ ($P6$, 168) 1; 2; 3; 4; 5; 6
- [2] $P321$ (150) 1; 2; 3; 7; 8; 9
- [2] $P312$ (149) 1; 2; 3; 10; 11; 12
- $\{$ [3] $P222$ ($C222$, 21) 1; 4; 7; 10
- [3] $P222$ ($C222$, 21) 1; 4; 8; 11
- [3] $P222$ ($C222$, 21) 1; 4; 9; 12

IIa none

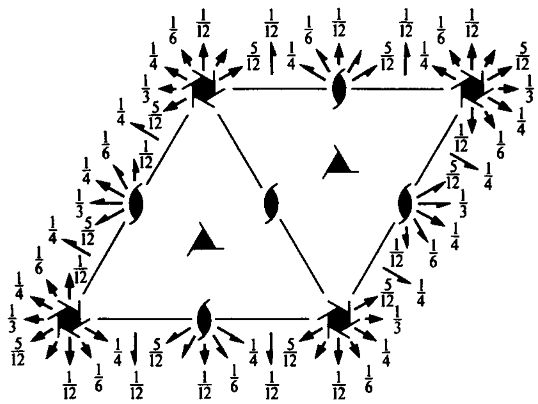
IIb [2] $P6_322$ ($\mathbf{c}' = 2\mathbf{c}$) (182); [3] $P6_422$ ($\mathbf{c}' = 3\mathbf{c}$) (181); [3] $P6_222$ ($\mathbf{c}' = 3\mathbf{c}$) (180)

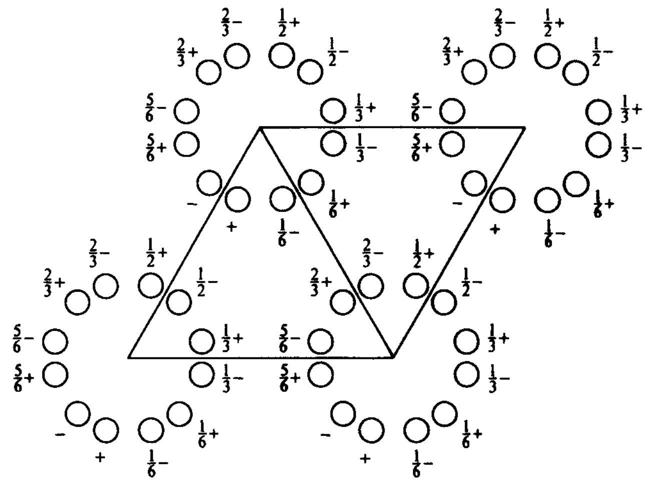
(*Continued on preceding page*)

International Tables for Crystallography (2006). Vol. A, Space group 178, pp. 568–569.

$P6_122$ D_6^2 622 Hexagonal

No. 178 $P6_122$ Patterson symmetry $P6/mmm$





Origin on $2[100]$ at $6_1\,(2,1,1)\,1$

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le \frac{1}{12}$

Vertices $0,0,0$ $1,0,0$ $1,1,0$ $0,1,0$

$0,0,\frac{1}{12}$ $1,0,\frac{1}{12}$ $1,1,\frac{1}{12}$ $0,1,\frac{1}{12}$

Symmetry operations

(1) 1	(2) $3^+(0,0,\frac{1}{3})$ $0,0,z$	(3) $3^-(0,0,\frac{2}{3})$ $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$	(5) $6^-(0,0,\frac{5}{6})$ $0,0,z$	(6) $6^+(0,0,\frac{1}{6})$ $0,0,z$
(7) 2 $x,x,\frac{1}{6}$	(8) 2 $x,0,0$	(9) 2 $0,y,\frac{1}{3}$
(10) 2 $x,\bar{x},\frac{5}{12}$	(11) 2 $x,2x,\frac{1}{4}$	(12) 2 $2x,x,\frac{1}{12}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	c	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$				$000l$: $l=6n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{5}{6}$	(6) $x-y,x,z+\frac{1}{6}$				
			(7) $y,x,\bar{z}+\frac{1}{3}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{2}{3}$				
			(10) $\bar{y},\bar{x},\bar{z}+\frac{5}{6}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{1}{6}$				
									Special: as above, plus
6	b	. . 2	$x,2x,\frac{1}{4}$	$2\bar{x},\bar{x},\frac{7}{12}$	$x,\bar{x},\frac{11}{12}$	$\bar{x},2\bar{x},\frac{3}{4}$	$2x,x,\frac{1}{12}$	$\bar{x},x,\frac{5}{12}$	$hh\overline{2h}l$: $l=2n$ or $l=3n+1$ or $l=3n+2$
6	a	. 2 .	$x,0,0$	$0,x,\frac{1}{3}$	$\bar{x},\bar{x},\frac{2}{3}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{5}{6}$	$x,x,\frac{1}{6}$	$h\bar{h}0l$: $l=2n$ or $l=3n+1$ or $l=3n+2$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{12}$

Maximal non-isomorphic subgroups

I [2] $P6_111$ ($P6_1$, 169) 1; 2; 3; 4; 5; 6
[2] $P3_121$ (152) 1; 2; 3; 7; 8; 9
[2] $P3_112$ (151) 1; 2; 3; 10; 11; 12
{ [3] $P2_122$ ($C222_1$, 20) 1; 4; 7; 10
[3] $P2_122$ ($C222_1$, 20) 1; 4; 8; 11
[3] $P2_122$ ($C222_1$, 20) 1; 4; 9; 12 }

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $H6_122$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6_122$, 178); [5] $P6_522$ ($\mathbf{c}'=5\mathbf{c}$) (179); [7] $P6_122$ ($\mathbf{c}'=7\mathbf{c}$) (178)

Minimal non-isomorphic supergroups

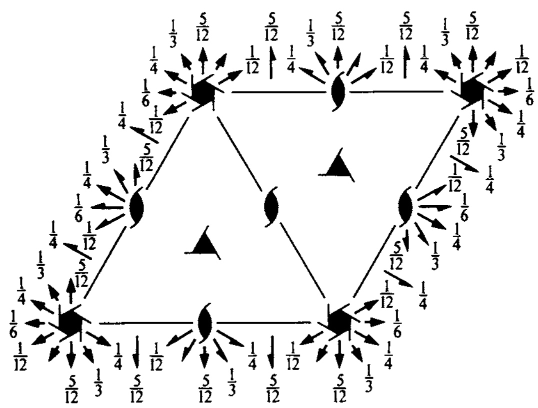
I none

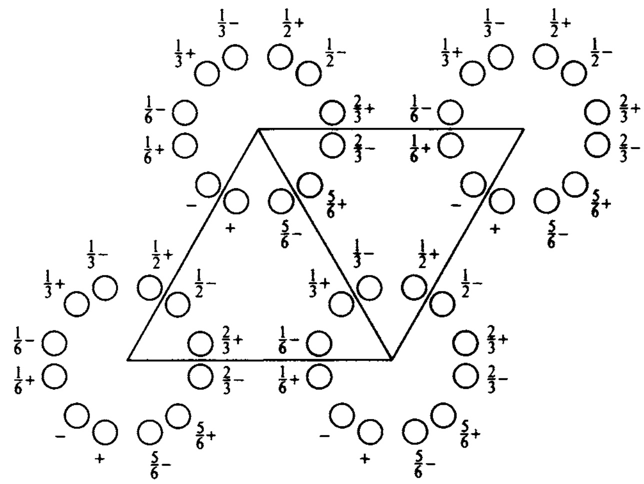
II [2] $P6_222$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (180); [3] $P6_322$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (182)

International Tables for Crystallography (2006). Vol. A, Space group 179, pp. 570–571.

$P6_522$ D_6^3 622 Hexagonal

No. 179 $P6_522$ Patterson symmetry $P6/mmm$





Origin on $2[100]$ at $6_5\,(2,1,1)\,1$

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le \frac{1}{12}$

Vertices $0,0,0$ $1,0,0$ $1,1,0$ $0,1,0$

$0,0,\frac{1}{12}$ $1,0,\frac{1}{12}$ $1,1,\frac{1}{12}$ $0,1,\frac{1}{12}$

Symmetry operations

(1) 1	(2) $3^+(0,0,\frac{2}{3})$ $0,0,z$	(3) $3^-(0,0,\frac{1}{3})$ $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$	(5) $6^-(0,0,\frac{1}{6})$ $0,0,z$	(6) $6^+(0,0,\frac{5}{6})$ $0,0,z$
(7) 2 $x,x,\frac{1}{3}$	(8) 2 $x,0,0$	(9) 2 $0,y,\frac{1}{6}$
(10) 2 $x,\bar{x},\frac{1}{12}$	(11) 2 $x,2x,\frac{1}{4}$	(12) 2 $2x,x,\frac{5}{12}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	c	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$				$000l$: $l=6n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{6}$	(6) $x-y,x,z+\frac{5}{6}$				
			(7) $y,x,\bar{z}+\frac{2}{3}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{3}$				
			(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{6}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{5}{6}$				
									Special: as above, plus
6	b	..2	$x,2x,\frac{3}{4}$	$2\bar{x},\bar{x},\frac{5}{12}$	$x,\bar{x},\frac{1}{12}$	$\bar{x},2\bar{x},\frac{1}{4}$	$2x,x,\frac{11}{12}$	$\bar{x},x,\frac{7}{12}$	$hh\overline{2h}l$: $l=2n$ or $l=3n+1$ or $l=3n+2$
6	a	.2.	$x,0,0$	$0,x,\frac{2}{3}$	$\bar{x},\bar{x},\frac{1}{3}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{6}$	$x,x,\frac{5}{6}$	$h\bar{h}0l$: $l=2n$ or $l=3n+1$ or $l=3n+2$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{5}{12}$

Maximal non-isomorphic subgroups

I
- [2] $P6_511$ ($P6_5$, 170) 1; 2; 3; 4; 5; 6
- [2] $P3_221$ (154) 1; 2; 3; 7; 8; 9
- [2] $P3_212$ (153) 1; 2; 3; 10; 11; 12
- { [3] $P2_122$ ($C222_1$, 20) 1; 4; 7; 10
- { [3] $P2_122$ ($C222_1$, 20) 1; 4; 8; 11
- { [3] $P2_122$ ($C222_1$, 20) 1; 4; 9; 12

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $H6_522$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6_522$, 179); [5] $P6_122$ ($\mathbf{c}'=5\mathbf{c}$) (178); [7] $P6_522$ ($\mathbf{c}'=7\mathbf{c}$) (179)

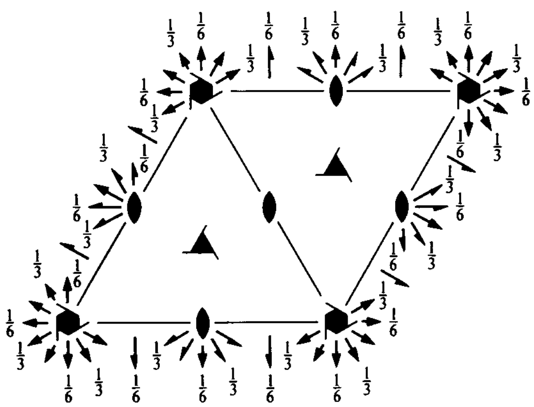
Minimal non-isomorphic supergroups

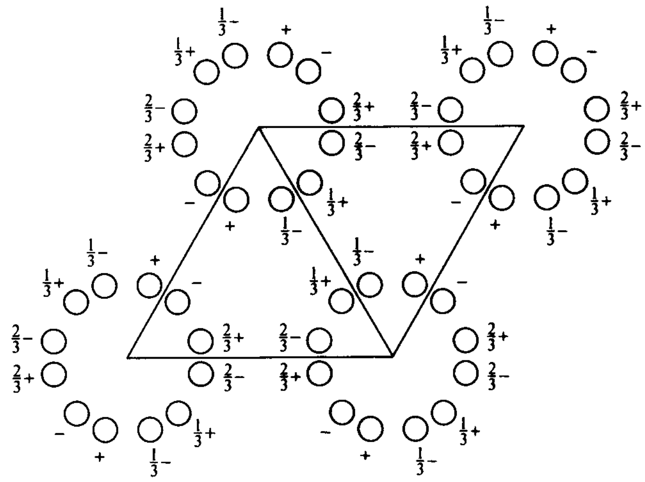
I none

II [2] $P6_422$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (181); [3] $P6_322$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (182)

$P6_222$ D_6^4 622 Hexagonal

No. 180 $P6_222$ Patterson symmetry $P6/mmm$





Origin at 222 at $6_2(2,1,1)(1,2,1)$

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le \frac{1}{6}$; $y \le x$

Vertices $0,0,0$ $1,0,0$ $1,1,0$

$0,0,\frac{1}{6}$ $1,0,\frac{1}{6}$ $1,1,\frac{1}{6}$

Symmetry operations

(1) 1	(2) $3^+(0,0,\frac{2}{3})$ $0,0,z$	(3) $3^-(0,0,\frac{1}{3})$ $0,0,z$
(4) 2 $0,0,z$	(5) $6^-(0,0,\frac{2}{3})$ $0,0,z$	(6) $6^+(0,0,\frac{1}{3})$ $0,0,z$
(7) 2 $x,x,\frac{1}{3}$	(8) 2 $x,0,0$	(9) 2 $0,y,\frac{1}{6}$
(10) 2 $x,\bar{x},\frac{1}{3}$	(11) 2 $x,2x,0$	(12) 2 $2x,x,\frac{1}{6}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	k	1	(1) x,y,z (4) $\bar{x},\bar{y},z$ (7) $y,x,\bar{z}+\frac{2}{3}$ (10) $\bar{y},\bar{x},\bar{z}+\frac{2}{3}$	(2) $\bar{y},x-y,z+\frac{2}{3}$ (5) $y,\bar{x}+y,z+\frac{2}{3}$ (8) $x-y,\bar{y},\bar{z}$ (11) $\bar{x}+y,y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$ (6) $x-y,x,z+\frac{1}{3}$ (9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{3}$ (12) $x,x-y,\bar{z}+\frac{1}{3}$				$000l$: $l=3n$
									Special: as above, plus
6	j	. . 2	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{6}$	$x,\bar{x},\frac{5}{6}$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{1}{6}$	$\bar{x},x,\frac{5}{6}$	no extra conditions
6	i	. . 2	$x,2x,0$	$2\bar{x},\bar{x},\frac{2}{3}$	$x,\bar{x},\frac{1}{3}$	$\bar{x},2\bar{x},0$	$2x,x,\frac{2}{3}$	$\bar{x},x,\frac{1}{3}$	no extra conditions
6	h	. 2 .	$x,0,\frac{1}{2}$	$0,x,\frac{1}{6}$	$\bar{x},\bar{x},\frac{5}{6}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{6}$	$x,x,\frac{5}{6}$	no extra conditions
6	g	. 2 .	$x,0,0$	$0,x,\frac{2}{3}$	$\bar{x},\bar{x},\frac{1}{3}$	$\bar{x},0,0$	$0,\bar{x},\frac{2}{3}$	$x,x,\frac{1}{3}$	no extra conditions
6	f	2 . .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z+\frac{2}{3}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{3}$	$0,\frac{1}{2},\bar{z}+\frac{2}{3}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{3}$	$hkil$: $h=2n+1$ or $k=2n+1$ or $l=3n$
6	e	2 . .	$0,0,z$	$0,0,z+\frac{2}{3}$	$0,0,z+\frac{1}{3}$	$0,0,\bar{z}+\frac{2}{3}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{3}$	$hkil$: $l=3n$
3	d	2 2 2	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{6}$	$\frac{1}{2},\frac{1}{2},\frac{5}{6}$				$hkil$: $h=2n+1$ or $k=2n+1$ or $l=3n$
3	c	2 2 2	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{2}{3}$	$\frac{1}{2},\frac{1}{2},\frac{1}{3}$				$hkil$: $h=2n+1$ or $k=2n+1$ or $l=3n$
3	b	2 2 2	$0,0,\frac{1}{2}$	$0,0,\frac{1}{6}$	$0,0,\frac{5}{6}$				$hkil$: $l=3n$
3	a	2 2 2	$0,0,0$	$0,0,\frac{2}{3}$	$0,0,\frac{1}{3}$				$hkil$: $l=3n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{6}$

Maximal non-isomorphic subgroups

I [2] $P6_211$ ($P6_2$, 171) 1; 2; 3; 4; 5; 6
[2] $P3_221$ (154) 1; 2; 3; 7; 8; 9
[2] $P3_212$ (153) 1; 2; 3; 10; 11; 12
{ [3] $P222$ ($C222$, 21) 1; 4; 7; 10
[3] $P222$ ($C222$, 21) 1; 4; 8; 11
[3] $P222$ ($C222$, 21) 1; 4; 9; 12 }

IIa none

IIb [2] $P6_122$ ($\mathbf{c}'=2\mathbf{c}$) (178)

Maximal isomorphic subgroups of lowest index

IIc [2] $P6_422$ ($\mathbf{c}'=2\mathbf{c}$) (181); [3] $H6_222$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6_222$, 180); [7] $P6_222$ ($\mathbf{c}'=7\mathbf{c}$) (180)

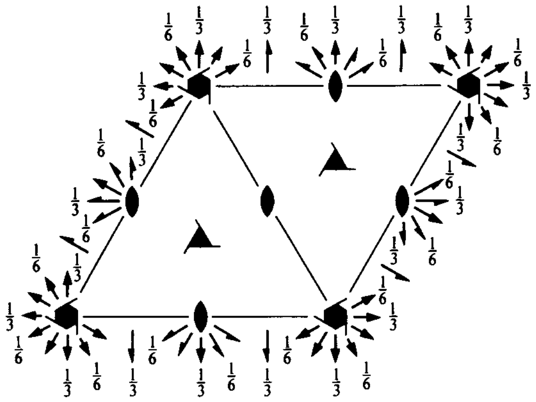
Minimal non-isomorphic supergroups

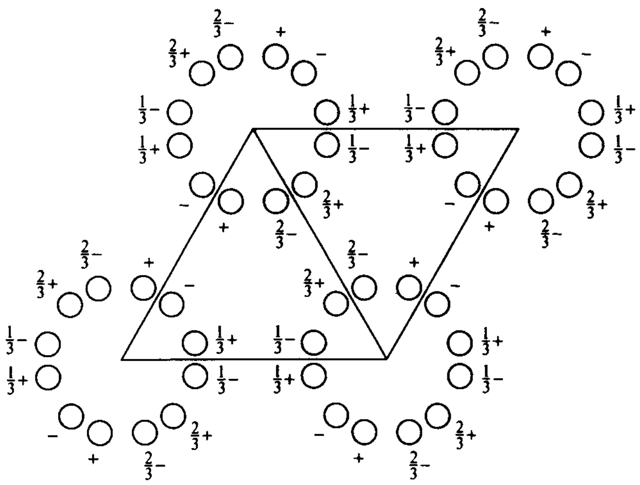
I none

II [3] $P622$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (177)

$P6_422$ D_6^5 622 Hexagonal

No. 181 $P6_422$ Patterson symmetry $P6/mmm$





Origin at 222 at $6_4(2,1,1)(1,2,1)$

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le \frac{1}{6}$; $y \le x$

Vertices $0,0,0$ $1,0,0$ $1,1,0$

$0,0,\frac{1}{6}$ $1,0,\frac{1}{6}$ $1,1,\frac{1}{6}$

Symmetry operations

(1) 1	(2) $3^+(0,0,\frac{1}{3})$ $0,0,z$	(3) $3^-(0,0,\frac{2}{3})$ $0,0,z$
(4) 2 $0,0,z$	(5) $6^-(0,0,\frac{1}{3})$ $0,0,z$	(6) $6^+(0,0,\frac{2}{3})$ $0,0,z$
(7) 2 $x,x,\frac{1}{6}$	(8) 2 $x,0,0$	(9) 2 $0,y,\frac{1}{3}$
(10) 2 $x,\bar{x},\frac{1}{6}$	(11) 2 $x,2x,0$	(12) 2 $2x,x,\frac{1}{3}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	k	1	(1) x,y,z (4) $\bar{x},\bar{y},z$ (7) $y,x,\bar{z}+\frac{1}{3}$ (10) $\bar{y},\bar{x},\bar{z}+\frac{1}{3}$	(2) $\bar{y},x-y,z+\frac{1}{3}$ (5) $y,\bar{x}+y,z+\frac{1}{3}$ (8) $x-y,\bar{y},\bar{z}$ (11) $\bar{x}+y,y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$ (6) $x-y,x,z+\frac{2}{3}$ (9) $\bar{x},\bar{x}+y,\bar{z}+\frac{2}{3}$ (12) $x,x-y,\bar{z}+\frac{2}{3}$				$000l$: $l=3n$
									Special: as above, plus
6	j	. . 2	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{5}{6}$	$x,\bar{x},\frac{1}{6}$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{5}{6}$	$\bar{x},x,\frac{1}{6}$	no extra conditions
6	i	. . 2	$x,2x,0$	$2\bar{x},\bar{x},\frac{1}{3}$	$x,\bar{x},\frac{2}{3}$	$\bar{x},2\bar{x},0$	$2x,x,\frac{1}{3}$	$\bar{x},x,\frac{2}{3}$	no extra conditions
6	h	. 2 .	$x,0,\frac{1}{2}$	$0,x,\frac{5}{6}$	$\bar{x},\bar{x},\frac{1}{6}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{5}{6}$	$x,x,\frac{1}{6}$	no extra conditions
6	g	. 2 .	$x,0,0$	$0,x,\frac{1}{3}$	$\bar{x},\bar{x},\frac{2}{3}$	$\bar{x},0,0$	$0,\bar{x},\frac{1}{3}$	$x,x,\frac{2}{3}$	no extra conditions
6	f	2 . .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z+\frac{1}{3}$	$\frac{1}{2},\frac{1}{2},z+\frac{2}{3}$	$0,\frac{1}{2},\bar{z}+\frac{1}{3}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{2}{3}$	$hkil$: $h=2n+1$ or $k=2n+1$ or $l=3n$
6	e	2 . .	$0,0,z$	$0,0,z+\frac{1}{3}$	$0,0,z+\frac{2}{3}$	$0,0,\bar{z}+\frac{1}{3}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{2}{3}$	$hkil$: $l=3n$
3	d	2 2 2	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{5}{6}$	$\frac{1}{2},\frac{1}{2},\frac{1}{6}$				$hkil$: $h=2n+1$ or $k=2n+1$ or $l=3n$
3	c	2 2 2	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{3}$	$\frac{1}{2},\frac{1}{2},\frac{2}{3}$				$hkil$: $h=2n+1$ or $k=2n+1$ or $l=3n$
3	b	2 2 2	$0,0,\frac{1}{2}$	$0,0,\frac{5}{6}$	$0,0,\frac{1}{6}$				$hkil$: $l=3n$
3	a	2 2 2	$0,0,0$	$0,0,\frac{1}{3}$	$0,0,\frac{2}{3}$				$hkil$: $l=3n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{3}$

Maximal non-isomorphic subgroups

I
- [2] $P6_411$ ($P6_4$, 172) 1; 2; 3; 4; 5; 6
- [2] $P3_121$ (152) 1; 2; 3; 7; 8; 9
- [2] $P3_112$ (151) 1; 2; 3; 10; 11; 12
- { [3] $P222$ ($C222$, 21) 1; 4; 7; 10
- [3] $P222$ ($C222$, 21) 1; 4; 8; 11
- [3] $P222$ ($C222$, 21) 1; 4; 9; 12 }

IIa none

IIb [2] $P6_522$ ($\mathbf{c}'=2\mathbf{c}$) (179)

Maximal isomorphic subgroups of lowest index

IIc [2] $P6_222$ ($\mathbf{c}'=2\mathbf{c}$) (180); [3] $H6_422$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6_422$, 181); [7] $P6_422$ ($\mathbf{c}'=7\mathbf{c}$) (181)

Minimal non-isomorphic supergroups

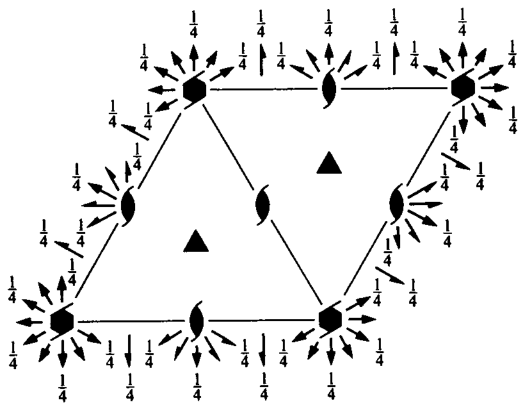
I none

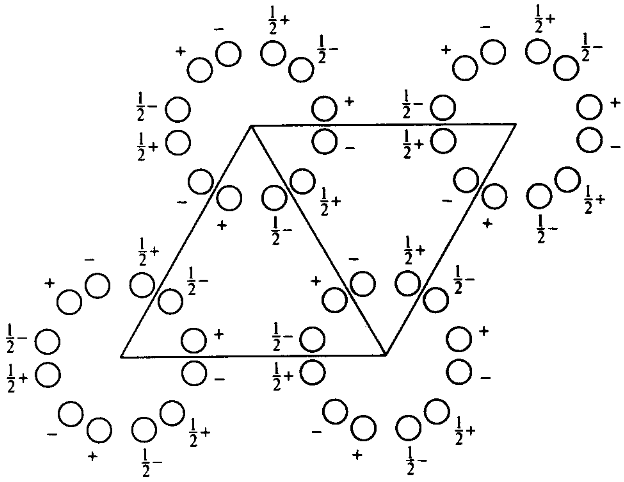
II [3] $P622$ ($\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (177)

International Tables for Crystallography (2006). Vol. A, Space group 182, pp. 576–577.

$P6_322$ D_6^6 622 Hexagonal

No. 182 $P6_322$ Patterson symmetry $P6/mmm$





Origin at 321 at 6_321

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{4}$; $x \le (1+y)/2$; $y \le \min(1-x, (1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$

$0,0,\frac{1}{4}$ $\frac{1}{2},0,\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\frac{1}{3},\frac{2}{3},\frac{1}{4}$ $0,\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$	(5) $6^-(0,0,\frac{1}{2})$ $0,0,z$	(6) $6^+(0,0,\frac{1}{2})$ $0,0,z$
(7) 2 $x,x,0$	(8) 2 $x,0,0$	(9) 2 $0,y,0$
(10) 2 $x,\bar{x},\frac{1}{4}$	(11) 2 $x,2x,\frac{1}{4}$	(12) 2 $2x,x,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	i	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$000l$: $l=2n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$				
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$				
			(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{1}{2}$				
									Special: as above, plus
6	h	..2	$x,2x,\frac{1}{4}$	$2\bar{x},\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},2\bar{x},\frac{3}{4}$	$2x,x,\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	$hh\overline{2h}l$: $l=2n$
6	g	.2.	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	$h\bar{h}0l$: $l=2n$
4	f	3..	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$			$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
4	e	3..	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$			$hkil$: $l=2n$
2	d	3.2	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	c	3.2	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	b	3.2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$
2	a	32.	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{4}$

Maximal non-isomorphic subgroups

I [2] $P6_311$ ($P6_3$, 173) 1; 2; 3; 4; 5; 6
[2] $P321$ (150) 1; 2; 3; 7; 8; 9
[2] $P312$ (149) 1; 2; 3; 10; 11; 12
{ [3] $P2_122$ ($C222_1$, 20) 1; 4; 7; 10
[3] $P2_122$ ($C222_1$, 20) 1; 4; 8; 11
[3] $P2_122$ ($C222_1$, 20) 1; 4; 9; 12 }

IIa none

IIb [3] $P6_522$ ($\mathbf{c}'=3\mathbf{c}$) (179); [3] $P6_122$ ($\mathbf{c}'=3\mathbf{c}$) (178)

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_322$ ($\mathbf{c}'=3\mathbf{c}$) (182); [3] $H6_322$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6_322$, 182)

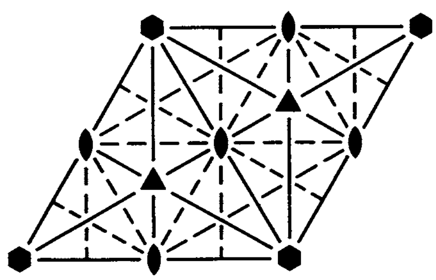
Minimal non-isomorphic supergroups

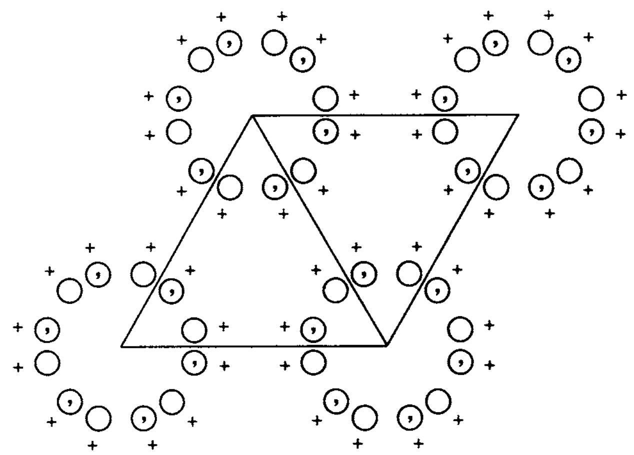
I [2] $P6_3/mcm$ (193); [2] $P6_3/mmc$ (194)

II [2] $P622$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (177)

$P6mm$ $\quad C_{6v}^{1}$ $\quad 6mm$ $\quad$ Hexagonal

No. 183 $\quad P6mm$ $\quad$ Patterson symmetry $P6/mmm$





Origin on $6mm$

Asymmetric unit $\quad 0 \le x \le \frac{2}{3}$; $\quad 0 \le y \le \frac{1}{3}$; $\quad 0 \le z \le 1$; $\quad x \le (1+y)/2$; $\quad y \le x/2$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0$

$0,0,1 \quad \frac{1}{2},0,1 \quad \frac{2}{3},\frac{1}{3},1$

Symmetry operations

(1) 1	(2) 3^{+} $0,0,z$	(3) 3^{-} $0,0,z$
(4) 2 $0,0,z$	(5) 6^{-} $0,0,z$	(6) 6^{+} $0,0,z$
(7) m $x,\bar{x},z$	(8) m $x,2x,z$	(9) m $2x,x,z$
(10) m x,x,z	(11) m $x,0,z$	(12) m $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	f	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				no conditions
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$				
			(7) $\bar{y},\bar{x},z$	(8) $\bar{x}+y,y,z$	(9) $x,x-y,z$				
			(10) y,x,z	(11) $x-y,\bar{y},z$	(12) $\bar{x},\bar{x}+y,z$				
									Special: no extra conditions
6	e	$.m.$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,z$	$\bar{x},2\bar{x},z$	$2x,x,z$	
6	d	$..m$	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$\bar{x},0,z$	$0,\bar{x},z$	x,x,z	
3	c	$2mm$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$				
2	b	$3m.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$					
1	a	$6mm$	$0,0,z$						

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P611$ ($P6$, 168) 1; 2; 3; 4; 5; 6
[2] $P31m$ (157) 1; 2; 3; 10; 11; 12
[2] $P3m1$ (156) 1; 2; 3; 7; 8; 9
$\left\{\begin{array}{ll} [3]\ P2mm\ (Cmm2, 35) & 1;\ 4;\ 7;\ 10 \\ [3]\ P2mm\ (Cmm2, 35) & 1;\ 4;\ 8;\ 11 \\ [3]\ P2mm\ (Cmm2, 35) & 1;\ 4;\ 9;\ 12 \end{array}\right.$

IIa none

IIb [2] $P6_3mc$ ($\mathbf{c}' = 2\mathbf{c}$) (186); [2] $P6_3cm$ ($\mathbf{c}' = 2\mathbf{c}$) (185); [2] $P6cc$ ($\mathbf{c}' = 2\mathbf{c}$) (184)

Maximal isomorphic subgroups of lowest index

IIc [2] $P6mm$ ($\mathbf{c}' = 2\mathbf{c}$) (183); [3] $H6mm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6mm$, 183)

Minimal non-isomorphic supergroups

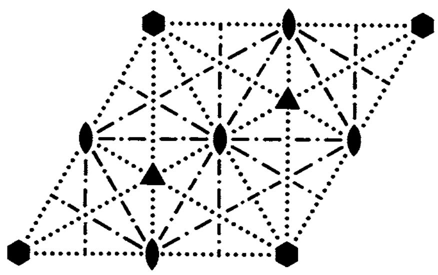
I [2] $P6/mmm$ (191)

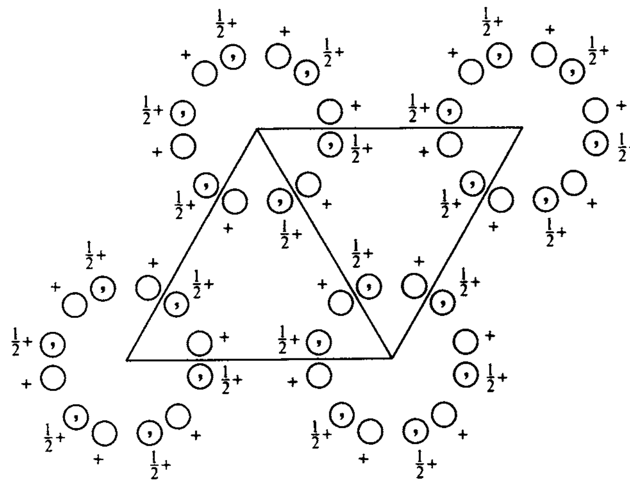
II none

International Tables for Crystallography (2006). Vol. A, Space group 184, pp. 580–581.

$P6cc$ $\quad$ C_{6v}^2 $\quad$ $6mm$ $\quad$ Hexagonal

No. 184 $\quad$ $P6cc$ $\quad$ Patterson symmetry $P6/mmm$





Origin on $6cc$

Asymmetric unit $\quad 0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2};\quad x \le (1+y)/2;\quad y \le \min(1-x, x)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{2},\frac{1}{2},0$

$\quad 0,0,\frac{1}{2} \quad \frac{1}{2},0,\frac{1}{2} \quad \frac{2}{3},\frac{1}{3},\frac{1}{2} \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) $3^+\ 0,0,z$	(3) $3^-\ 0,0,z$
(4) $2\ \ 0,0,z$	(5) $6^-\ 0,0,z$	(6) $6^+\ 0,0,z$
(7) $c\ \ x,\bar{x},z$	(8) $c\ \ x,2x,z$	(9) $c\ \ 2x,x,z$
(10) $c\ \ x,x,z$	(11) $c\ \ x,0,z$	(12) $c\ \ 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$hh\overline{2h}l$: $l=2n$
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$				$h\bar{h}0l$: $l=2n$
			(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $\bar{x}+y,y,z+\frac{1}{2}$	(9) $x,x-y,z+\frac{1}{2}$				$000l$: $l=2n$
			(10) $y,x,z+\frac{1}{2}$	(11) $x-y,\bar{y},z+\frac{1}{2}$	(12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$				
									Special: as above, plus
6	c	$2\,.\,.$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$hkil$: $l=2n$
4	b	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$	$\frac{1}{3},\frac{2}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$			$hkil$: $l=2n$
2	a	$6\,.\,.$	$0,0,z$	$0,0,z+\frac{1}{2}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P611$ ($P6$, 168) 1; 2; 3; 4; 5; 6
[2] $P31c$ (159) 1; 2; 3; 10; 11; 12
[2] $P3c1$ (158) 1; 2; 3; 7; 8; 9
{ [3] $P2cc$ ($Ccc2$, 37) 1; 4; 7; 10
{ [3] $P2cc$ ($Ccc2$, 37) 1; 4; 8; 11
{ [3] $P2cc$ ($Ccc2$, 37) 1; 4; 9; 12

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P6cc$ ($\mathbf{c}'=3\mathbf{c}$) (184); [3] $H6cc$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6cc$, 184)

Minimal non-isomorphic supergroups

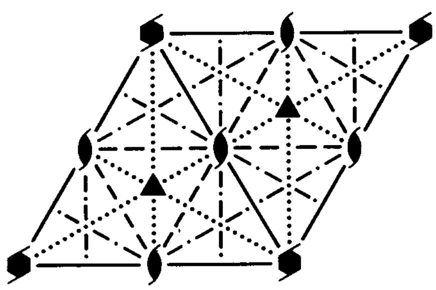
I [2] $P6/mcc$ (192)

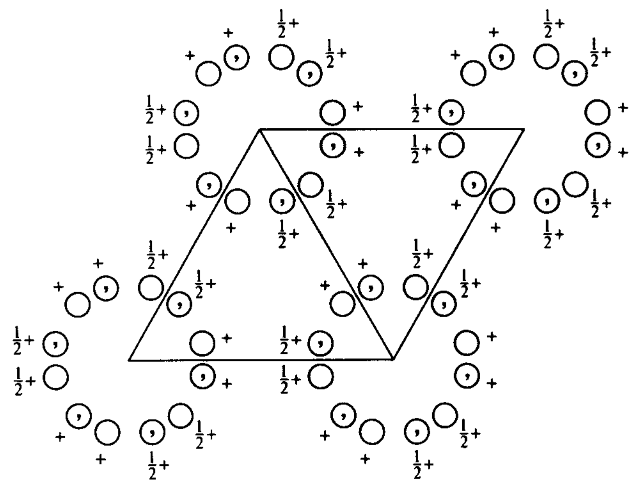
II [2] $P6mm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (183)

International Tables for Crystallography (2006). Vol. A, Space group 185, pp. 582–583.

$P6_3cm$ $\quad C_{6v}^3$ $\quad 6mm$ $\quad$ Hexagonal

No. 185 $\quad P6_3cm$ $\quad$ Patterson symmetry $P6/mmm$





Origin on $31m$ on 6_3cm

Asymmetric unit $\quad 0 \le x \le \frac{2}{3}$; $\quad 0 \le y \le \frac{1}{2}$; $\quad 0 \le z \le \frac{1}{2}$; $\quad x \le (1+y)/2$; $\quad y \le \min(1-x, x)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{2},\frac{1}{2},0$

$\quad 0,0,\frac{1}{2} \quad \frac{1}{2},0,\frac{1}{2} \quad \frac{2}{3},\frac{1}{3},\frac{1}{2} \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) $3^+ \ 0,0,z$	(3) $3^- \ 0,0,z$
(4) $2(0,0,\frac{1}{2}) \quad 0,0,z$	(5) $6^-(0,0,\frac{1}{2}) \quad 0,0,z$	(6) $6^+(0,0,\frac{1}{2}) \quad 0,0,z$
(7) $c \quad x,\bar{x},z$	(8) $c \quad x,2x,z$	(9) $c \quad 2x,x,z$
(10) $m \quad x,x,z$	(11) $m \quad x,0,z$	(12) $m \quad 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	*d*	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$h\bar{h}0l$: $l=2n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$				$000l$: $l=2n$
			(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $\bar{x}+y,y,z+\frac{1}{2}$	(9) $x,x-y,z+\frac{1}{2}$				
			(10) y,x,z	(11) $x-y,\bar{y},z$	(12) $\bar{x},\bar{x}+y,z$				
									Special: as above, plus
6	*c*	$. . m$	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$\bar{x},0,z+\frac{1}{2}$	$0,\bar{x},z+\frac{1}{2}$	$x,x,z+\frac{1}{2}$	no extra conditions
4	*b*	$3 . .$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$\frac{1}{3},\frac{2}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},z$			$hkil$: $l=2n$
2	*a*	$3 . m$	$0,0,z$	$0,0,z+\frac{1}{2}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1g1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I	[2] $P6_311$ ($P6_3$, 173)	1; 2; 3; 4; 5; 6
	[2] $P3c1$ (158)	1; 2; 3; 7; 8; 9
	[2] $P31m$ (157)	1; 2; 3; 10; 11; 12
	$\{$ [3] $P2_1cm$ ($Cmc2_1$, 36)	1; 4; 7; 10
	[3] $P2_1cm$ ($Cmc2_1$, 36)	1; 4; 8; 11
	[3] $P2_1cm$ ($Cmc2_1$, 36)	1; 4; 9; 12

IIa none

IIb [3] $H6_3cm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6_3mc$, 186)

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_3cm$ ($\mathbf{c}'=3\mathbf{c}$) (185); [4] $P6_3cm$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (185)

Minimal non-isomorphic supergroups

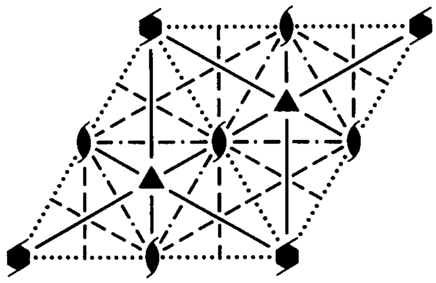
I [2] $P6_3/mcm$ (193)

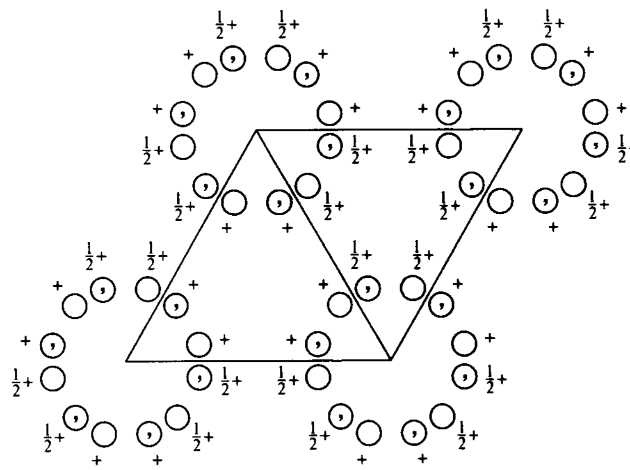
II [3] $H6_3cm$ ($P6_3mc$, 186); [2] $P6mm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (183)

International Tables for Crystallography (2006). Vol. A, Space group 186, pp. 584–585.

$P6_3mc$ $\quad C_{6v}^4$ $\quad 6mm$ $\quad$ Hexagonal

No. 186 $\quad P6_3mc$ $\quad$ Patterson symmetry $P6/mmm$





Origin on $3m1$ on 6_3mc

Asymmetric unit $\quad 0 \le x \le \frac{2}{3}$; $\quad 0 \le y \le \frac{1}{3}$; $\quad 0 \le z \le 1$; $\quad x \le (1+y)/2$; $\quad y \le x/2$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0$

$0,0,1 \quad \frac{1}{2},0,1 \quad \frac{2}{3},\frac{1}{3},1$

Symmetry operations

(1) 1	(2) $3^+\ 0,0,z$	(3) $3^-\ 0,0,z$
(4) $2(0,0,\frac{1}{2})\quad 0,0,z$	(5) $6^-(0,0,\frac{1}{2})\quad 0,0,z$	(6) $6^+(0,0,\frac{1}{2})\quad 0,0,z$
(7) $m\ \ x,\bar{x},z$	(8) $m\ \ x,2x,z$	(9) $m\ \ 2x,x,z$
(10) $c\ \ x,x,z$	(11) $c\ \ x,0,z$	(12) $c\ \ 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$hh\overline{2h}l$: $l=2n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$				$000l$: $l=2n$
			(7) $\bar{y},\bar{x},z$	(8) $\bar{x}+y,y,z$	(9) $x,x-y,z$				
			(10) $y,x,z+\frac{1}{2}$	(11) $x-y,\bar{y},z+\frac{1}{2}$	(12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$				
									Special: as above, plus
6	c	$.m.$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,z+\frac{1}{2}$	$\bar{x},2\bar{x},z+\frac{1}{2}$	$2x,x,z+\frac{1}{2}$	no extra conditions
2	b	$3m.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	a	$3m.$	$0,0,z$	$0,0,z+\frac{1}{2}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I	[2] $P6_311$ ($P6_3$, 173)	1; 2; 3; 4; 5; 6
	[2] $P31c$ (159)	1; 2; 3; 10; 11; 12
	[2] $P3m1$ (156)	1; 2; 3; 7; 8; 9
	[3] $P2_1mc$ ($Cmc2_1$, 36)	1; 4; 7; 10
	[3] $P2_1mc$ ($Cmc2_1$, 36)	1; 4; 8; 11
	[3] $P2_1mc$ ($Cmc2_1$, 36)	1; 4; 9; 12

IIa none

IIb [3] $H6_3mc$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P6_3cm$, 185)

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_3mc$ ($\mathbf{c}'=3\mathbf{c}$) (186); [4] $P6_3mc$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (186)

Minimal non-isomorphic supergroups

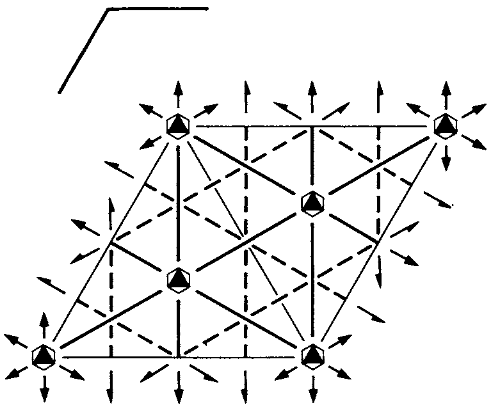
I [2] $P6_3/mmc$ (194)

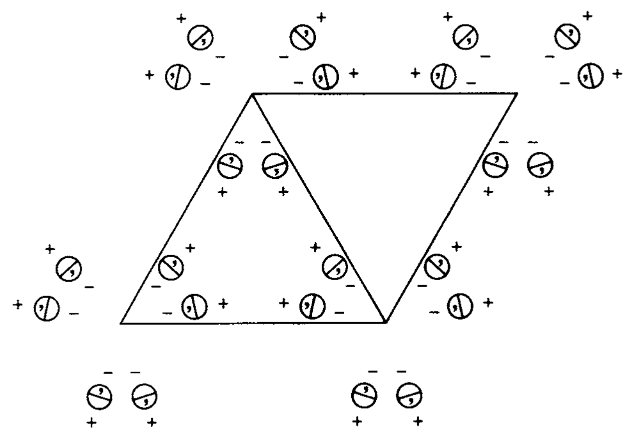
II [3] $H6_3mc$ ($P6_3cm$, 185); [2] $P6mm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (183)

International Tables for Crystallography (2006). Vol. A, Space group 187, pp. 586–587.

$P\bar{6}m2$ D_{3h}^{1} $\bar{6}m2$ Hexagonal

No. 187 $P\bar{6}m2$ Patterson symmetry $P6/mmm$





Origin at $\bar{6}m2$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{2}$; $x \le 2y$; $y \le \min(1-x, 2x)$

Vertices $0,0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$

$0,0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) m $x,y,0$	(5) $\bar{6}^-$ $0,0,z$; $0,0,0$	(6) $\bar{6}^+$ $0,0,z$; $0,0,0$
(7) m $x,\bar{x},z$	(8) m $x,2x,z$	(9) m $2x,x,z$
(10) 2 $x,\bar{x},0$	(11) 2 $x,2x,0$	(12) 2 $2x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{6}11$ ($P\bar{6}$, 174)	1; 2; 3; 4; 5; 6
	[2] $P3m1$ (156)	1; 2; 3; 7; 8; 9
	[2] $P312$ (149)	1; 2; 3; 10; 11; 12
	[3] $Pmm2$ ($Amm2$, 38)	1; 4; 7; 10
	[3] $Pmm2$ ($Amm2$, 38)	1; 4; 8; 11
	[3] $Pmm2$ ($Amm2$, 38)	1; 4; 9; 12

IIa none

IIb [2] $P\bar{6}c2$ ($\mathbf{c}' = 2\mathbf{c}$) (188); [3] $H\bar{6}m2$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P\bar{6}2m$, 189)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{6}m2$ ($\mathbf{c}' = 2\mathbf{c}$) (187); [4] $P\bar{6}m2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (187)

Minimal non-isomorphic supergroups

I [2] $P6/mmm$ (191); [2] $P6_3/mmc$ (194)

II [3] $H\bar{6}m2$ ($P\bar{6}2m$, 189)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	o	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				no conditions
			(4) $x,y,\bar{z}$	(5) $\bar{y},x-y,\bar{z}$	(6) $\bar{x}+y,\bar{x},\bar{z}$				
			(7) $\bar{y},\bar{x},z$	(8) $\bar{x}+y,y,z$	(9) $x,x-y,z$				
			(10) $\bar{y},\bar{x},\bar{z}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}$				
									Special: no extra conditions
6	n	$.m.$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$x,\bar{x},\bar{z}$	$x,2x,\bar{z}$	$2\bar{x},\bar{x},\bar{z}$	
6	m	$m..$	$x,y,\frac{1}{2}$	$\bar{y},x-y,\frac{1}{2}$	$\bar{x}+y,\bar{x},\frac{1}{2}$	$\bar{y},\bar{x},\frac{1}{2}$	$\bar{x}+y,y,\frac{1}{2}$	$x,x-y,\frac{1}{2}$	
6	l	$m..$	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$\bar{y},\bar{x},0$	$\bar{x}+y,y,0$	$x,x-y,0$	
3	k	$mm2$	$x,\bar{x},\frac{1}{2}$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$				
3	j	$mm2$	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$				
2	i	$3m.$	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$					
2	h	$3m.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$					
2	g	$3m.$	$0,0,z$	$0,0,\bar{z}$					
1	f	$\bar{6}m2$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$						
1	e	$\bar{6}m2$	$\frac{2}{3},\frac{1}{3},0$						
1	d	$\bar{6}m2$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$						
1	c	$\bar{6}m2$	$\frac{1}{3},\frac{2}{3},0$						
1	b	$\bar{6}m2$	$0,0,\frac{1}{2}$						
1	a	$\bar{6}m2$	$0,0,0$						

Symmetry of special projections

Along [001] $p3m1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

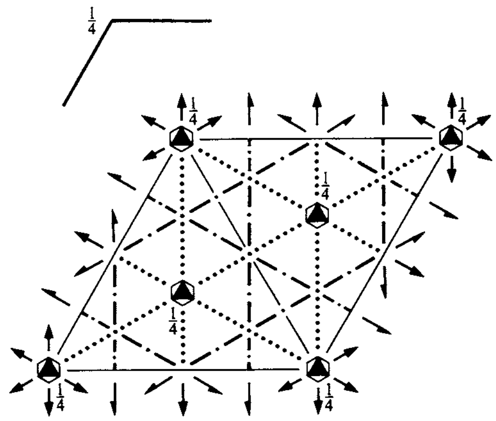
Along [100] $p11m$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

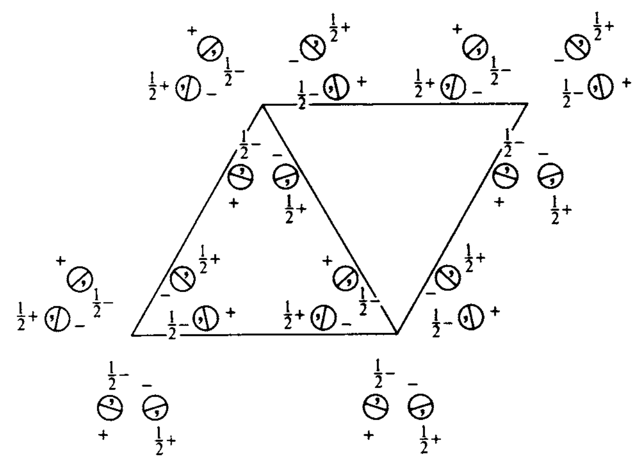
Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

(*Continued on preceding page*)

$P\bar{6}c2$ $\quad D_{3h}^{2}$ $\quad \bar{6}m2$ $\quad$ Hexagonal

No. 188 $\quad P\bar{6}c2$ $\quad$ Patterson symmetry $P6/mmm$





Origin at $3c2$

Asymmetric unit $\quad 0 \le x \le \frac{2}{3}; \quad 0 \le y \le \frac{2}{3}; \quad 0 \le z \le \frac{1}{4}; \quad x \le (1+y)/2; \quad y \le \min(1-x,(1+x)/2)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0 \quad 0,\frac{1}{2},0$

$0,0,\frac{1}{4} \quad \frac{1}{2},0,\frac{1}{4} \quad \frac{2}{3},\frac{1}{3},\frac{1}{4} \quad \frac{1}{3},\frac{2}{3},\frac{1}{4} \quad 0,\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1	(2) $3^{+}\ 0,0,z$	(3) $3^{-}\ 0,0,z$
(4) $m\ \ x,y,\frac{1}{4}$	(5) $\bar{6}^{-}\ 0,0,z;\ \ 0,0,\frac{1}{4}$	(6) $\bar{6}^{+}\ 0,0,z;\ \ 0,0,\frac{1}{4}$
(7) $c\ \ x,\bar{x},z$	(8) $c\ \ x,2x,z$	(9) $c\ \ 2x,x,z$
(10) $2\ \ x,\bar{x},0$	(11) $2\ \ x,2x,0$	(12) $2\ \ 2x,x,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$h\bar{h}0l$: $l=2n$
			(4) $x,y,\bar{z}+\frac{1}{2}$	(5) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(6) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$				$000l$: $l=2n$
			(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $\bar{x}+y,y,z+\frac{1}{2}$	(9) $x,x-y,z+\frac{1}{2}$				
			(10) $\bar{y},\bar{x},\bar{z}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}$				
									Special: as above, plus
6	k	$m\,.\,.$	$x,y,\frac{1}{4}$	$\bar{y},x-y,\frac{1}{4}$	$\bar{x}+y,\bar{x},\frac{1}{4}$	$\bar{y},\bar{x},\frac{3}{4}$	$\bar{x}+y,y,\frac{3}{4}$	$x,x-y,\frac{3}{4}$	no extra conditions
6	j	$.\,.\,2$	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	$x,\bar{x},\frac{1}{2}$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	$hkil$: $l=2n$
4	i	$3\,.\,.$	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}$			$hkil$: $l=2n$
4	h	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$	$\frac{1}{3},\frac{2}{3},z+\frac{1}{2}$	$\frac{1}{3},\frac{2}{3},\bar{z}$			$hkil$: $l=2n$
4	g	$3\,.\,.$	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$			$hkil$: $l=2n$
2	f	$\bar{6}\,.\,.$	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$					$hkil$: $l=2n$
2	e	$3\,.\,2$	$\frac{2}{3},\frac{1}{3},0$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$					$hkil$: $l=2n$
2	d	$\bar{6}\,.\,.$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$					$hkil$: $l=2n$
2	c	$3\,.\,2$	$\frac{1}{3},\frac{2}{3},0$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$					$hkil$: $l=2n$
2	b	$\bar{6}\,.\,.$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$
2	a	$3\,.\,2$	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p3m1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p11m$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{6}11$ ($P\bar{6}$, 174)	1; 2; 3; 4; 5; 6
	[2] $P3c1$ (158)	1; 2; 3; 7; 8; 9
	[2] $P312$ (149)	1; 2; 3; 10; 11; 12
	{ [3] $Pmc2$ ($Ama2$, 40)	1; 4; 7; 10
	{ [3] $Pmc2$ ($Ama2$, 40)	1; 4; 8; 11
	{ [3] $Pmc2$ ($Ama2$, 40)	1; 4; 9; 12

IIa none

IIb [3] $H\bar{6}c2$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P\bar{6}2c$, 190)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{6}c2$ ($\mathbf{c}'=3\mathbf{c}$) (188); [4] $P\bar{6}c2$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (188)

Minimal non-isomorphic supergroups

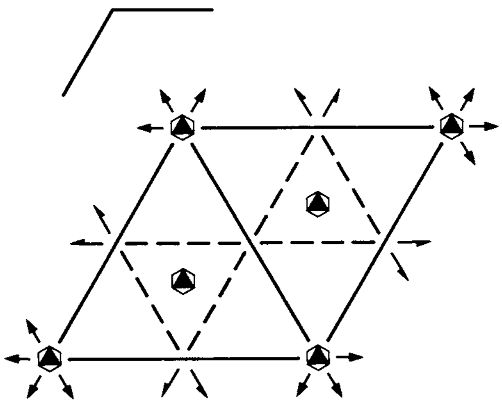
I [2] $P6/mcc$ (192); [2] $P6_3/mcm$ (193)

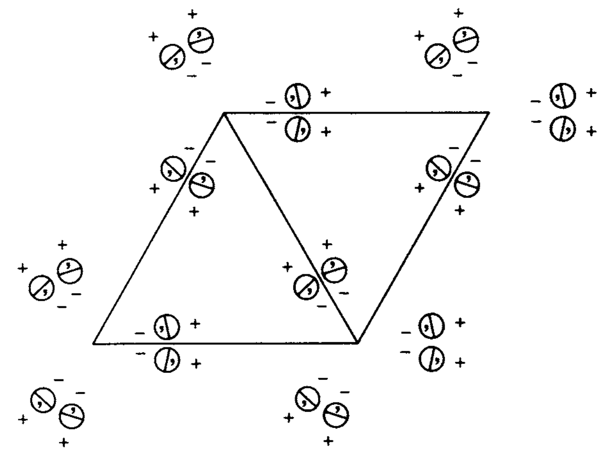
II [3] $H\bar{6}c2$ ($P\bar{6}2c$, 190); [2] $P\bar{6}m2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (187)

International Tables for Crystallography (2006). Vol. A, Space group 189, pp. 590–591.

$P\bar{6}2m$ D_{3h}^3 $\bar{6}2m$ Hexagonal

No. 189 $P\bar{6}2m$ Patterson symmetry $P6/mmm$





Origin at $\bar{6}2m$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x, x)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{2},\frac{1}{2},0$

$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) m $x,y,0$	(5) $\bar{6}^-$ $0,0,z$; $0,0,0$	(6) $\bar{6}^+$ $0,0,z$; $0,0,0$
(7) 2 $x,x,0$	(8) 2 $x,0,0$	(9) 2 $0,y,0$
(10) m x,x,z	(11) m $x,0,z$	(12) m $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				no conditions
			(4) $x,y,\bar{z}$	(5) $\bar{y},x-y,\bar{z}$	(6) $\bar{x}+y,\bar{x},\bar{z}$				
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$				
			(10) y,x,z	(11) $x-y,\bar{y},z$	(12) $\bar{x},\bar{x}+y,z$				
									Special: no extra conditions
6	k	$m\,.\,.$	$x,y,\frac{1}{2}$	$\bar{y},x-y,\frac{1}{2}$	$\bar{x}+y,\bar{x},\frac{1}{2}$	$y,x,\frac{1}{2}$	$x-y,\bar{y},\frac{1}{2}$	$\bar{x},\bar{x}+y,\frac{1}{2}$	
6	j	$m\,.\,.$	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$y,x,0$	$x-y,\bar{y},0$	$\bar{x},\bar{x}+y,0$	
6	i	$.\,.\,m$	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$x,0,\bar{z}$	$0,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
4	h	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},z$			
3	g	$m\,2\,m$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$				
3	f	$m\,2\,m$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$				
2	e	$3\,.\,m$	$0,0,z$	$0,0,\bar{z}$					
2	d	$\bar{6}\,.\,.$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$					
2	c	$\bar{6}\,.\,.$	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$					
1	b	$\bar{6}\,2\,m$	$0,0,\frac{1}{2}$						
1	a	$\bar{6}\,2\,m$	$0,0,0$						

Symmetry of special projections

Along [001] $p\,3\,1\,m$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,2\,m\,m$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p\,1\,1\,m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{6}\,1\,1$ ($P\bar{6}$, 174)	1; 2; 3; 4; 5; 6
	[2] $P\,3\,1\,m$ (157)	1; 2; 3; 10; 11; 12
	[2] $P\,3\,2\,1$ (150)	1; 2; 3; 7; 8; 9
	[3] $P\,m\,2\,m$ ($A\,m\,m\,2$, 38)	1; 4; 7; 10
	[3] $P\,m\,2\,m$ ($A\,m\,m\,2$, 38)	1; 4; 8; 11
	[3] $P\,m\,2\,m$ ($A\,m\,m\,2$, 38)	1; 4; 9; 12

IIa none

IIb [2] $P\bar{6}2c$ ($\mathbf{c}'=2\mathbf{c}$) (190); [3] $H\bar{6}2m$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P\bar{6}m2$, 187)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{6}2m$ ($\mathbf{c}'=2\mathbf{c}$) (189); [4] $P\bar{6}2m$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (189)

Minimal non-isomorphic supergroups

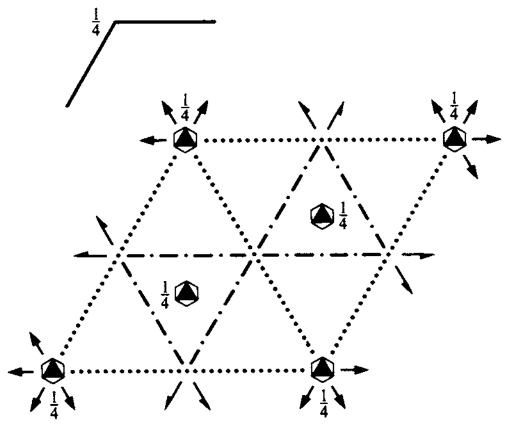
I [2] $P6/mmm$ (191); [2] $P6_3/mcm$ (193)

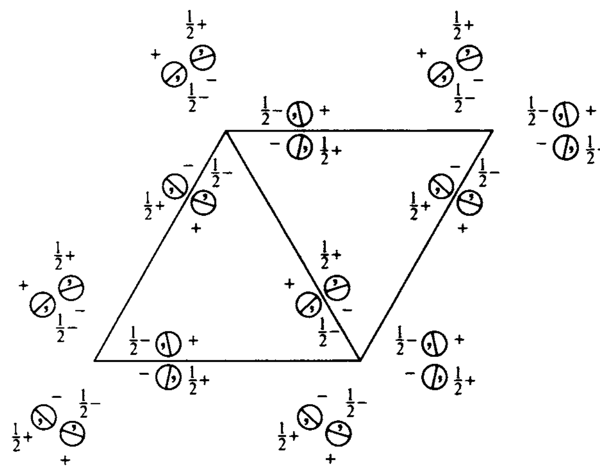
II [3] $H\bar{6}2m$ ($P\bar{6}m2$, 187)

International Tables for Crystallography (2006). Vol. A, Space group 190, pp. 592–593.

$P\bar{6}2c$ D_{3h}^{4} $\bar{6}2m$ Hexagonal

No. 190 $P\bar{6}2c$ Patterson symmetry $P6/mmm$





Origin at $32c$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{4}$; $x \le (1+y)/2$; $y \le \min(1-x, (1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$

$0,0,\frac{1}{4}$ $\frac{1}{2},0,\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\frac{1}{3},\frac{2}{3},\frac{1}{4}$ $0,\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1	(2) 3^{+} $0,0,z$	(3) 3^{-} $0,0,z$
(4) m $x,y,\frac{1}{4}$	(5) $\bar{6}^{-}$ $0,0,z$; $0,0,\frac{1}{4}$	(6) $\bar{6}^{+}$ $0,0,z$; $0,0,\frac{1}{4}$
(7) 2 $x,x,0$	(8) 2 $x,0,0$	(9) 2 $0,y,0$
(10) c x,x,z	(11) c $x,0,z$	(12) c $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	i	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$hh\overline{2h}l$: $l=2n$
			(4) $x,y,\bar{z}+\frac{1}{2}$	(5) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(6) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$				$000l$: $l=2n$
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$				
			(10) $y,x,z+\frac{1}{2}$	(11) $x-y,\bar{y},z+\frac{1}{2}$	(12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$				
									Special: as above, plus
6	h	$m\,.\,.$	$x,y,\frac{1}{4}$	$\bar{y},x-y,\frac{1}{4}$	$\bar{x}+y,\bar{x},\frac{1}{4}$	$y,x,\frac{3}{4}$	$x-y,\bar{y},\frac{3}{4}$	$\bar{x},\bar{x}+y,\frac{3}{4}$	no extra conditions
6	g	$.\,2\,.$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$hkil$: $l=2n$
4	f	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$			$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
4	e	$3\,.\,.$	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$			$hkil$: $l=2n$
2	d	$\bar{6}\,.\,.$	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	c	$\bar{6}\,.\,.$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	b	$\bar{6}\,.\,.$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$
2	a	$3\,2\,.$	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p\,3\,1\,m$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,2\,g\,m$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p\,1\,1\,m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I
- [2] $P\bar{6}11$ ($P\bar{6}$, 174) 1; 2; 3; 4; 5; 6
- [2] $P31c$ (159) 1; 2; 3; 10; 11; 12
- [2] $P321$ (150) 1; 2; 3; 7; 8; 9
- [3] $Pm2c$ ($Ama2$, 40) 1; 4; 7; 10
- [3] $Pm2c$ ($Ama2$, 40) 1; 4; 8; 11
- [3] $Pm2c$ ($Ama2$, 40) 1; 4; 9; 12

IIa none

IIb [3] $H\bar{6}2c$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P\bar{6}c2$, 188)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{6}2c$ ($\mathbf{c}'=3\mathbf{c}$) (190); [4] $P\bar{6}2c$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (190)

Minimal non-isomorphic supergroups

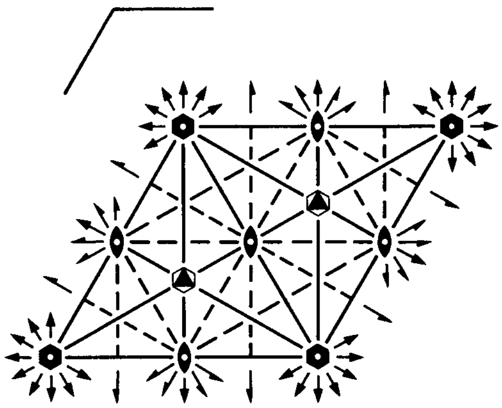
I [2] $P6/mcc$ (192); [2] $P6_3/mmc$ (194)

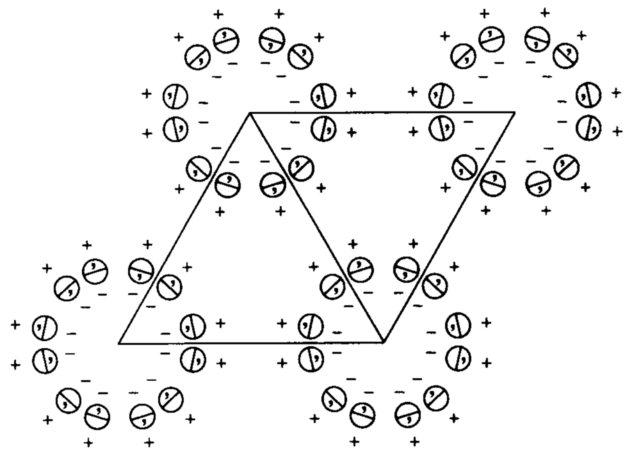
II [3] $H\bar{6}2c$ ($P\bar{6}c2$, 188); [2] $P\bar{6}2m$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (189)

International Tables for Crystallography (2006). Vol. A, Space group 191, pp. 594–595.

$P6/mmm$ $\quad D^1_{6h}$ $\quad 6/mmm$ $\quad$ Hexagonal

No. 191 $\quad P\ 6/m\ 2/m\ 2/m$ $\quad$ Patterson symmetry $P6/mmm$





Origin at centre $(6/mmm)$

Asymmetric unit $\quad 0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{1}{3};\quad 0 \le z \le \frac{1}{2};\quad x \le (1+y)/2;\quad y \le x/2$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0$

$0,0,\frac{1}{2} \quad \frac{1}{2},0,\frac{1}{2} \quad \frac{2}{3},\frac{1}{3},\frac{1}{2}$

Symmetry operations

(1) 1	(2) $3^+\ 0,0,z$	(3) $3^-\ 0,0,z$
(4) $2\ \ 0,0,z$	(5) $6^-\ 0,0,z$	(6) $6^+\ 0,0,z$
(7) $2\ \ x,x,0$	(8) $2\ \ x,0,0$	(9) $2\ \ 0,y,0$
(10) $2\ \ x,\bar{x},0$	(11) $2\ \ x,2x,0$	(12) $2\ \ 2x,x,0$
(13) $\bar{1}\ \ 0,0,0$	(14) $\bar{3}^+\ 0,0,z;\ 0,0,0$	(15) $\bar{3}^-\ 0,0,z;\ 0,0,0$
(16) $m\ \ x,y,0$	(17) $\bar{6}^-\ 0,0,z;\ 0,0,0$	(18) $\bar{6}^+\ 0,0,z;\ 0,0,0$
(19) $m\ \ x,\bar{x},z$	(20) $m\ \ x,2x,z$	(21) $m\ \ 2x,x,z$
(22) $m\ \ x,x,z$	(23) $m\ \ x,0,z$	(24) $m\ \ 0,y,z$

Maximal non-isomorphic subgroups

I	[2] $P\bar{6}2m$ (189)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
	[2] $P\bar{6}m2$ (187)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
	[2] $P6mm$ (183)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
	[2] $P622$ (177)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[2] $P6/m11$ ($P6/m$, 175)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
	[2] $P\bar{3}m1$ (164)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
	[2] $P\bar{3}1m$ (162)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
	{ [3] $Pmmm$ ($Cmmm$, 65)	1; 4; 7; 10; 13; 16; 19; 22
	{ [3] $Pmmm$ ($Cmmm$, 65)	1; 4; 8; 11; 13; 16; 20; 23
	{ [3] $Pmmm$ ($Cmmm$, 65)	1; 4; 9; 12; 13; 16; 21; 24

IIa none

IIb [2] $P6_3/mmc$ ($\mathbf{c}' = 2\mathbf{c}$) (194); [2] $P6_3/mcm$ ($\mathbf{c}' = 2\mathbf{c}$) (193); [2] $P6/mcc$ ($\mathbf{c}' = 2\mathbf{c}$) (192)

Maximal isomorphic subgroups of lowest index

IIc [2] $P6/mmm$ ($\mathbf{c}' = 2\mathbf{c}$) (191); [3] $H6/mmm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6/mmm$, 191)

Minimal non-isomorphic supergroups

I none

II none

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
24	r	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				no conditions
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$				
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$				
			(10) $\bar{y},\bar{x},\bar{z}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}$				
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$				
			(16) $x,y,\bar{z}$	(17) $\bar{y},x-y,\bar{z}$	(18) $\bar{x}+y,\bar{x},\bar{z}$				
			(19) $\bar{y},\bar{x},z$	(20) $\bar{x}+y,y,z$	(21) $x,x-y,z$				
			(22) y,x,z	(23) $x-y,\bar{y},z$	(24) $\bar{x},\bar{x}+y,z$				
									Special: no extra conditions
12	q	$m\,.\,.$	$x,y,\frac{1}{2}$	$\bar{y},x-y,\frac{1}{2}$	$\bar{x}+y,\bar{x},\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$y,\bar{x}+y,\frac{1}{2}$	$x-y,x,\frac{1}{2}$	
			$y,x,\frac{1}{2}$	$x-y,\bar{y},\frac{1}{2}$	$\bar{x},\bar{x}+y,\frac{1}{2}$	$\bar{y},\bar{x},\frac{1}{2}$	$\bar{x}+y,y,\frac{1}{2}$	$x,x-y,\frac{1}{2}$	
12	p	$m\,.\,.$	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$\bar{x},\bar{y},0$	$y,\bar{x}+y,0$	$x-y,x,0$	
			$y,x,0$	$x-y,\bar{y},0$	$\bar{x},\bar{x}+y,0$	$\bar{y},\bar{x},0$	$\bar{x}+y,y,0$	$x,x-y,0$	
12	o	$.\,m\,.$	$x,2x,z$	$2\bar{x},\bar{x},z$	$x,\bar{x},z$	$\bar{x},2\bar{x},z$	$2x,x,z$	$\bar{x},x,z$	
			$2x,x,\bar{z}$	$\bar{x},2\bar{x},\bar{z}$	$\bar{x},x,\bar{z}$	$2\bar{x},\bar{x},\bar{z}$	$x,2x,\bar{z}$	$x,\bar{x},\bar{z}$	
12	n	$.\,.\,m$	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$\bar{x},0,z$	$0,\bar{x},z$	x,x,z	
			$0,x,\bar{z}$	$x,0,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$0,\bar{x},\bar{z}$	$\bar{x},0,\bar{z}$	$x,x,\bar{z}$	
6	m	$m\,m\,2$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	
6	l	$m\,m\,2$	$x,2x,0$	$2\bar{x},\bar{x},0$	$x,\bar{x},0$	$\bar{x},2\bar{x},0$	$2x,x,0$	$\bar{x},x,0$	
6	k	$m\,2\,m$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	
6	j	$m\,2\,m$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	
6	i	$2\,m\,m$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	
4	h	$3\,m\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}$			
3	g	$m\,m\,m$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
3	f	$m\,m\,m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$				
2	e	$6\,m\,m$	$0,0,z$	$0,0,\bar{z}$					
2	d	$\bar{6}\,m\,2$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$					
2	c	$\bar{6}\,m\,2$	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$					
1	b	$6/m\,m\,m$	$0,0,\frac{1}{2}$						
1	a	$6/m\,m\,m$	$0,0,0$						

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

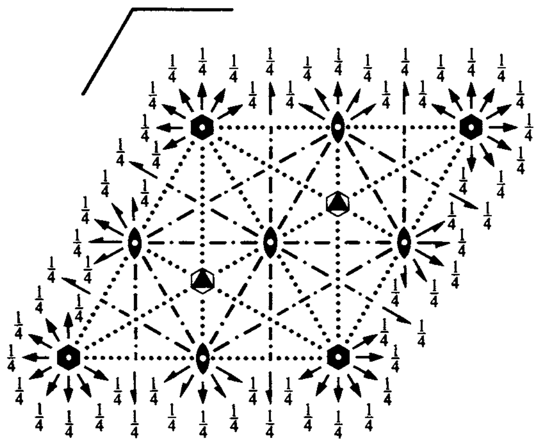
Along [210] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

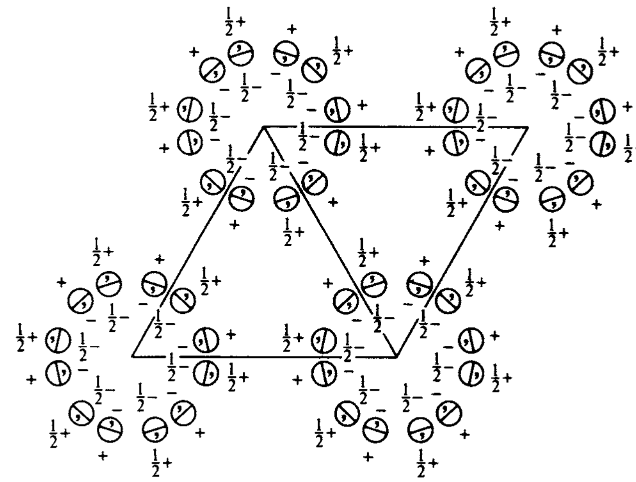
(*Continued on preceding page*)

International Tables for Crystallography (2006). Vol. A, Space group 192, pp. 596–597.

$P6/mcc$ $\quad D_{6h}^2$ $\quad 6/mmm$ $\quad$ Hexagonal

No. 192 $\quad P\ 6/m\ 2/c\ 2/c$ $\quad$ Patterson symmetry $P6/mmm$





Origin at centre $(6/m)$ at $6/mcc$

Asymmetric unit $\quad 0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{4};\quad x \le (1+y)/2;\quad y \le \min(1-x, x)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{2},\frac{1}{2},0$

$0,0,\frac{1}{4} \quad \frac{1}{2},0,\frac{1}{4} \quad \frac{2}{3},\frac{1}{3},\frac{1}{4} \quad \frac{1}{2},\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1	(2) $3^+\ 0,0,z$	(3) $3^-\ 0,0,z$
(4) $2\ \ 0,0,z$	(5) $6^-\ 0,0,z$	(6) $6^+\ 0,0,z$
(7) $2\ \ x,x,\frac{1}{4}$	(8) $2\ \ x,0,\frac{1}{4}$	(9) $2\ \ 0,y,\frac{1}{4}$
(10) $2\ \ x,\bar{x},\frac{1}{4}$	(11) $2\ \ x,2x,\frac{1}{4}$	(12) $2\ \ 2x,x,\frac{1}{4}$
(13) $\bar{1}\ \ 0,0,0$	(14) $\bar{3}^+\ 0,0,z;\ 0,0,0$	(15) $\bar{3}^-\ 0,0,z;\ 0,0,0$
(16) $m\ \ x,y,0$	(17) $\bar{6}^-\ 0,0,z;\ 0,0,0$	(18) $\bar{6}^+\ 0,0,z;\ 0,0,0$
(19) $c\ \ x,\bar{x},z$	(20) $c\ \ x,2x,z$	(21) $c\ \ 2x,x,z$
(22) $c\ \ x,x,z$	(23) $c\ \ x,0,z$	(24) $c\ \ 0,y,z$

Maximal non-isomorphic subgroups

I	[2] $P\bar{6}2c$ (190)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
	[2] $P\bar{6}c2$ (188)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
	[2] $P6cc$ (184)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
	[2] $P622$ (177)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[2] $P6/m11$ ($P6/m$, 175)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
	[2] $P\bar{3}c1$ (165)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
	[2] $P\bar{3}1c$ (163)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
	{ [3] $Pmcc$ ($Cccm$, 66)	1; 4; 7; 10; 13; 16; 19; 22
	{ [3] $Pmcc$ ($Cccm$, 66)	1; 4; 8; 11; 13; 16; 20; 23
	{ [3] $Pmcc$ ($Cccm$, 66)	1; 4; 9; 12; 13; 16; 21; 24

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P6/mcc$ ($\mathbf{c}' = 3\mathbf{c}$) (192); [3] $H6/mcc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6/mcc$, 192)

Minimal non-isomorphic supergroups

I none

II [2] $P6/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (191)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	Reflection conditions
				General:
24	m	1	(1) x,y,z (2) $\bar{y},x-y,z$ (3) $\bar{x}+y,\bar{x},z$ (4) $\bar{x},\bar{y},z$ (5) $y,\bar{x}+y,z$ (6) $x-y,x,z$ (7) $y,x,\bar{z}+\frac{1}{2}$ (8) $x-y,\bar{y},\bar{z}+\frac{1}{2}$ (9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$ (10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$ (11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$ (12) $x,x-y,\bar{z}+\frac{1}{2}$ (13) $\bar{x},\bar{y},\bar{z}$ (14) $y,\bar{x}+y,\bar{z}$ (15) $x-y,x,\bar{z}$ (16) $x,y,\bar{z}$ (17) $\bar{y},x-y,\bar{z}$ (18) $\bar{x}+y,\bar{x},\bar{z}$ (19) $\bar{y},\bar{x},z+\frac{1}{2}$ (20) $\bar{x}+y,y,z+\frac{1}{2}$ (21) $x,x-y,z+\frac{1}{2}$ (22) $y,x,z+\frac{1}{2}$ (23) $x-y,\bar{y},z+\frac{1}{2}$ (24) $\bar{x},\bar{x}+y,z+\frac{1}{2}$	$hh\overline{2h}l$: $l=2n$ $h\bar{h}0l$: $l=2n$ $000l$: $l=2n$
				Special: as above, plus
12	l	$m\,.\,.$	$x,y,0$ $\bar{y},x-y,0$ $\bar{x}+y,\bar{x},0$ $\bar{x},\bar{y},0$ $y,\bar{x}+y,0$ $x-y,x,0$ $y,x,\frac{1}{2}$ $x-y,\bar{y},\frac{1}{2}$ $\bar{x},\bar{x}+y,\frac{1}{2}$ $\bar{y},\bar{x},\frac{1}{2}$ $\bar{x}+y,y,\frac{1}{2}$ $x,x-y,\frac{1}{2}$	no extra conditions
12	k	$.\,.\,2$	$x,2x,\frac{1}{4}$ $2\bar{x},\bar{x},\frac{1}{4}$ $x,\bar{x},\frac{1}{4}$ $\bar{x},2\bar{x},\frac{1}{4}$ $2x,x,\frac{1}{4}$ $\bar{x},x,\frac{1}{4}$ $\bar{x},2\bar{x},\frac{3}{4}$ $2x,x,\frac{3}{4}$ $\bar{x},x,\frac{3}{4}$ $x,2x,\frac{3}{4}$ $2\bar{x},\bar{x},\frac{3}{4}$ $x,\bar{x},\frac{3}{4}$	$hkil$: $l=2n$
12	j	$.\,2\,.$	$x,0,\frac{1}{4}$ $0,x,\frac{1}{4}$ $\bar{x},\bar{x},\frac{1}{4}$ $\bar{x},0,\frac{1}{4}$ $0,\bar{x},\frac{1}{4}$ $x,x,\frac{1}{4}$ $\bar{x},0,\frac{3}{4}$ $0,\bar{x},\frac{3}{4}$ $x,x,\frac{3}{4}$ $x,0,\frac{3}{4}$ $0,x,\frac{3}{4}$ $\bar{x},\bar{x},\frac{3}{4}$	$hkil$: $l=2n$
12	i	$2\,.\,.$	$\frac{1}{2},0,z$ $0,\frac{1}{2},z$ $\frac{1}{2},\frac{1}{2},z$ $0,\frac{1}{2},\bar{z}+\frac{1}{2}$ $\frac{1}{2},0,\bar{z}+\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$ $\frac{1}{2},0,\bar{z}$ $0,\frac{1}{2},\bar{z}$ $\frac{1}{2},\frac{1}{2},\bar{z}$ $0,\frac{1}{2},z+\frac{1}{2}$ $\frac{1}{2},0,z+\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$hkil$: $l=2n$
8	h	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$ $\frac{2}{3},\frac{1}{3},z$ $\frac{2}{3},\frac{1}{3},\bar{z}+\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\bar{z}$ $\frac{1}{3},\frac{2}{3},\bar{z}$ $\frac{1}{3},\frac{2}{3},z+\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$hkil$: $l=2n$
6	g	$2/m\,.\,.$	$\frac{1}{2},0,0$ $0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
6	f	$2\,2\,2$	$\frac{1}{2},0,\frac{1}{4}$ $0,\frac{1}{2},\frac{1}{4}$ $\frac{1}{2},\frac{1}{2},\frac{1}{4}$ $\frac{1}{2},0,\frac{3}{4}$ $0,\frac{1}{2},\frac{3}{4}$ $\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$hkil$: $l=2n$
4	e	$6\,.\,.$	$0,0,z$ $0,0,\bar{z}+\frac{1}{2}$ $0,0,\bar{z}$ $0,0,z+\frac{1}{2}$	$hkil$: $l=2n$
4	d	$\bar{6}\,.\,.$	$\frac{1}{3},\frac{2}{3},0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},\frac{1}{2}$	$hkil$: $l=2n$
4	c	$3\,.\,2$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{3}{4}$ $\frac{1}{3},\frac{2}{3},\frac{3}{4}$	$hkil$: $l=2n$
2	b	$6/m\,.\,.$	$0,0,0$ $0,0,\frac{1}{2}$	$hkil$: $l=2n$
2	a	$6\,2\,2$	$0,0,\frac{1}{4}$ $0,0,\frac{3}{4}$	$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

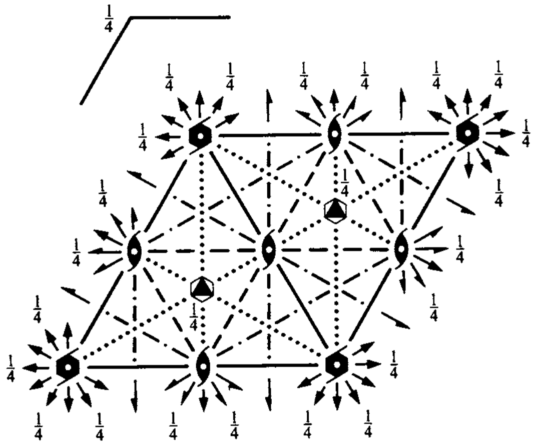
Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

(*Continued on preceding page*)

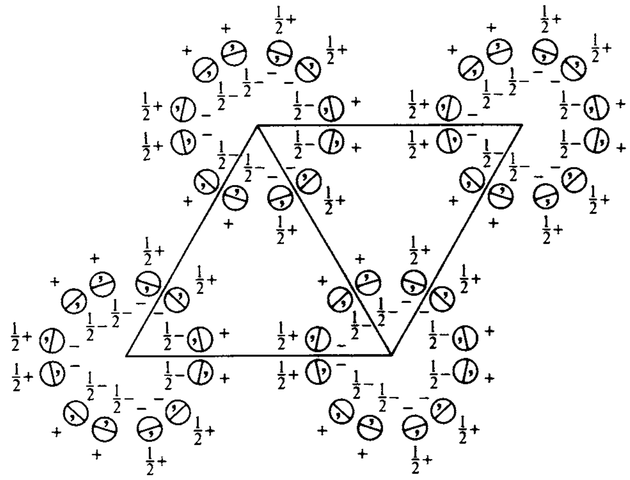
International Tables for Crystallography (2006). Vol. A, Space group 193, pp. 598–599.

$P6_3/mcm$ $\quad D_{6h}^3$ $\quad 6/mmm$ $\quad$ Hexagonal

No. 193 $\quad P\ 6_3/m\ 2/c\ 2/m$ $\quad$ Patterson symmetry $P6/mmm$



For $\bar{1}$ and $\bar{6}$ see $P6_3/m$ (No. 176)



Origin at centre ($\bar{3}1m$) at $\bar{3}c2/m$

Asymmetric unit $\quad 0 \le x \le \frac{2}{3};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{4};\quad x \le (1+y)/2;\quad y \le \min(1-x, x)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{2},\frac{1}{2},0$

$0,0,\frac{1}{4} \quad \frac{1}{2},0,\frac{1}{4} \quad \frac{2}{3},\frac{1}{3},\frac{1}{4} \quad \frac{1}{2},\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1	(2) $3^+\ 0,0,z$	(3) $3^-\ 0,0,z$
(4) $2(0,0,\frac{1}{2})\ \ 0,0,z$	(5) $6^-(0,0,\frac{1}{2})\ \ 0,0,z$	(6) $6^+(0,0,\frac{1}{2})\ \ 0,0,z$
(7) $2\ \ x,x,\frac{1}{4}$	(8) $2\ \ x,0,\frac{1}{4}$	(9) $2\ \ 0,y,\frac{1}{4}$
(10) $2\ \ x,\bar{x},0$	(11) $2\ \ x,2x,0$	(12) $2\ \ 2x,x,0$
(13) $\bar{1}\ \ 0,0,0$	(14) $\bar{3}^+\ 0,0,z;\ 0,0,0$	(15) $\bar{3}^-\ 0,0,z;\ 0,0,0$
(16) $m\ \ x,y,\frac{1}{4}$	(17) $\bar{6}^-\ 0,0,z;\ 0,0,\frac{1}{4}$	(18) $\bar{6}^+\ 0,0,z;\ 0,0,\frac{1}{4}$
(19) $c\ \ x,\bar{x},z$	(20) $c\ \ x,2x,z$	(21) $c\ \ 2x,x,z$
(22) $m\ \ x,x,z$	(23) $m\ \ x,0,z$	(24) $m\ \ 0,y,z$

Maximal non-isomorphic subgroups

I	[2] $P\bar{6}2m$ (189)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
	[2] $P\bar{6}c2$ (188)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
	[2] $P6_3cm$ (185)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
	[2] $P6_322$ (182)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[2] $P6_3/m11$ ($P6_3/m$, 176)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
	[2] $P\bar{3}c1$ (165)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
	[2] $P\bar{3}1m$ (162)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
	{ [3] $Pmcm$ ($Cmcm$, 63)	1; 4; 7; 10; 13; 16; 19; 22
	{ [3] $Pmcm$ ($Cmcm$, 63)	1; 4; 8; 11; 13; 16; 20; 23
	{ [3] $Pmcm$ ($Cmcm$, 63)	1; 4; 9; 12; 13; 16; 21; 24

IIa none

IIb [3] $H6_3/mcm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6_3/mmc$, 194)

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_3/mcm$ ($\mathbf{c}' = 3\mathbf{c}$) (193); [4] $P6_3/mcm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (193)

Minimal non-isomorphic supergroups

I none

II [3] $H6_3/mcm$ ($P6_3/mmc$, 194); [2] $P6/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (191)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
24	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$h\bar{h}0l$: $l=2n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$	$000l$: $l=2n$
			(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $x-y,\bar{y},\bar{z}+\frac{1}{2}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$	
			(10) $\bar{y},\bar{x},\bar{z}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}$	
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$	
			(16) $x,y,\bar{z}+\frac{1}{2}$	(17) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(18) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$	
			(19) $\bar{y},\bar{x},z+\frac{1}{2}$	(20) $\bar{x}+y,y,z+\frac{1}{2}$	(21) $x,x-y,z+\frac{1}{2}$	
			(22) y,x,z	(23) $x-y,\bar{y},z$	(24) $\bar{x},\bar{x}+y,z$	

									Special: as above, plus
12	k	$..m$	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$\bar{x},0,z+\frac{1}{2}$			no extra conditions
			$0,\bar{x},z+\frac{1}{2}$	$x,x,z+\frac{1}{2}$	$0,x,\bar{z}+\frac{1}{2}$	$x,0,\bar{z}+\frac{1}{2}$			
			$\bar{x},\bar{x},\bar{z}+\frac{1}{2}$	$0,\bar{x},\bar{z}$	$\bar{x},0,\bar{z}$	$x,x,\bar{z}$			
12	j	$m..$	$x,y,\frac{1}{4}$	$\bar{y},x-y,\frac{1}{4}$	$\bar{x}+y,\bar{x},\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$y,\bar{x}+y,\frac{3}{4}$	$x-y,x,\frac{3}{4}$	no extra conditions
			$y,x,\frac{1}{4}$	$x-y,\bar{y},\frac{1}{4}$	$\bar{x},\bar{x}+y,\frac{1}{4}$	$\bar{y},\bar{x},\frac{3}{4}$	$\bar{x}+y,y,\frac{3}{4}$	$x,x-y,\frac{3}{4}$	
12	i	$..2$	$x,2x,0$	$2\bar{x},\bar{x},0$	$x,\bar{x},0$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$hkil$: $l=2n$
			$\bar{x},2\bar{x},0$	$2x,x,0$	$\bar{x},x,0$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	
8	h	$3..$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}+\frac{1}{2}$	$\frac{1}{3},\frac{2}{3},\bar{z}$			$hkil$: $l=2n$
			$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$	$\frac{1}{3},\frac{2}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},z$			
6	g	$m2m$	$x,0,\frac{1}{4}$	$0,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$0,\bar{x},\frac{3}{4}$	$x,x,\frac{3}{4}$	no extra conditions
6	f	$..2/m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
4	e	$3.m$	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$			$hkil$: $l=2n$
4	d	3.2	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},0$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$			$hkil$: $l=2n$
4	c	$\bar{6}..$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$			$hkil$: $l=2n$
2	b	$\bar{3}.m$	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$
2	a	$\bar{6}2m$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

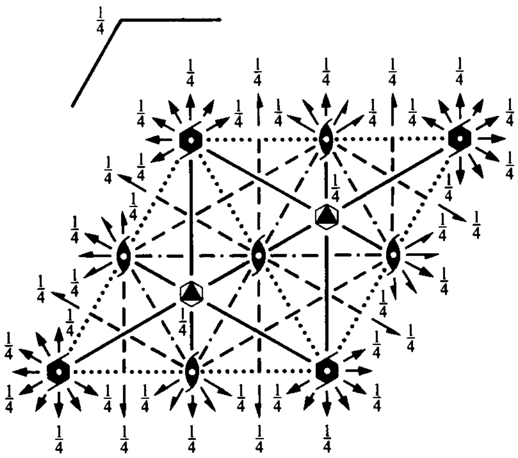
Along [210] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

(*Continued on preceding page*)

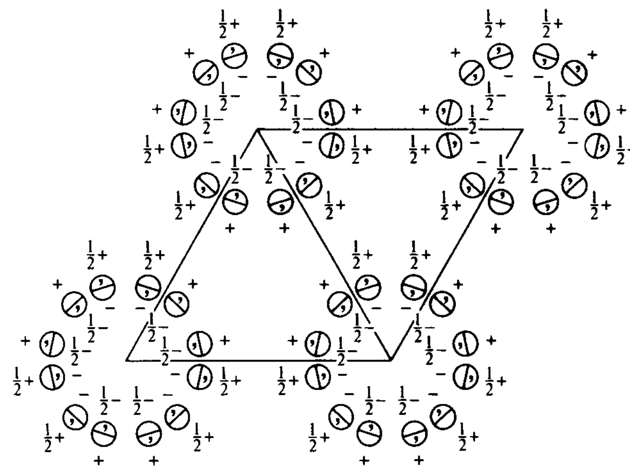
International Tables for Crystallography (2006). Vol. A, Space group 194, pp. 600–601.

$P6_3/mmc$ D_{6h}^4 $6/mmm$ Hexagonal

No. 194 $P\ 6_3/m\ 2/m\ 2/c$ Patterson symmetry $P6/mmm$



For $\bar{1}$ and $\bar{6}$ see $P6_3/m$ (No. 176)



Origin at centre ($\bar{3}m1$) at $\bar{3}2/mc$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{4}$; $x \le 2y$; $y \le \min(1-x, 2x)$

Vertices $0,0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$

$0,0,\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\frac{1}{3},\frac{2}{3},\frac{1}{4}$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$	(5) $6^-(0,0,\frac{1}{2})$ $0,0,z$	(6) $6^+(0,0,\frac{1}{2})$ $0,0,z$
(7) 2 $x,x,0$	(8) 2 $x,0,0$	(9) 2 $0,y,0$
(10) 2 $x,\bar{x},\frac{1}{4}$	(11) 2 $x,2x,\frac{1}{4}$	(12) 2 $2x,x,\frac{1}{4}$
(13) $\bar{1}$ $0,0,0$	(14) $\bar{3}^+$ $0,0,z$; $0,0,0$	(15) $\bar{3}^-$ $0,0,z$; $0,0,0$
(16) m $x,y,\frac{1}{4}$	(17) $\bar{6}^-$ $0,0,z$; $0,0,\frac{1}{4}$	(18) $\bar{6}^+$ $0,0,z$; $0,0,\frac{1}{4}$
(19) m $x,\bar{x},z$	(20) m $x,2x,z$	(21) m $2x,x,z$
(22) c x,x,z	(23) c $x,0,z$	(24) c $0,y,z$

Maximal non-isomorphic subgroups

I	[2] $P\bar{6}2c$ (190)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
	[2] $P\bar{6}m2$ (187)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
	[2] $P6_3mc$ (186)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
	[2] $P6_322$ (182)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[2] $P6_3/m11$ ($P6_3/m$, 176)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
	[2] $P\bar{3}m1$ (164)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
	[2] $P\bar{3}1c$ (163)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
	[3] $Pmmc$ ($Cmcm$, 63)	1; 4; 7; 10; 13; 16; 19; 22
	[3] $Pmmc$ ($Cmcm$, 63)	1; 4; 8; 11; 13; 16; 20; 23
	[3] $Pmmc$ ($Cmcm$, 63)	1; 4; 9; 12; 13; 16; 21; 24

IIa none

IIb [3] $H6_3/mmc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P6_3/mcm$, 193)

Maximal isomorphic subgroups of lowest index

IIc [3] $P6_3/mmc$ ($\mathbf{c}' = 3\mathbf{c}$) (194); [4] $P6_3/mmc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (194)

Minimal non-isomorphic supergroups

I none

II [3] $H6_3/mmc$ ($P6_3/mcm$, 193); [2] $P6/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (191)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
24	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$hh\overline{2h}l$: $l=2n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$				$000l$: $l=2n$
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$				
			(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{1}{2}$				
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$				
			(16) $x,y,\bar{z}+\frac{1}{2}$	(17) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(18) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$				
			(19) $\bar{y},\bar{x},z$	(20) $\bar{x}+y,y,z$	(21) $x,x-y,z$				
			(22) $y,x,z+\frac{1}{2}$	(23) $x-y,\bar{y},z+\frac{1}{2}$	(24) $\bar{x},\bar{x}+y,z+\frac{1}{2}$				
									Special: as above, plus
12	k	$.m.$	$x,2x,z$	$2\bar{x},\bar{x},z$	$x,\bar{x},z$	$\bar{x},2\bar{x},z+\frac{1}{2}$			no extra conditions
			$2x,x,z+\frac{1}{2}$	$\bar{x},x,z+\frac{1}{2}$	$2x,x,\bar{z}$	$\bar{x},2\bar{x},\bar{z}$			
			$\bar{x},x,\bar{z}$	$2\bar{x},\bar{x},\bar{z}+\frac{1}{2}$	$x,2x,\bar{z}+\frac{1}{2}$	$x,\bar{x},\bar{z}+\frac{1}{2}$			
12	j	$m..$	$x,y,\frac{1}{4}$	$\bar{y},x-y,\frac{1}{4}$	$\bar{x}+y,\bar{x},\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$y,\bar{x}+y,\frac{3}{4}$	$x-y,x,\frac{3}{4}$	no extra conditions
			$y,x,\frac{3}{4}$	$x-y,\bar{y},\frac{3}{4}$	$\bar{x},\bar{x}+y,\frac{3}{4}$	$\bar{y},\bar{x},\frac{1}{4}$	$\bar{x}+y,y,\frac{1}{4}$	$x,x-y,\frac{1}{4}$	
12	i	$.2.$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	$hkil$: $l=2n$
			$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	
6	h	$mm2$	$x,2x,\frac{1}{4}$	$2\bar{x},\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},2\bar{x},\frac{3}{4}$	$2x,x,\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	no extra conditions
6	g	$.2/m.$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
4	f	$3m.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$			$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
4	e	$3m.$	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$			$hkil$: $l=2n$
2	d	$\bar{6}m2$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$ (for d and c)
2	c	$\bar{6}m2$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$					
2	b	$\bar{6}m2$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$
2	a	$\bar{3}m.$	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

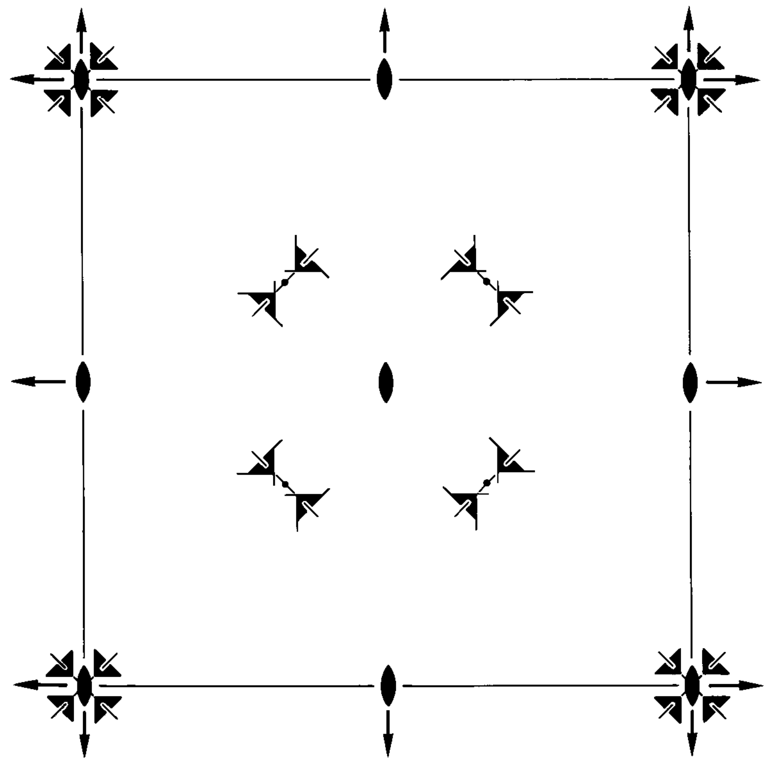
Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

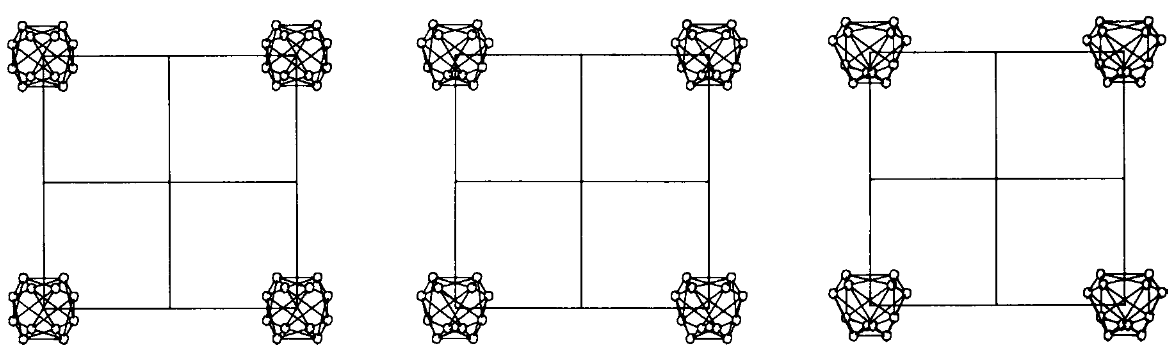
(*Continued on preceding page*)

International Tables for Crystallography (2006). Vol. A, Space group 195, pp. 602–603.

$P23$ | T^1 | 23 | Cubic

No. 195 | $P23$ | Patterson symmetry $Pm\bar{3}$





Origin at 23

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}; \quad y \le 1-x; \quad z \le \min(x,y)$

Vertices $\quad 0,0,0 \quad 1,0,0 \quad 0,1,0 \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) $2 \quad 0,0,z$	(3) $2 \quad 0,y,0$	(4) $2 \quad x,0,0$
(5) $3^+ \; x,x,x$	(6) $3^+ \; \bar{x},x,\bar{x}$	(7) $3^+ \; x,\bar{x},\bar{x}$	(8) $3^+ \; \bar{x},\bar{x},x$
(9) $3^- \; x,x,x$	(10) $3^- \; x,\bar{x},\bar{x}$	(11) $3^- \; \bar{x},\bar{x},x$	(12) $3^- \; \bar{x},x,\bar{x}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									h,k,l cyclically permutable
									General:
12	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			no conditions
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			
									Special: no extra conditions
6	i	$2\,.\,.$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$	
6	h	$2\,.\,.$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$	
6	g	$2\,.\,.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$0,\frac{1}{2},x$	$0,\frac{1}{2},\bar{x}$	
6	f	$2\,.\,.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	
4	e	$.\,3\,.$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			
3	d	$2\,2\,2\,.\,.$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$				
3	c	$2\,2\,2\,.\,.$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$				
1	b	$2\,3\,.$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						
1	a	$2\,3\,.$	$0,0,0$						

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [111] $p3$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [3] $P21$ ($P222$, 16) 1; 2; 3; 4
[4] $P13$ ($R3$, 146) 1; 5; 9
[4] $P13$ ($R3$, 146) 1; 6; 12
[4] $P13$ ($R3$, 146) 1; 7; 10
[4] $P13$ ($R3$, 146) 1; 8; 11

IIa none

IIb [2] $F23$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (196); [4] $I2_13$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (199); [4] $I23$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (197)

Maximal isomorphic subgroups of lowest index

IIc [27] $P23$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (195)

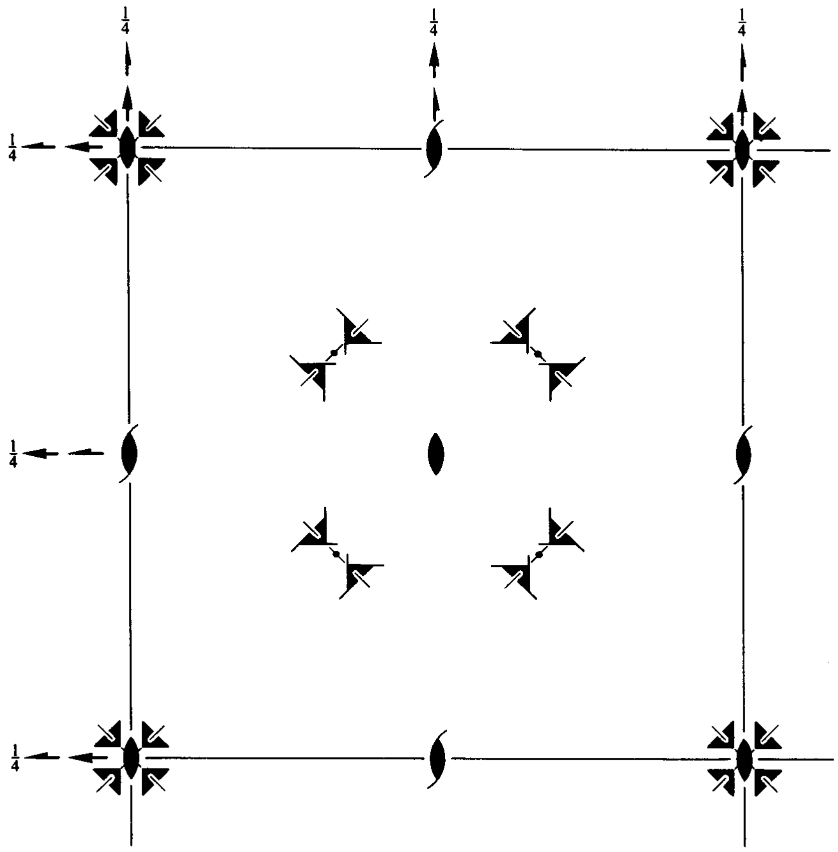
Minimal non-isomorphic supergroups

I [2] $Pm\bar{3}$ (200); [2] $Pn\bar{3}$ (201); [2] $P432$ (207); [2] $P4_232$ (208); [2] $P\bar{4}3m$ (215); [2] $P\bar{4}3n$ (218)

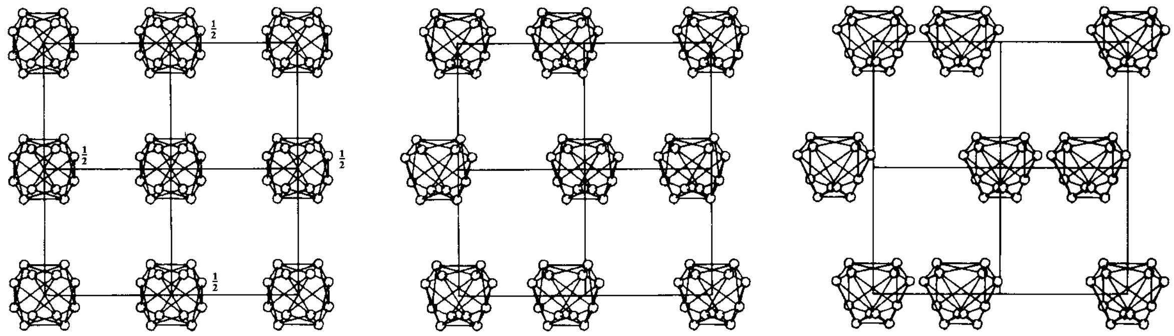
II [2] $I23$ (197); [4] $F23$ (196)

$F\,2\,3$ T^2 $2\,3$ Cubic

No. 196 $F\,2\,3$ Patterson symmetry $F\,m\,\bar{3}$



Upper left quadrant only



Origin at 2 3

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $-\frac{1}{4} \le z \le \frac{1}{4}$; $y \le x$; $\max(x-\frac{1}{2}, -y) \le z \le \min(\frac{1}{2}-x, y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $3^{+}\ x,x,x$	(6) $3^{+}\ \bar{x},x,\bar{x}$	(7) $3^{+}\ x,\bar{x},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x},x$
(9) $3^{-}\ x,x,x$	(10) $3^{-}\ x,\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x},\bar{x},x$	(12) $3^{-}\ \bar{x},x,\bar{x}$

For $(0,\frac{1}{2},\frac{1}{2})$+ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2\quad x,\frac{1}{4},\frac{1}{4}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{3},x-\frac{1}{6},x$	(6) $3^{+}\ \bar{x},x+\frac{1}{2},\bar{x}$	(7) $3^{+}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x+\frac{1}{6},x$	(10) $3^{-}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) $3^{-}\ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$

For $(\frac{1}{2},0,\frac{1}{2})$+ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,0,\frac{1}{4}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x-\frac{1}{6},x$	(6) $3^{+}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^{+}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x-\frac{1}{3},x$	(10) $3^{-}\ x+\frac{1}{2},\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{1}{2},\bar{x},x$	(12) $3^{-}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$

For $(\frac{1}{2},\frac{1}{2},0)$+ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x+\frac{1}{3},x$	(6) $3^{+}\ \bar{x}+\frac{1}{2},x,\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x},\bar{x}$	(8) $3^{+}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{3},x+\frac{1}{6},x$	(10) $3^{-}\ x,\bar{x}+\frac{1}{2},\bar{x}$	(11) $3^{-}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^{-}\ \bar{x},x+\frac{1}{2},\bar{x}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad (0,\frac{1}{2},\frac{1}{2})+\quad (\frac{1}{2},0,\frac{1}{2})+\quad (\frac{1}{2},\frac{1}{2},0)+$						Reflection conditions h,k,l cyclically permutable General:
48	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			hkl : $h+k,h+l,k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			hhl : $h+l=2n$
									$h00$: $h=2n$
									Special: no extra conditions
24	g	$2\,.\,.$	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}$	
24	f	$2\,.\,.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	
16	e	$.\,3\,.$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			
4	d	$2\,3\,.$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$						
4	c	$2\,3\,.$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$						
4	b	$2\,3\,.$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						
4	a	$2\,3\,.$	$0,0,0$						

Symmetry of special projections

Along [001] $p\,2\,m\,m$	Along [111] $p\,3$	Along [110] $c\,1\,m\,1$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}\quad \mathbf{b}'=\frac{1}{2}\mathbf{b}$	$\mathbf{a}'=\frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})\quad \mathbf{b}'=\frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$	$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})\quad \mathbf{b}'=\mathbf{c}$
Origin at $0,0,z$	Origin at x,x,x	Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[3] $F\,2\,1$ ($F\,2\,2\,2$, 22)	(1; 2; 3; 4)+
	[4] $F\,1\,3$ ($R\,3$, 146)	(1; 5; 9)+
	[4] $F\,1\,3$ ($R\,3$, 146)	(1; 6; 12)+
	[4] $F\,1\,3$ ($R\,3$, 146)	(1; 7; 10)+
	[4] $F\,1\,3$ ($R\,3$, 146)	(1; 8; 11)+
IIa	[4] $P\,2_1\,3$ (198)	1; 5; 9; (2; 7; 12) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 6; 11) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 8; 10) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\,2_1\,3$ (198)	1; 7; 10; (2; 5; 11) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 8; 12) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 6; 9) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\,2_1\,3$ (198)	1; 8; 11; (2; 6; 10) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 7; 9) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 5; 12) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\,2_1\,3$ (198)	1; 6; 12; (2; 8; 9) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 5; 10) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 7; 11) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\,2_1\,3$ (198)	1; 5; 9; (3; 8; 10) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 7; 12) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 6; 11) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\,2_1\,3$ (198)	1; 7; 10; (3; 6; 9) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 5; 11) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 8; 12) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\,2_1\,3$ (198)	1; 8; 11; (3; 5; 12) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 6; 10) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 7; 9) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\,2_1\,3$ (198)	1; 6; 12; (3; 7; 11) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 8; 9) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 5; 10) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\,2\,3$ (195)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[4] $P\,2\,3$ (195)	1; 2; 3; 4; (5; 6; 7; 8) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\,2\,3$ (195)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},0,\frac{1}{2})$; (9; 10; 11; 12) + $(0,\frac{1}{2},\frac{1}{2})$
	[4] $P\,2\,3$ (195)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$; (9; 10; 11; 12) + $(\frac{1}{2},0,\frac{1}{2})$
	[4] $P\,2\,3$ (195)	1; 5; 9; (4; 6; 11) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 8; 10) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 7; 12) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\,2\,3$ (195)	1; 7; 10; (4; 8; 12) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 6; 9) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 5; 11) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\,2\,3$ (195)	1; 8; 11; (4; 7; 9) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 5; 12) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 6; 10) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\,2\,3$ (195)	1; 6; 12; (4; 5; 10) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 7; 11) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 8; 9) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $F\,2\,3$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (196)

Minimal non-isomorphic supergroups

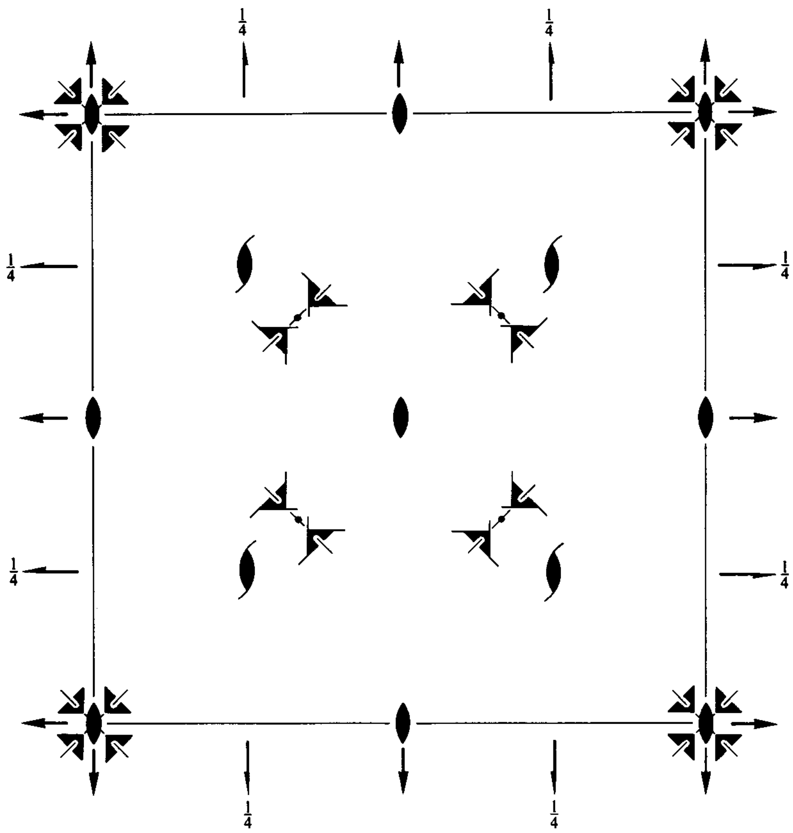
I [2] $F\,m\,\bar{3}$ (202); [2] $F\,d\,\bar{3}$ (203); [2] $F\,4\,3\,2$ (209); [2] $F\,4_1\,3\,2$ (210); [2] $F\,\bar{4}\,3\,m$ (216); [2] $F\,\bar{4}\,3\,c$ (219)

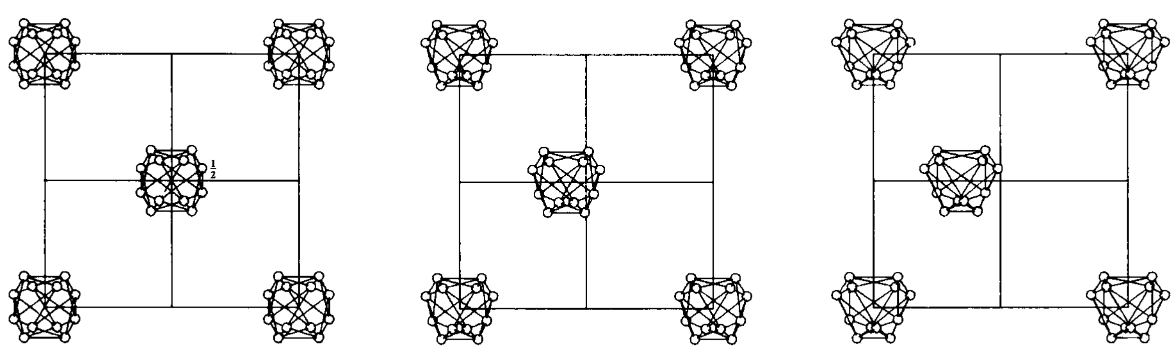
II [2] $P\,2\,3$ ($\mathbf{a}' = \frac{1}{2}\mathbf{c}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (195)

International Tables for Crystallography (2006). Vol. A, Space group 197, pp. 608–609.

$I23$ T^3 23 Cubic

No. 197 $I23$ Patterson symmetry $Im\bar{3}$





Origin at 23

Asymmetric unit $0 \le x \le 1$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le \min(x, 1-x)$; $z \le y$

Vertices $0,0,0$ $1,0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\ \ 0,0,z$	(3) $2\ \ 0,y,0$	(4) $2\ \ x,0,0$
(5) $3^+\ x,x,x$	(6) $3^+\ \bar{x},x,\bar{x}$	(7) $3^+\ x,\bar{x},\bar{x}$	(8) $3^+\ \bar{x},\bar{x},x$
(9) $3^-\ x,x,x$	(10) $3^-\ x,\bar{x},\bar{x}$	(11) $3^-\ \bar{x},\bar{x},x$	(12) $3^-\ \bar{x},x,\bar{x}$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\ \ \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,x,x$	(6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})\ \ \bar{x}+\frac{1}{3},x+\frac{1}{3},\bar{x}$	(7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\ \ x+\frac{2}{3},\bar{x}-\frac{1}{3},\bar{x}$	(8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})\ \ \bar{x}+\frac{1}{3},\bar{x}+\frac{2}{3},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,x,x$	(10) $3^-(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\ \ x+\frac{1}{3},\bar{x}+\frac{1}{3},\bar{x}$	(11) $3^-(\frac{1}{6},\frac{1}{6},-\frac{1}{6})\ \ \bar{x}+\frac{2}{3},\bar{x}+\frac{1}{3},x$	(12) $3^-(\frac{1}{6},-\frac{1}{6},\frac{1}{6})\ \ \bar{x}-\frac{1}{3},x+\frac{2}{3},\bar{x}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$					h,k,l cyclically permutable General:
24	f	1	(1) x,y,z (5) z,x,y (9) y,z,x	(2) $\bar{x},\bar{y},z$ (6) $z,\bar{x},\bar{y}$ (10) $\bar{y},z,\bar{x}$	(3) $\bar{x},y,\bar{z}$ (7) $\bar{z},\bar{x},y$ (11) $y,\bar{z},\bar{x}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{z},x,\bar{y}$ (12) $\bar{y},\bar{z},x$			hkl : $h+k+l=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $h00$: $h=2n$ Special: no extra conditions
12	e	$2\,.\,.$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$	
12	d	$2\,.\,.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	
8	c	$.\,3\,.$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			
6	b	$2\,2\,2\,.\,.$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$				
2	a	$2\,3\,.$	$0,0,0$						

Symmetry of special projections

Along [001] $c2mm$	Along [111] $p3$	Along [110] $p1m1$
$\mathbf{a}'=\mathbf{a}$ $\quad \mathbf{b}'=\mathbf{b}$	$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\quad \mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$	$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad \mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $0,0,z$	Origin at x,x,x	Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[3] $I121$ ($I222$, 23)	(1; 2; 3; 4)+
	[4] $I13$ ($R3$, 146)	(1; 5; 9)+
	[4] $I13$ ($R3$, 146)	(1; 6; 12)+
	[4] $I13$ ($R3$, 146)	(1; 7; 10)+
	[4] $I13$ ($R3$, 146)	(1; 8; 11)+
IIa	[2] $P23$ (195)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $I23$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (197)

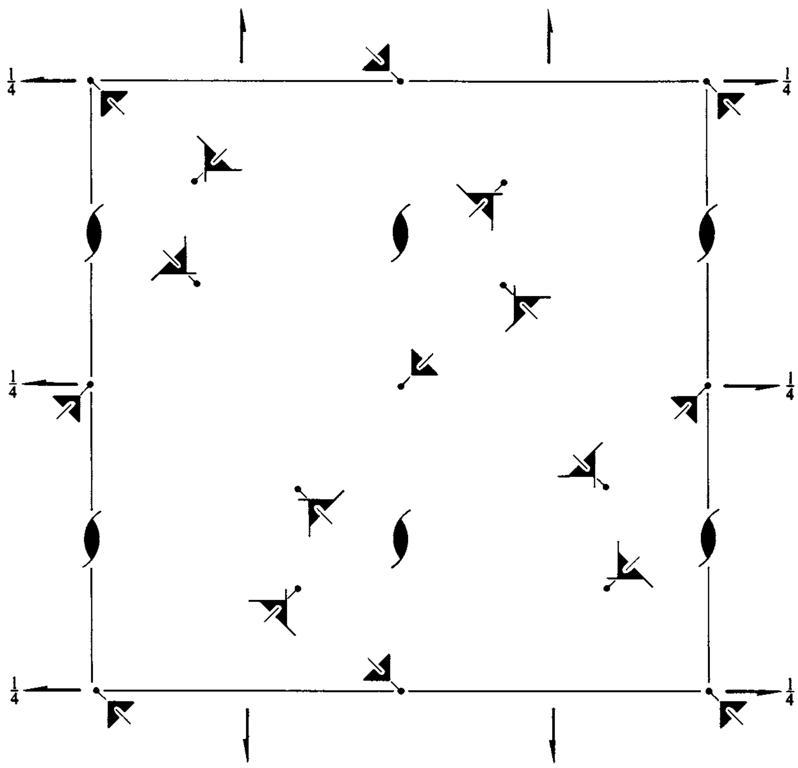
Minimal non-isomorphic supergroups

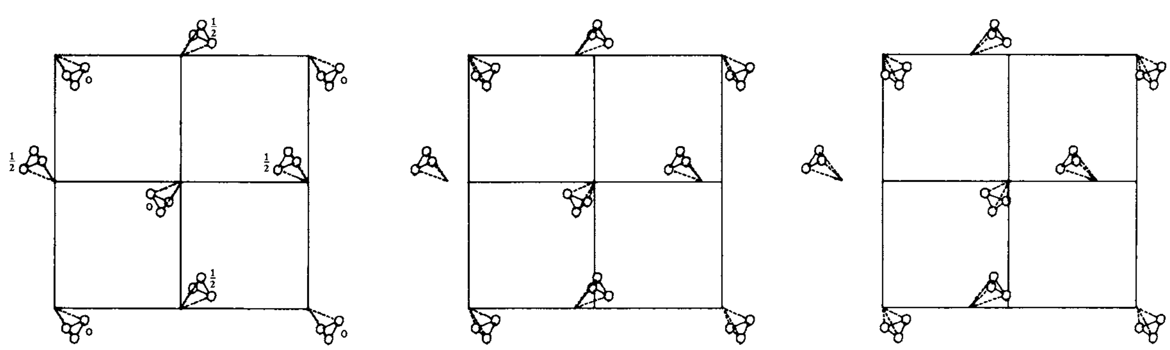
I [2] $Im\bar{3}$ (204); [2] $I432$ (211); [2] $I\bar{4}3m$ (217)

II [4] $P23$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (195)

$P2_13$ T^4 23 Cubic

No. 198 $P2_13$ Patterson symmetry $Pm\bar{3}$





Origin on 3[111] at midpoint of three non-intersecting pairs of parallel 2_1 axes

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad -\frac{1}{2} \le z \le \frac{1}{2};\quad \max(x-\frac{1}{2}, -y) \le z \le \min(x,y)$

Vertices $0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad 0,\frac{1}{2},0 \quad \frac{1}{2},\frac{1}{2},\frac{1}{2} \quad 0,\frac{1}{2},-\frac{1}{2}$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},0$
(5) $3^+\ \ x,x,x$	(6) $3^+\ \ \bar{x}+\frac{1}{2},x,\bar{x}$	(7) $3^+\ \ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^+\ \ \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^-\ \ x,x,x$	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\ \ \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\ \ \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							h,k,l cyclically permutable General:
12	b	1	(1) x,y,z (5) z,x,y (9) y,z,x	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$ (10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$ (11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$ (12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	$h00: \ h=2n$
							Special: no extra conditions
4	a	$.3.$	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$	

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},0,z$

Along [111] $p3$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p1g1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x+\frac{1}{4},x,0$

Maximal non-isomorphic subgroups

I [3] $P2_11$ ($P2_12_12_1$, 19) 1; 2; 3; 4
$\left\{\begin{array}{ll} [4]\ P13\ (R3,\ 146) & 1;\ 5;\ 9 \\ [4]\ P13\ (R3,\ 146) & 1;\ 6;\ 12 \\ [4]\ P13\ (R3,\ 146) & 1;\ 7;\ 10 \\ [4]\ P13\ (R3,\ 146) & 1;\ 8;\ 11 \end{array}\right.$

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $P2_13$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (198)

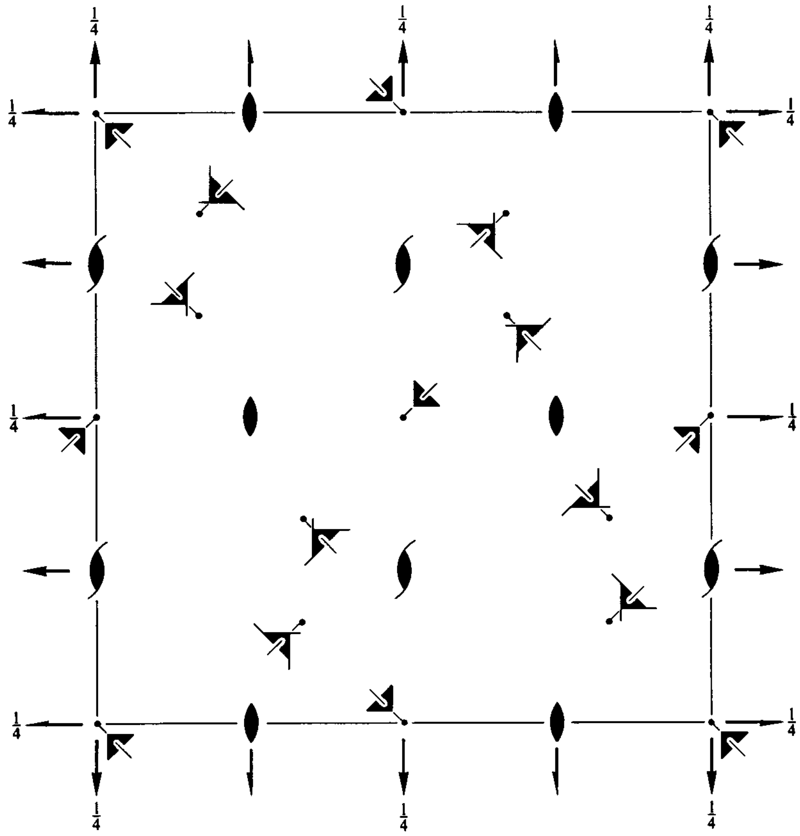
Minimal non-isomorphic supergroups

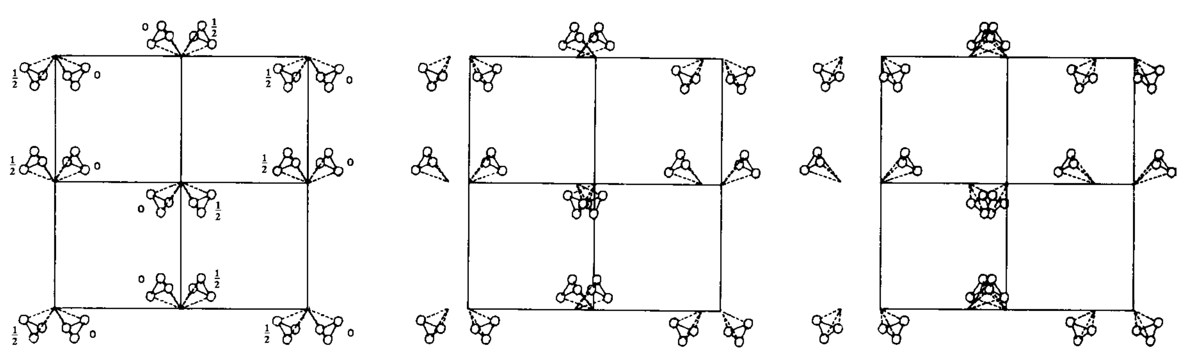
I [2] $Pa\bar{3}$ (205); [2] $P4_332$ (212); [2] $P4_132$ (213)

II [2] $I2_13$ (199); [4] $F23$ (196)

International Tables for Crystallography (2006). Vol. A, Space group 199, pp. 612–613.

$I\,2_1\,3$	T^5	$2\,3$	Cubic
No. 199	$I\,2_1\,3$		Patterson symmetry $I\,m\,\bar{3}$





Origin on 3[111] at midpoint of three non-intersecting pairs of parallel 2 axes and of three non-intersecting pairs of parallel 2_1 axes

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $z \le \min(x,y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$	(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) 3^- x,x,x	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,\frac{1}{4},z$	(3) 2 $\frac{1}{4},y,0$	(4) 2 $x,0,\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$	(7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(10) $3^-(\frac{1}{6},-\frac{1}{6},-\frac{1}{6})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-(-\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^-(-\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				h,k,l cyclically permutable General:
24	c	1	(1) x,y,z (5) z,x,y (9) y,z,x	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$ (10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$ (11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$ (12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	hkl : $h+k+l=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $h00$: $h=2n$
							Special: no extra conditions
12	b	$2\,.\,.$	$x,0,\frac{1}{4}$ $\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{4},x,0$ $\frac{3}{4},\bar{x}+\frac{1}{2},0$	$0,\frac{1}{4},x$ $0,\frac{3}{4},\bar{x}+\frac{1}{2}$		
8	a	$.\,3\,.$	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$	

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\quad \mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},0,z$

Along [111] $p3$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\quad \mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad \mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x+\frac{1}{4},0$

Maximal non-isomorphic subgroups

I [3] $I2_11$ ($I2_12_12_1$, 24) (1; 2; 3; 4)+
{ [4] $I13$ ($R3$, 146) (1; 5; 9)+
[4] $I13$ ($R3$, 146) (1; 6; 12)+
[4] $I13$ ($R3$, 146) (1; 7; 10)+
[4] $I13$ ($R3$, 146) (1; 8; 11)+

IIa [2] $P2_13$ (198) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $I2_13$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (199)

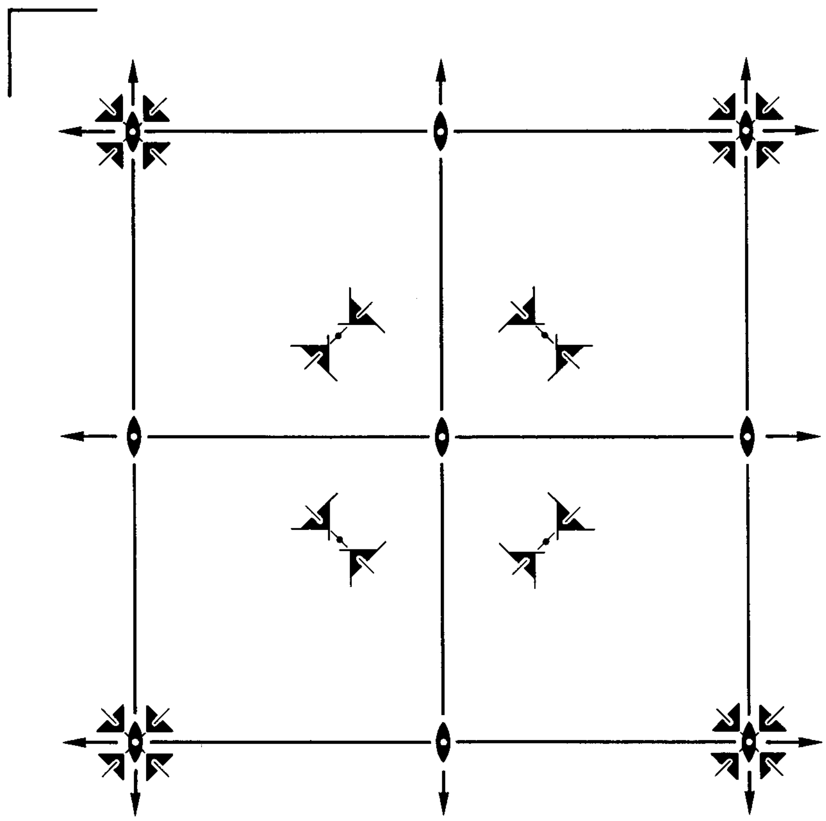
Minimal non-isomorphic supergroups

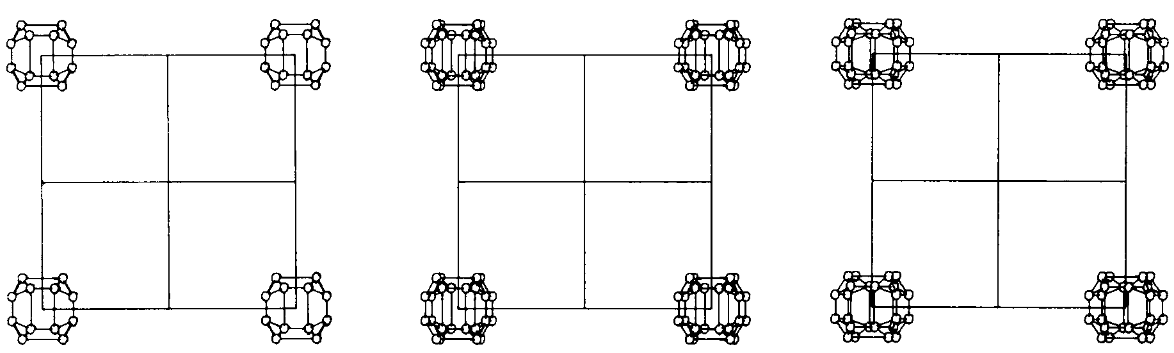
I [2] $Ia\bar{3}$ (206); [2] $I4_132$ (214); [2] $I\bar{4}3d$ (220)

II [4] $P23$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (195)

$Pm\bar{3}$ T_h^1 $m\bar{3}$ Cubic

No. 200 $P2/m\bar{3}$ Patterson symmetry $Pm\bar{3}$





Origin at centre ($m\bar{3}$)

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $z \le \min(x, y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) $\bar{1}$ $0,0,0$	(14) m $x,y,0$	(15) m $x,0,z$	(16) m $0,y,z$
(17) $\bar{3}^+$ x,x,x; $0,0,0$	(18) $\bar{3}^+$ $\bar{x},x,\bar{x}$; $0,0,0$	(19) $\bar{3}^+$ $x,\bar{x},\bar{x}$; $0,0,0$	(20) $\bar{3}^+$ $\bar{x},\bar{x},x$; $0,0,0$
(21) $\bar{3}^-$ x,x,x; $0,0,0$	(22) $\bar{3}^-$ $x,\bar{x},\bar{x}$; $0,0,0$	(23) $\bar{3}^-$ $\bar{x},\bar{x},x$; $0,0,0$	(24) $\bar{3}^-$ $\bar{x},x,\bar{x}$; $0,0,0$

Minimal non-isomorphic supergroups

I [2] $Pm\bar{3}m$ (221); [2] $Pm\bar{3}n$ (223)

II [2] $Im\bar{3}$ (204); [4] $Fm\bar{3}$ (202)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

h,k,l cyclically permutable

General:

							Reflection conditions
24	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	no conditions
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x,y,\bar{z}$	(15) $x,\bar{y},z$	(16) $\bar{x},y,z$	
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z},x,y$	(19) $z,x,\bar{y}$	(20) $z,\bar{x},y$	
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z},x$	(23) $\bar{y},z,x$	(24) $y,z,\bar{x}$	

Special: no extra conditions

12	k	$m\,.\,.$	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$	$\frac{1}{2},y,\bar{z}$	$\frac{1}{2},\bar{y},\bar{z}$	$z,\frac{1}{2},y$	$z,\frac{1}{2},\bar{y}$
			$\bar{z},\frac{1}{2},y$	$\bar{z},\frac{1}{2},\bar{y}$	$y,z,\frac{1}{2}$	$\bar{y},z,\frac{1}{2}$	$y,\bar{z},\frac{1}{2}$	$\bar{y},\bar{z},\frac{1}{2}$
12	j	$m\,.\,.$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$z,0,y$	$z,0,\bar{y}$
			$\bar{z},0,y$	$\bar{z},0,\bar{y}$	$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$
8	i	$.\,3\,.$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$		
			$\bar{x},\bar{x},\bar{x}$	$x,x,\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$		
6	h	$m\,m\,2\,.\,.$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$
6	g	$m\,m\,2\,.\,.$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$
6	f	$m\,m\,2\,.\,.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$0,\frac{1}{2},x$	$0,\frac{1}{2},\bar{x}$
6	e	$m\,m\,2\,.\,.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
3	d	$m\,m\,m\,.\,.$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$			
3	c	$m\,m\,m\,.\,.$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			
1	b	$m\,\bar{3}\,.$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
1	a	$m\,\bar{3}\,.$	$0,0,0$					

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [111] $p6$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P23$ (195)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[3] $Pm1$ ($Pmmm$, 47)	1; 2; 3; 4; 13; 14; 15; 16
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 5; 9; 13; 17; 21
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 6; 12; 13; 18; 24
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 7; 10; 13; 19; 22
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 8; 11; 13; 20; 23

IIa none

IIb [2] $Fm\bar{3}$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (202); [4] $Ia\bar{3}$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (206); [4] $Im\bar{3}$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (204)

Maximal isomorphic subgroups of lowest index

IIc [27] $Pm\bar{3}$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (200)

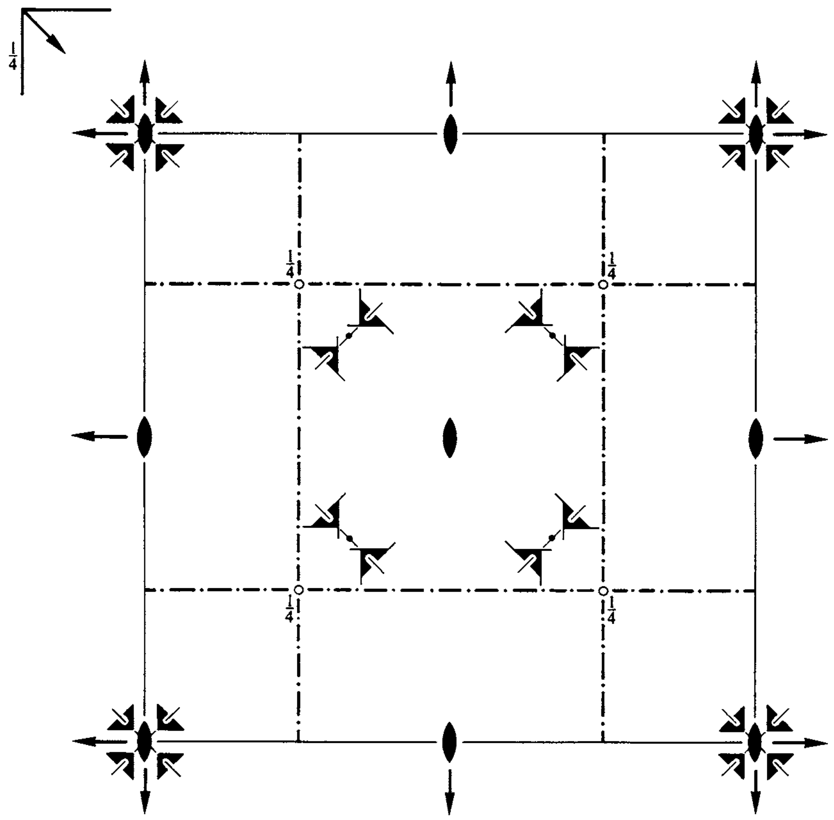
(*Continued on preceding page*)

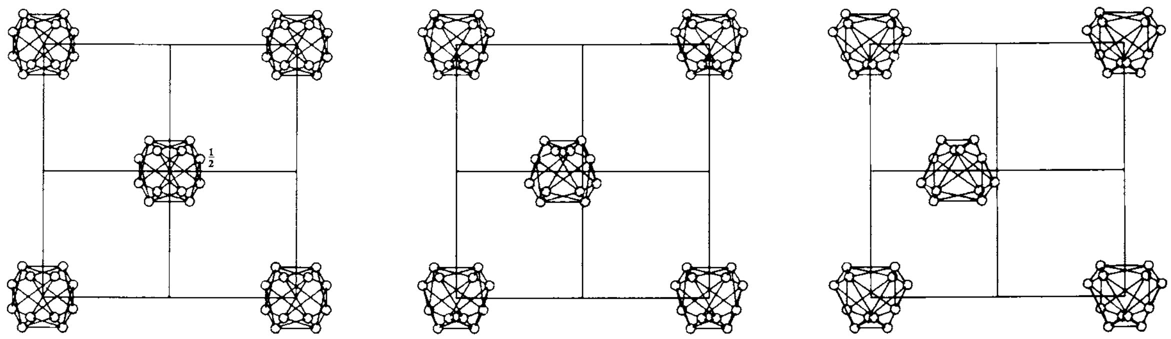
International Tables for Crystallography (2006). Vol. A, Space group 201, pp. 616–619.

$Pn\bar{3}$ T_h^2 $m\bar{3}$ Cubic

No. 201 $P2/n\bar{3}$ Patterson symmetry $Pm\bar{3}$

ORIGIN CHOICE 1





Origin at 23, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from centre ($\bar{3}$)

Asymmetric unit $\quad 0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}; \quad y \le \min(x, 1-x); \quad z \le y$

Vertices $\quad 0,0,0 \quad 1,0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $\quad 0,0,z$	(3) 2 $\quad 0,y,0$	(4) 2 $\quad x,0,0$
(5) $3^+ \; x,x,x$	(6) $3^+ \; \bar{x},x,\bar{x}$	(7) $3^+ \; x,\bar{x},\bar{x}$	(8) $3^+ \; \bar{x},\bar{x},x$
(9) $3^- \; x,x,x$	(10) $3^- \; x,\bar{x},\bar{x}$	(11) $3^- \; \bar{x},\bar{x},x$	(12) $3^- \; \bar{x},x,\bar{x}$
(13) $\bar{1} \quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(14) $n(\frac{1}{2},\frac{1}{2},0) \quad x,y,\frac{1}{4}$	(15) $n(\frac{1}{2},0,\frac{1}{2}) \quad x,\frac{1}{4},z$	(16) $n(0,\frac{1}{2},\frac{1}{2}) \quad \frac{1}{4},y,z$
(17) $\bar{3}^+ \; x,x,x; \quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(18) $\bar{3}^+ \; \bar{x}-1,x+1,\bar{x}; \quad -\frac{1}{4},\frac{1}{4},\frac{3}{4}$	(19) $\bar{3}^+ \; x,\bar{x}+1,\bar{x}; \quad \frac{1}{4},\frac{3}{4},-\frac{1}{4}$	(20) $\bar{3}^+ \; \bar{x}+1,\bar{x},x; \quad \frac{3}{4},-\frac{1}{4},\frac{1}{4}$
(21) $\bar{3}^- \; x,x,x; \quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(22) $\bar{3}^- \; x+1,\bar{x}-1,\bar{x}; \quad \frac{1}{4},-\frac{1}{4},\frac{3}{4}$	(23) $\bar{3}^- \; \bar{x},\bar{x}+1,x; \quad -\frac{1}{4},\frac{3}{4},\frac{1}{4}$	(24) $\bar{3}^- \; \bar{x}+1,x,\bar{x}; \quad \frac{3}{4},\frac{1}{4},-\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	Reflection conditions
				h,k,l cyclically permutable General:
24	h	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}$ (4) $x,\bar{y},\bar{z}$	$0kl$: $k+l=2n$
			(5) z,x,y (6) $z,\bar{x},\bar{y}$ (7) $\bar{z},\bar{x},y$ (8) $\bar{z},x,\bar{y}$	$h00$: $h=2n$
			(9) y,z,x (10) $\bar{y},z,\bar{x}$ (11) $y,\bar{z},\bar{x}$ (12) $\bar{y},\bar{z},x$	
			(13) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (14) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (15) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (16) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	
			(17) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$ (18) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y+\frac{1}{2}$ (19) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}+\frac{1}{2}$ (20) $z+\frac{1}{2},\bar{x}+\frac{1}{2},y+\frac{1}{2}$	
			(21) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$ (22) $y+\frac{1}{2},\bar{z}+\frac{1}{2},x+\frac{1}{2}$ (23) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x+\frac{1}{2}$ (24) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	
				Special: as above, plus
12	g	$2\,.\,.$	$x,\frac{1}{2},0$ $\bar{x},\frac{1}{2},0$ $0,x,\frac{1}{2}$ $0,\bar{x},\frac{1}{2}$ $\frac{1}{2},0,x$ $\frac{1}{2},0,\bar{x}$	hkl : $h+k+l=2n$
			$\bar{x}+\frac{1}{2},0,\frac{1}{2}$ $x+\frac{1}{2},0,\frac{1}{2}$ $\frac{1}{2},\bar{x}+\frac{1}{2},0$ $\frac{1}{2},x+\frac{1}{2},0$ $0,\frac{1}{2},\bar{x}+\frac{1}{2}$ $0,\frac{1}{2},x+\frac{1}{2}$	
12	f	$2\,.\,.$	$x,0,0$ $\bar{x},0,0$ $0,x,0$ $0,\bar{x},0$ $0,0,x$ $0,0,\bar{x}$	hkl : $h+k+l=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$	
8	e	$.\,3\,.$	x,x,x $\bar{x},\bar{x},x$	no extra conditions
			$\bar{x},x,\bar{x}$ $x,\bar{x},\bar{x}$	
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$ $x+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	
			$x+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	
6	d	$2\,2\,2\,.\,.$	$0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},0,0$ $0,\frac{1}{2},0$ $0,0,\frac{1}{2}$	hkl : $h+k+l=2n$
4	c	$.\,\bar{3}\,.$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$ $\frac{1}{4},\frac{1}{4},\frac{3}{4}$ $\frac{1}{4},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\frac{1}{4},\frac{1}{4}$	hkl : $h+k,h+l,k+l=2n$
4	b	$.\,\bar{3}\,.$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\frac{1}{4},\frac{3}{4}$ $\frac{1}{4},\frac{3}{4},\frac{3}{4}$	hkl : $h+k,h+l,k+l=2n$
2	a	$2\,3\,.$	$0,0,0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [111] $p6$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{1}{4}$

Maximal non-isomorphic subgroups

I [2] $P23$ (195) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
[3] $Pn1$ ($Pnnn$, 48) 1; 2; 3; 4; 13; 14; 15; 16
$\left\{\begin{array}{ll} [4]\ P1\bar{3}\ (R\bar{3}, 148) & 1;\ 5;\ 9;\ 13;\ 17;\ 21 \\ [4]\ P1\bar{3}\ (R\bar{3}, 148) & 1;\ 6;\ 12;\ 13;\ 18;\ 24 \\ [4]\ P1\bar{3}\ (R\bar{3}, 148) & 1;\ 7;\ 10;\ 13;\ 19;\ 22 \\ [4]\ P1\bar{3}\ (R\bar{3}, 148) & 1;\ 8;\ 11;\ 13;\ 20;\ 23 \end{array}\right.$

IIa none

IIb [2] $Fd\bar{3}$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (203)

Maximal isomorphic subgroups of lowest index

IIc [27] $Pn\bar{3}$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (201)

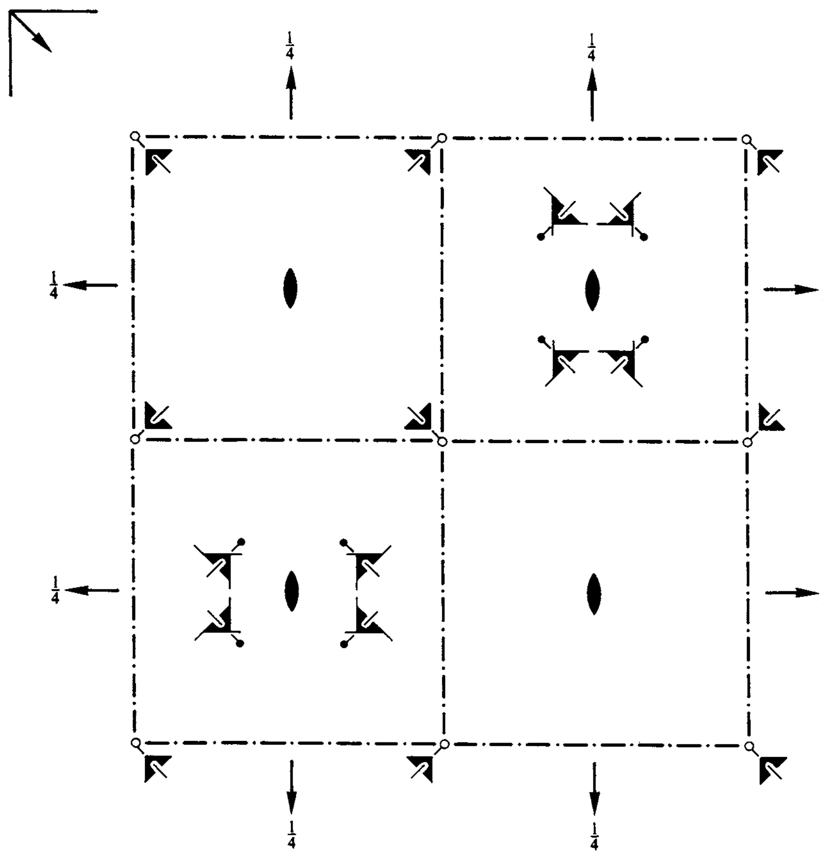
Minimal non-isomorphic supergroups

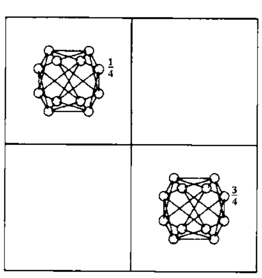
I [2] $Pn\bar{3}n$ (222); [2] $Pn\bar{3}m$ (224)

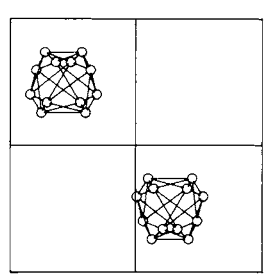
II [2] $Im\bar{3}$ (204); [4] $Fm\bar{3}$ (202)

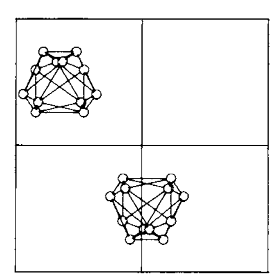
$Pn\bar{3}$	T_h^2	$m\bar{3}$	Cubic
No. 201	$P2/n\bar{3}$		Patterson symmetry $Pm\bar{3}$

ORIGIN CHOICE 2









Origin at centre ($\bar{3}$), at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from 23

Asymmetric unit $-\frac{1}{4} \le x \le \frac{3}{4};\quad -\frac{1}{4} \le y \le \frac{1}{4};\quad -\frac{1}{4} \le z \le \frac{1}{4};\quad y \le \min(x, \frac{1}{2}-x);\quad z \le y$

Vertices $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}\quad \frac{3}{4},-\frac{1}{4},-\frac{1}{4}\quad \frac{1}{4},\frac{1}{4},-\frac{1}{4}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\ \ \frac{1}{4},\frac{1}{4},z$	(3) $2\ \ \frac{1}{4},y,\frac{1}{4}$	(4) $2\ \ x,\frac{1}{4},\frac{1}{4}$
(5) $3^{+}\ x,x,x$	(6) $3^{+}\ \bar{x},x+\frac{1}{2},\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x},\bar{x}$	(8) $3^{+}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^{-}\ x,x,x$	(10) $3^{-}\ x+\frac{1}{2},\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) $3^{-}\ \bar{x},x+\frac{1}{2},\bar{x}$
(13) $\bar{1}\ \ 0,0,0$	(14) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$	(15) $n(\frac{1}{2},0,\frac{1}{2})\ \ x,0,z$	(16) $n(0,\frac{1}{2},\frac{1}{2})\ \ 0,y,z$
(17) $\bar{3}^{+}\ x,x,x;\ 0,0,0$	(18) $\bar{3}^{+}\ \bar{x}-1,x+\frac{1}{2},\bar{x};\ -\frac{1}{2},0,\frac{1}{2}$	(19) $\bar{3}^{+}\ x-\frac{1}{2},\bar{x}+1,\bar{x};\ 0,\frac{1}{2},-\frac{1}{2}$	(20) $\bar{3}^{+}\ \bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x;\ \frac{1}{2},-\frac{1}{2},0$
(21) $\bar{3}^{-}\ x,x,x;\ 0,0,0$	(22) $\bar{3}^{-}\ x+\frac{1}{2},\bar{x}-1,\bar{x};\ 0,-\frac{1}{2},\frac{1}{2}$	(23) $\bar{3}^{-}\ \bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x;\ -\frac{1}{2},\frac{1}{2},0$	(24) $\bar{3}^{-}\ \bar{x}+1,x-\frac{1}{2},\bar{x};\ \frac{1}{2},0,-\frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

h,k,l cyclically permutable

General:

Mult.	Wyckoff	Site symmetry	Coordinates				Reflection conditions
24	*h*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0kl$: $k+l=2n$
			(5) z,x,y	(6) $z,\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(7) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},y$	(8) $\bar{z}+\frac{1}{2},x,\bar{y}+\frac{1}{2}$	$h00$: $h=2n$
			(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	(11) $y,\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},x$	
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(15) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(16) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$	
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z},x+\frac{1}{2},y+\frac{1}{2}$	(19) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}$	(20) $z+\frac{1}{2},\bar{x},y+\frac{1}{2}$	
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y+\frac{1}{2},\bar{z},x+\frac{1}{2}$	(23) $\bar{y},z+\frac{1}{2},x+\frac{1}{2}$	(24) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}$	

Special: as above, plus

Mult.	Wyckoff	Site symmetry	Coordinates						Reflection conditions
12	*g*	2 . .	$x,\frac{3}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{3}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$	hkl : $h+k+l=2n$
			$\bar{x},\frac{1}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{1}{4}$	$\frac{3}{4},x+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\bar{x}$	$\frac{1}{4},\frac{3}{4},x+\frac{1}{2}$	
12	*f*	2 . .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{1}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$	hkl : $h+k+l=2n$
			$\bar{x},\frac{3}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{3}{4}$	$\frac{3}{4},x+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\bar{x}$	$\frac{3}{4},\frac{3}{4},x+\frac{1}{2}$	
8	*e*	. 3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	$\bar{x}+\frac{1}{2},x,\bar{x}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$			no extra conditions
			$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{x}$	$x+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},x+\frac{1}{2}$			
6	*d*	2 2 2 . .	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	hkl : $h+k+l=2n$
4	*c*	. $\bar{3}$.	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $h+k,h+l,k+l=2n$
4	*b*	. $\bar{3}$.	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $h+k,h+l,k+l=2n$
2	*a*	2 3 .	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$					hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [111] $p6$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I
- [2] $P23$ (195) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
- [3] $Pn1$ ($Pnnn$, 48) 1; 2; 3; 4; 13; 14; 15; 16
- {[4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 5; 9; 13; 17; 21
- [4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 6; 12; 13; 18; 24
- [4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 7; 10; 13; 19; 22
- [4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 8; 11; 13; 20; 23}

IIa none

IIb [2] $Fd\bar{3}$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (203)

Maximal isomorphic subgroups of lowest index

IIc [27] $Pn\bar{3}$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (201)

Minimal non-isomorphic supergroups

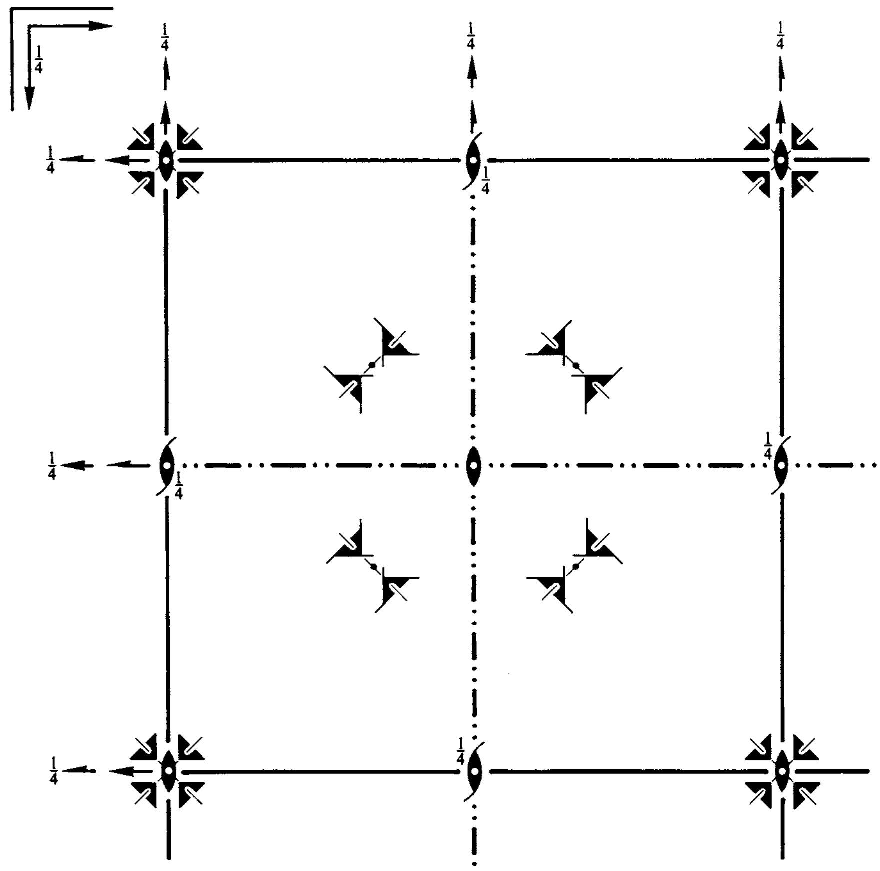
I [2] $Pn\bar{3}n$ (222); [2] $Pn\bar{3}m$ (224)

II [2] $Im\bar{3}$ (204); [4] $Fm\bar{3}$ (202)

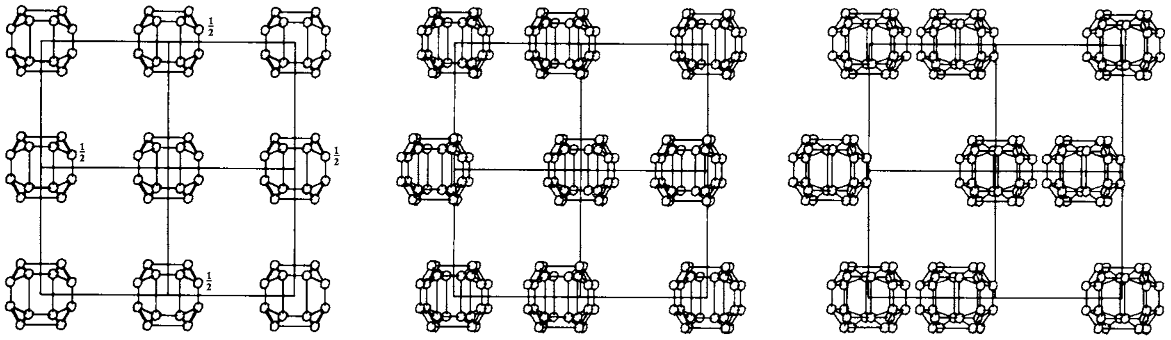
International Tables for Crystallography (2006). Vol. A, Space group 202, pp. 620–622.

$Fm\bar{3}$ T_h^3 $m\bar{3}$ Cubic

No. 202 $F2/m\bar{3}$ Patterson symmetry $Fm\bar{3}$



Upper left quadrant only



Origin at centre ($m\bar{3}$)

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$; $y \le x$; $z \le \min(\frac{1}{2} - x, y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) $\bar{1}$ 0,0,0	(14) m $x,y,0$	(15) m $x,0,z$	(16) m $0,y,z$
(17) $\bar{3}^+$ x,x,x; 0,0,0	(18) $\bar{3}^+$ $\bar{x},x,\bar{x}$; 0,0,0	(19) $\bar{3}^+$ $x,\bar{x},\bar{x}$; 0,0,0	(20) $\bar{3}^+$ $\bar{x},\bar{x},x$; 0,0,0
(21) $\bar{3}^-$ x,x,x; 0,0,0	(22) $\bar{3}^-$ $x,\bar{x},\bar{x}$; 0,0,0	(23) $\bar{3}^-$ $\bar{x},\bar{x},x$; 0,0,0	(24) $\bar{3}^-$ $\bar{x},x,\bar{x}$; 0,0,0

Symmetry operations *(continued)*

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\ \ 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{4}$	(4) $2\ \ x,\frac{1}{4},\frac{1}{4}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x-\frac{1}{3},x-\frac{1}{6},x$	(6) $3^{+}\ \ \bar{x},x+\frac{1}{2},\bar{x}$	(7) $3^{+}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$	(8) $3^{+}\ \ \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x-\frac{1}{6},x+\frac{1}{6},x$	(10) $3^{-}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^{-}\ \ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) $3^{-}\ \ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $\bar{1}\ \ 0,\frac{1}{4},\frac{1}{4}$	(14) $b\ \ x,y,\frac{1}{4}$	(15) $c\ \ x,\frac{1}{4},z$	(16) $n(0,\frac{1}{2},\frac{1}{2})\ \ 0,y,z$
(17) $\bar{3}^{+}\ \ x,x+\frac{1}{2},x;\ 0,\frac{1}{2},0$	(18) $\bar{3}^{+}\ \ \bar{x}-1,x+\frac{1}{2},\bar{x};\ -\frac{1}{2},0,\frac{1}{2}$	(19) $\bar{3}^{+}\ \ x,\bar{x}+\frac{1}{2},\bar{x};\ 0,\frac{1}{2},0$	(20) $\bar{3}^{+}\ \ \bar{x}+1,\bar{x}+\frac{1}{2},x;\ \frac{1}{2},0,\frac{1}{2}$
(21) $\bar{3}^{-}\ \ x-\frac{1}{2},x-\frac{1}{2},x;\ 0,0,\frac{1}{2}$	(22) $\bar{3}^{-}\ \ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};\ 0,0,\frac{1}{2}$	(23) $\bar{3}^{-}\ \ \bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x;\ -\frac{1}{2},\frac{1}{2},0$	(24) $\bar{3}^{-}\ \ \bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x};\ \frac{1}{2},\frac{1}{2},0$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},0,z$	(3) $2\ \ \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\ \ x,0,\frac{1}{4}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{6},x-\frac{1}{6},x$	(6) $3^{+}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\ \ \bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$	(7) $3^{+}\ \ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^{+}\ \ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x-\frac{1}{6},x-\frac{1}{3},x$	(10) $3^{-}\ \ x+\frac{1}{2},\bar{x},\bar{x}$	(11) $3^{-}\ \ \bar{x}+\frac{1}{2},\bar{x},x$	(12) $3^{-}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\ \ \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $\bar{1}\ \ \frac{1}{4},0,\frac{1}{4}$	(14) $a\ \ x,y,\frac{1}{4}$	(15) $n(\frac{1}{2},0,\frac{1}{2})\ \ x,0,z$	(16) $c\ \ \frac{1}{4},y,z$
(17) $\bar{3}^{+}\ \ x-\frac{1}{2},x-\frac{1}{2},x;\ 0,0,\frac{1}{2}$	(18) $\bar{3}^{+}\ \ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x};\ 0,0,\frac{1}{2}$	(19) $\bar{3}^{+}\ \ x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x};\ \frac{1}{2},\frac{1}{2},0$	(20) $\bar{3}^{+}\ \ \bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x;\ \frac{1}{2},-\frac{1}{2},0$
(21) $\bar{3}^{-}\ \ x+\frac{1}{2},x,x;\ \frac{1}{2},0,0$	(22) $\bar{3}^{-}\ \ x+\frac{1}{2},\bar{x}-1,\bar{x};\ 0,-\frac{1}{2},\frac{1}{2}$	(23) $\bar{3}^{-}\ \ \bar{x}+\frac{1}{2},\bar{x}+1,x;\ 0,\frac{1}{2},\frac{1}{2}$	(24) $\bar{3}^{-}\ \ \bar{x}+\frac{1}{2},x,\bar{x};\ \frac{1}{2},0,0$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\ \ \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\ \ \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},0$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{6},x+\frac{1}{3},x$	(6) $3^{+}\ \ \bar{x}+\frac{1}{2},x,\bar{x}$	(7) $3^{+}\ \ x+\frac{1}{2},\bar{x},\bar{x}$	(8) $3^{+}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\ \ \bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{3},x+\frac{1}{6},x$	(10) $3^{-}\ \ x,\bar{x}+\frac{1}{2},\bar{x}$	(11) $3^{-}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\ \ \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^{-}\ \ \bar{x},x+\frac{1}{2},\bar{x}$
(13) $\bar{1}\ \ \frac{1}{4},\frac{1}{4},0$	(14) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$	(15) $a\ \ x,\frac{1}{4},z$	(16) $b\ \ \frac{1}{4},y,z$
(17) $\bar{3}^{+}\ \ x+\frac{1}{2},x,x;\ \frac{1}{2},0,0$	(18) $\bar{3}^{+}\ \ \bar{x}-\frac{1}{2},x+1,\bar{x};\ 0,\frac{1}{2},\frac{1}{2}$	(19) $\bar{3}^{+}\ \ x-\frac{1}{2},\bar{x}+1,\bar{x};\ 0,\frac{1}{2},-\frac{1}{2}$	(20) $\bar{3}^{+}\ \ \bar{x}+\frac{1}{2},\bar{x},x;\ \frac{1}{2},0,0$
(21) $\bar{3}^{-}\ \ x,x+\frac{1}{2},x;\ 0,\frac{1}{2},0$	(22) $\bar{3}^{-}\ \ x+1,\bar{x}-\frac{1}{2},\bar{x};\ \frac{1}{2},0,\frac{1}{2}$	(23) $\bar{3}^{-}\ \ \bar{x},\bar{x}+\frac{1}{2},x;\ 0,\frac{1}{2},0$	(24) $\bar{3}^{-}\ \ \bar{x}+1,x-\frac{1}{2},\bar{x};\ \frac{1}{2},0,-\frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\ \ (0,\frac{1}{2},\frac{1}{2})+\ \ (\frac{1}{2},0,\frac{1}{2})+\ \ (\frac{1}{2},\frac{1}{2},0)+$						Reflection conditions h,k,l cyclically permutable General:
96	i	1	(1) x,y,z (5) z,x,y (9) y,z,x (13) $\bar{x},\bar{y},\bar{z}$ (17) $\bar{z},\bar{x},\bar{y}$ (21) $\bar{y},\bar{z},\bar{x}$	(2) $\bar{x},\bar{y},z$ (6) $z,\bar{x},\bar{y}$ (10) $\bar{y},z,\bar{x}$ (14) $x,y,\bar{z}$ (18) $\bar{z},x,y$ (22) $y,\bar{z},x$	(3) $\bar{x},y,\bar{z}$ (7) $\bar{z},\bar{x},y$ (11) $y,\bar{z},\bar{x}$ (15) $x,\bar{y},z$ (19) $z,x,\bar{y}$ (23) $\bar{y},z,x$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{z},x,\bar{y}$ (12) $\bar{y},\bar{z},x$ (16) $\bar{x},y,z$ (20) $z,\bar{x},y$ (24) $y,z,\bar{x}$			hkl : $h+k,h+l,k+l=2n$ $0kl$: $k,l=2n$ hhl : $h+l=2n$ $h00$: $h=2n$
									Special: as above, plus
48	h	$m\,.\,.$	$0,y,z$ $\bar{z},0,y$	$0,\bar{y},z$ $\bar{z},0,\bar{y}$	$0,y,\bar{z}$ $y,z,0$	$0,\bar{y},\bar{z}$ $\bar{y},z,0$	$z,0,y$ $y,\bar{z},0$	$z,0,\bar{y}$ $\bar{y},\bar{z},0$	no extra conditions
48	g	$2\,.\,.$	$x,\frac{1}{4},\frac{1}{4}$ $\bar{x},\frac{3}{4},\frac{3}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$ $x,\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},x,\frac{1}{4}$ $\frac{3}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$ $\frac{3}{4},x,\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},x$ $\frac{3}{4},\frac{3}{4},\bar{x}$	$\frac{3}{4},\frac{1}{4},\bar{x}$ $\frac{1}{4},\frac{3}{4},x$	hkl : $h=2n$
32	f	$.\,3\,.$	x,x,x $\bar{x},\bar{x},\bar{x}$	$\bar{x},\bar{x},x$ $x,x,\bar{x}$	$\bar{x},x,\bar{x}$ $x,\bar{x},x$	$x,\bar{x},\bar{x}$ $\bar{x},x,x$			no extra conditions
24	e	$m\,m\,2\,.\,.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	no extra conditions
24	d	$2/m\,.\,.$	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl : $h=2n$
8	c	$2\,3\,.$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$					hkl : $h=2n$
4	b	$m\,\bar{3}\,.$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						no extra conditions
4	a	$m\,\bar{3}\,.$	$0,0,0$						no extra conditions

Symmetry of special projections

Along [001] $p2mm$	Along [111] $p6$	Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\quad \mathbf{b}' = \frac{1}{2}\mathbf{b}$	$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\quad \mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$	$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad \mathbf{b}' = \mathbf{c}$
Origin at $0,0,z$	Origin at x,x,x	Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $F23$ (196)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
	[3] $Fm1$ ($Fmmm$, 69)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[4] $F1\bar{3}$ ($R\bar{3}$, 148)	(1; 5; 9; 13; 17; 21)+
	[4] $F1\bar{3}$ ($R\bar{3}$, 148)	(1; 6; 12; 13; 18; 24)+
	[4] $F1\bar{3}$ ($R\bar{3}$, 148)	(1; 7; 10; 13; 19; 22)+
	[4] $F1\bar{3}$ ($R\bar{3}$, 148)	(1; 8; 11; 13; 20; 23)+
IIa	[4] $Pa\bar{3}$ (205)	1; 5; 9; 13; 17; 21; (2; 7; 12; 14; 19; 24) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 6; 11; 16; 18; 23) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 8; 10; 15; 20; 22) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pa\bar{3}$ (205)	1; 7; 10; 13; 19; 22; (2; 5; 11; 14; 17; 23) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 8; 12; 16; 20; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 6; 9; 15; 18; 21) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pa\bar{3}$ (205)	1; 8; 11; 13; 20; 23; (2; 6; 10; 14; 18; 22) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 7; 9; 16; 19; 21) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 5; 12; 15; 17; 24) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pa\bar{3}$ (205)	1; 6; 12; 13; 18; 24; (2; 8; 9; 14; 20; 21) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 5; 10; 16; 17; 22) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 7; 11; 15; 19; 23) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pa\bar{3}$ (205)	1; 5; 9; 13; 17; 21; (3; 8; 10; 15; 20; 22) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 7; 12; 14; 19; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 6; 11; 16; 18; 23) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pa\bar{3}$ (205)	1; 7; 10; 13; 19; 22; (3; 6; 9; 15; 18; 21) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 5; 11; 14; 17; 23) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 8; 12; 16; 20; 24) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pa\bar{3}$ (205)	1; 8; 11; 13; 20; 23; (3; 5; 12; 15; 17; 24) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 6; 10; 14; 18; 22) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 7; 9; 16; 19; 21) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pa\bar{3}$ (205)	1; 6; 12; 13; 18; 24; (3; 7; 11; 15; 19; 23) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 8; 9; 14; 20; 21) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 5; 10; 16; 17; 22) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pn\bar{3}$ (201)	1; 5; 9; 13; 17; 21; (4; 6; 11; 16; 18; 23) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 8; 10; 15; 20; 22) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 7; 12; 14; 19; 24) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pn\bar{3}$ (201)	1; 7; 10; 13; 19; 22; (4; 8; 12; 16; 20; 24) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 6; 9; 15; 18; 21) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 5; 11; 14; 17; 23) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pn\bar{3}$ (201)	1; 8; 11; 13; 20; 23; (4; 7; 9; 16; 19; 21) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 5; 12; 15; 17; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 6; 10; 14; 18; 22) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pn\bar{3}$ (201)	1; 6; 12; 13; 18; 24; (4; 5; 10; 16; 17; 22) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 7; 11; 15; 19; 23) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 8; 9; 14; 20; 21) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pm\bar{3}$ (200)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[4] $Pm\bar{3}$ (200)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pm\bar{3}$ (200)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 17; 18; 19; 20) + $(\frac{1}{2},0,\frac{1}{2})$; (9; 10; 11; 12; 21; 22; 23; 24) + $(0,\frac{1}{2},\frac{1}{2})$
	[4] $Pm\bar{3}$ (200)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 17; 18; 19; 20) + $(\frac{1}{2},\frac{1}{2},0)$; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $Fm\bar{3}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (202)

Minimal non-isomorphic supergroups

I [2] $Fm\bar{3}m$ (225); [2] $Fm\bar{3}c$ (226)

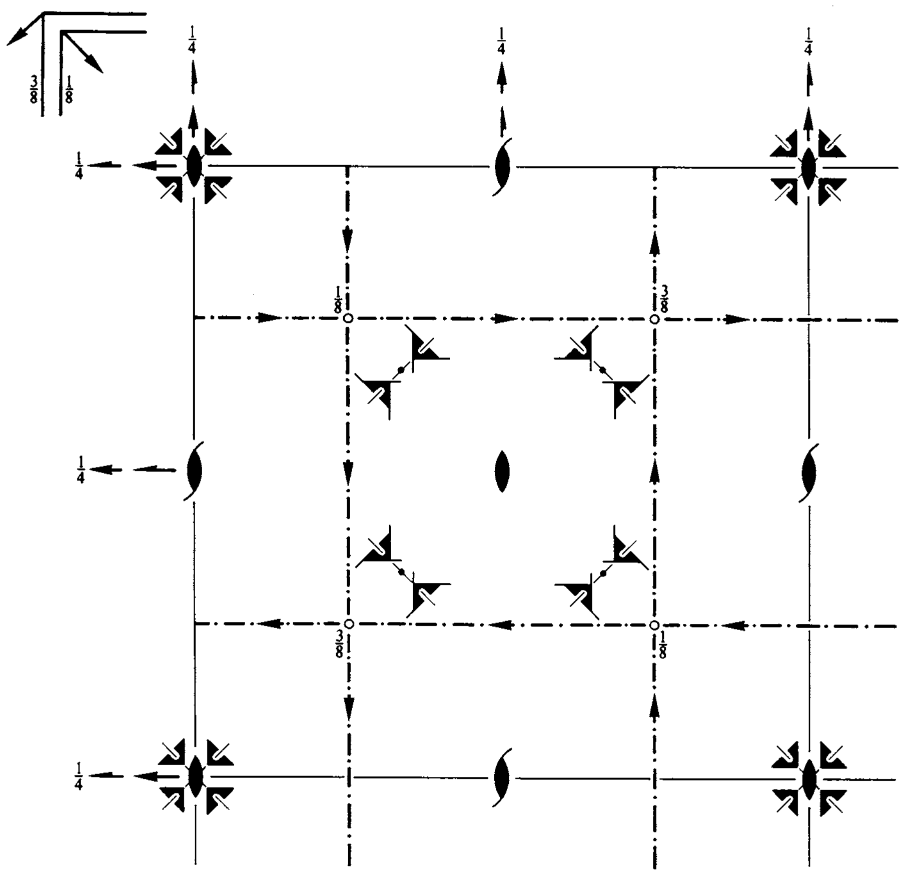
II [2] $Pm\bar{3}$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (200)

International Tables for Crystallography (2006). Vol. A, Space group 203, pp. 623–627.

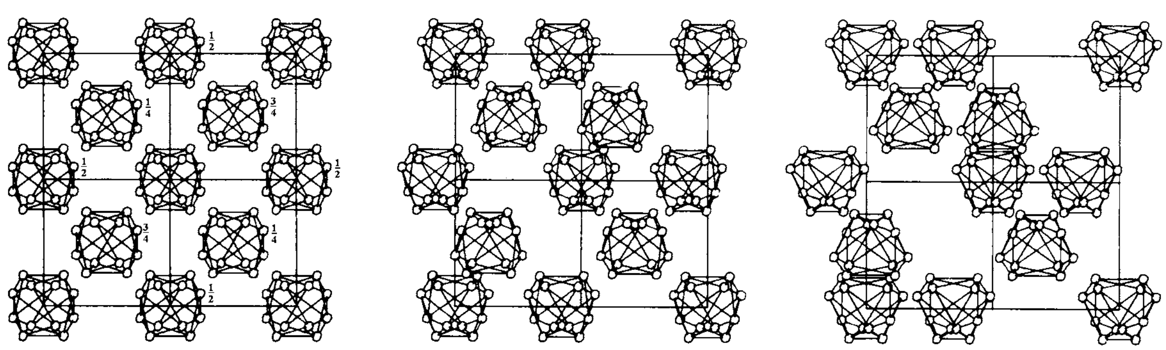
$F\,d\,\bar{3}$ $\quad T_h^4 \quad m\bar{3} \quad$ Cubic

No. 203 $\quad F\,2/d\,\bar{3} \quad$ Patterson symmetry $F\,m\,\bar{3}$

ORIGIN CHOICE 1



Upper left quadrant only



Origin at 23, at $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ from centre ($\bar{3}$)

Asymmetric unit $\quad 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{4}; \quad -\frac{1}{4} \leq z \leq \frac{1}{4}; \quad y \leq \min(x, \frac{1}{2}-x); \quad -y \leq z \leq y$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{4},\frac{1}{4},\frac{1}{4} \quad \frac{1}{4},\frac{1}{4},-\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $3^{+}\ x,x,x$	(6) $3^{+}\ \bar{x},x,\bar{x}$	(7) $3^{+}\ x,\bar{x},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x},x$
(9) $3^{-}\ x,x,x$	(10) $3^{-}\ x,\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x},\bar{x},x$	(12) $3^{-}\ \bar{x},x,\bar{x}$
(13) $\bar{1}\quad \frac{1}{8},\frac{1}{8},\frac{1}{8}$	(14) $d(\frac{1}{4},\frac{1}{4},0)\quad x,y,\frac{1}{8}$	(15) $d(\frac{1}{4},0,\frac{1}{4})\quad x,\frac{1}{8},z$	(16) $d(0,\frac{1}{4},\frac{1}{4})\quad \frac{1}{8},y,z$
(17) $\bar{3}^{+}\ x,x,x;\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$	(18) $\bar{3}^{+}\ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x};\ -\frac{1}{8},\frac{1}{8},\frac{3}{8}$	(19) $\bar{3}^{+}\ x,\bar{x}+\frac{1}{2},\bar{x};\ \frac{1}{8},\frac{3}{8},-\frac{1}{8}$	(20) $\bar{3}^{+}\ \bar{x}+\frac{1}{2},\bar{x},x;\ \frac{3}{8},-\frac{1}{8},\frac{1}{8}$
(21) $\bar{3}^{-}\ x,x,x;\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$	(22) $\bar{3}^{-}\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};\ \frac{1}{8},-\frac{1}{8},\frac{3}{8}$	(23) $\bar{3}^{-}\ \bar{x},\bar{x}+\frac{1}{2},x;\ -\frac{1}{8},\frac{3}{8},\frac{1}{8}$	(24) $\bar{3}^{-}\ \bar{x}+\frac{1}{2},x,\bar{x};\ \frac{3}{8},\frac{1}{8},-\frac{1}{8}$

For $(0,\frac{1}{2},\frac{1}{2})$+ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2\quad x,\frac{1}{4},\frac{1}{4}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{3},x-\frac{1}{6},x$	(6) $3^{+}\ \bar{x},x+\frac{1}{2},\bar{x}$	(7) $3^{+}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x+\frac{1}{6},x$	(10) $3^{-}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) $3^{-}\ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $\bar{1}\quad \frac{1}{8},\frac{3}{8},\frac{3}{8}$	(14) $d(\frac{1}{4},\frac{3}{4},0)\quad x,y,\frac{3}{8}$	(15) $d(\frac{1}{4},0,\frac{3}{4})\quad x,\frac{3}{8},z$	(16) $d(0,\frac{3}{4},\frac{3}{4})\quad \frac{1}{8},y,z$
(17) $\bar{3}^{+}\ x,x+\frac{1}{2},x;\ \frac{1}{8},\frac{5}{8},\frac{1}{8}$	(18) $\bar{3}^{+}\ \bar{x}-\frac{3}{2},x+1,\bar{x};\ -\frac{5}{8},\frac{1}{8},\frac{7}{8}$	(19) $\bar{3}^{+}\ x,\bar{x}+1,\bar{x};\ \frac{1}{8},\frac{7}{8},-\frac{1}{8}$	(20) $\bar{3}^{+}\ \bar{x}+\frac{3}{2},\bar{x}+\frac{1}{2},x;\ \frac{7}{8},-\frac{1}{8},\frac{5}{8}$
(21) $\bar{3}^{-}\ x-\frac{1}{2},x-\frac{1}{2},x;\ \frac{1}{8},\frac{1}{8},\frac{5}{8}$	(22) $\bar{3}^{-}\ x+1,\bar{x}-1,\bar{x};\ \frac{1}{8},-\frac{1}{8},\frac{7}{8}$	(23) $\bar{3}^{-}\ \bar{x}-\frac{1}{2},\bar{x}+1,x;\ -\frac{5}{8},\frac{7}{8},\frac{1}{8}$	(24) $\bar{3}^{-}\ \bar{x}+1,x+\frac{1}{2},\bar{x};\ \frac{7}{8},\frac{5}{8},-\frac{1}{8}$

For $(\frac{1}{2},0,\frac{1}{2})$+ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,0,\frac{1}{4}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x-\frac{1}{6},x$	(6) $3^{+}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^{+}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x-\frac{1}{3},x$	(10) $3^{-}\ x+\frac{1}{2},\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{1}{2},\bar{x},x$	(12) $3^{-}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $\bar{1}\quad \frac{3}{8},\frac{1}{8},\frac{3}{8}$	(14) $d(\frac{3}{4},\frac{1}{4},0)\quad x,y,\frac{3}{8}$	(15) $d(\frac{3}{4},0,\frac{3}{4})\quad x,\frac{1}{8},z$	(16) $d(0,\frac{1}{4},\frac{3}{4})\quad \frac{3}{8},y,z$
(17) $\bar{3}^{+}\ x-\frac{1}{2},x-\frac{1}{2},x;\ \frac{1}{8},\frac{1}{8},\frac{5}{8}$	(18) $\bar{3}^{+}\ \bar{x}-1,x+1,\bar{x};\ -\frac{1}{8},\frac{1}{8},\frac{7}{8}$	(19) $\bar{3}^{+}\ x+\frac{1}{2},\bar{x}+1,\bar{x};\ \frac{5}{8},\frac{7}{8},-\frac{1}{8}$	(20) $\bar{3}^{+}\ \bar{x}+1,\bar{x}-\frac{1}{2},x;\ \frac{7}{8},-\frac{5}{8},\frac{1}{8}$
(21) $\bar{3}^{-}\ x+\frac{1}{2},x,x;\ \frac{5}{8},\frac{1}{8},\frac{1}{8}$	(22) $\bar{3}^{-}\ x+1,\bar{x}-\frac{3}{2},\bar{x};\ \frac{1}{8},-\frac{5}{8},\frac{7}{8}$	(23) $\bar{3}^{-}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{3}{2},x;\ -\frac{1}{8},\frac{7}{8},\frac{5}{8}$	(24) $\bar{3}^{-}\ \bar{x}+1,x,\bar{x};\ \frac{7}{8},\frac{1}{8},-\frac{1}{8}$

For $(\frac{1}{2},\frac{1}{2},0)$+ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x+\frac{1}{3},x$	(6) $3^{+}\ \bar{x}+\frac{1}{2},x,\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x},\bar{x}$	(8) $3^{+}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{3},x+\frac{1}{6},x$	(10) $3^{-}\ x,\bar{x}+\frac{1}{2},\bar{x}$	(11) $3^{-}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^{-}\ \bar{x},x+\frac{1}{2},\bar{x}$
(13) $\bar{1}\quad \frac{3}{8},\frac{3}{8},\frac{1}{8}$	(14) $d(\frac{3}{4},\frac{3}{4},0)\quad x,y,\frac{1}{8}$	(15) $d(\frac{3}{4},0,\frac{1}{4})\quad x,\frac{3}{8},z$	(16) $d(0,\frac{3}{4},\frac{1}{4})\quad \frac{3}{8},y,z$
(17) $\bar{3}^{+}\ x+\frac{1}{2},x,x;\ \frac{5}{8},\frac{1}{8},\frac{1}{8}$	(18) $\bar{3}^{+}\ \bar{x}-1,x+\frac{3}{2},\bar{x};\ -\frac{1}{8},\frac{5}{8},\frac{7}{8}$	(19) $\bar{3}^{+}\ x-\frac{1}{2},\bar{x}+\frac{3}{2},\bar{x};\ \frac{1}{8},\frac{7}{8},-\frac{5}{8}$	(20) $\bar{3}^{+}\ \bar{x}+1,\bar{x},x;\ \frac{7}{8},-\frac{1}{8},\frac{1}{8}$
(21) $\bar{3}^{-}\ x,x+\frac{1}{2},x;\ \frac{1}{8},\frac{5}{8},\frac{1}{8}$	(22) $\bar{3}^{-}\ x+\frac{3}{2},\bar{x}-1,\bar{x};\ \frac{5}{8},-\frac{1}{8},\frac{7}{8}$	(23) $\bar{3}^{-}\ \bar{x},\bar{x}+1,x;\ -\frac{1}{8},\frac{7}{8},\frac{1}{8}$	(24) $\bar{3}^{-}\ \bar{x}+\frac{3}{2},x-\frac{1}{2},\bar{x};\ \frac{7}{8},\frac{1}{8},-\frac{5}{8}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
			$(0,0,0)+\quad (0,\frac{1}{2},\frac{1}{2})+\quad (\frac{1}{2},0,\frac{1}{2})+\quad (\frac{1}{2},\frac{1}{2},0)+$						h,k,l cyclically permutable General:
96	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			hkl : $h+k=2n$ and $h+l,k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			$0kl$: $k+l=4n$ and $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			hhl : $h+l=2n$
			(13) $\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(14) $x+\frac{1}{4},y+\frac{1}{4},\bar{z}+\frac{1}{4}$	(15) $x+\frac{1}{4},\bar{y}+\frac{1}{4},z+\frac{1}{4}$	(16) $\bar{x}+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$			$h00$: $h=4n$
			(17) $\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(18) $\bar{z}+\frac{1}{4},x+\frac{1}{4},y+\frac{1}{4}$	(19) $z+\frac{1}{4},x+\frac{1}{4},\bar{y}+\frac{1}{4}$	(20) $z+\frac{1}{4},\bar{x}+\frac{1}{4},y+\frac{1}{4}$			
			(21) $\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4}$	(22) $y+\frac{1}{4},\bar{z}+\frac{1}{4},x+\frac{1}{4}$	(23) $\bar{y}+\frac{1}{4},z+\frac{1}{4},x+\frac{1}{4}$	(24) $y+\frac{1}{4},z+\frac{1}{4},\bar{x}+\frac{1}{4}$			
									Special: as above, plus
48	f	2 . .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	hkl : $h=2n+1$ or $h+k+l=4n$
			$\bar{x}+\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$x+\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},x+\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\bar{x}+\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},x+\frac{1}{4}$	
32	e	. 3 .	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			no extra conditions
			$\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4}$	$x+\frac{1}{4},x+\frac{1}{4},\bar{x}+\frac{1}{4}$	$x+\frac{1}{4},\bar{x}+\frac{1}{4},x+\frac{1}{4}$	$\bar{x}+\frac{1}{4},x+\frac{1}{4},x+\frac{1}{4}$			
16	d	. $\bar{3}$.	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{3}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{3}{8}$	$\frac{5}{8},\frac{3}{8},\frac{3}{8}$			hkl : $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16	c	. $\bar{3}$.	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{7}{8},\frac{1}{8}$	$\frac{7}{8},\frac{1}{8},\frac{7}{8}$	$\frac{1}{8},\frac{7}{8},\frac{7}{8}$			
8	b	2 3 .	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$					hkl : $h=2n+1$ or $h+k+l=4n$
8	a	2 3 .	$0,0,0$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$					

(*Continued on page 623*)

ORIGIN CHOICE 1

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0, 0, z$

Along [111] $p6$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
Origin at x, x, x

Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, x, \frac{1}{8}$

ORIGIN CHOICE 2

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{8}, \frac{1}{8}, z$

Along [111] $p6$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
Origin at x, x, x

Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, x, 0$

ORIGIN CHOICES 1 AND 2

Maximal non-isomorphic subgroups

I [2] $F23$ (196) (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
[3] $Fd1$ ($Fddd$, 70) (1; 2; 3; 4; 13; 14; 15; 16)+
{ [4] $F1\bar{3}$ ($R\bar{3}$, 148) (1; 5; 9; 13; 17; 21)+
[4] $F1\bar{3}$ ($R\bar{3}$, 148) (1; 6; 12; 13; 18; 24)+
[4] $F1\bar{3}$ ($R\bar{3}$, 148) (1; 7; 10; 13; 19; 22)+
[4] $F1\bar{3}$ ($R\bar{3}$, 148) (1; 8; 11; 13; 20; 23)+ }

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $Fd\bar{3}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (203)

Minimal non-isomorphic supergroups

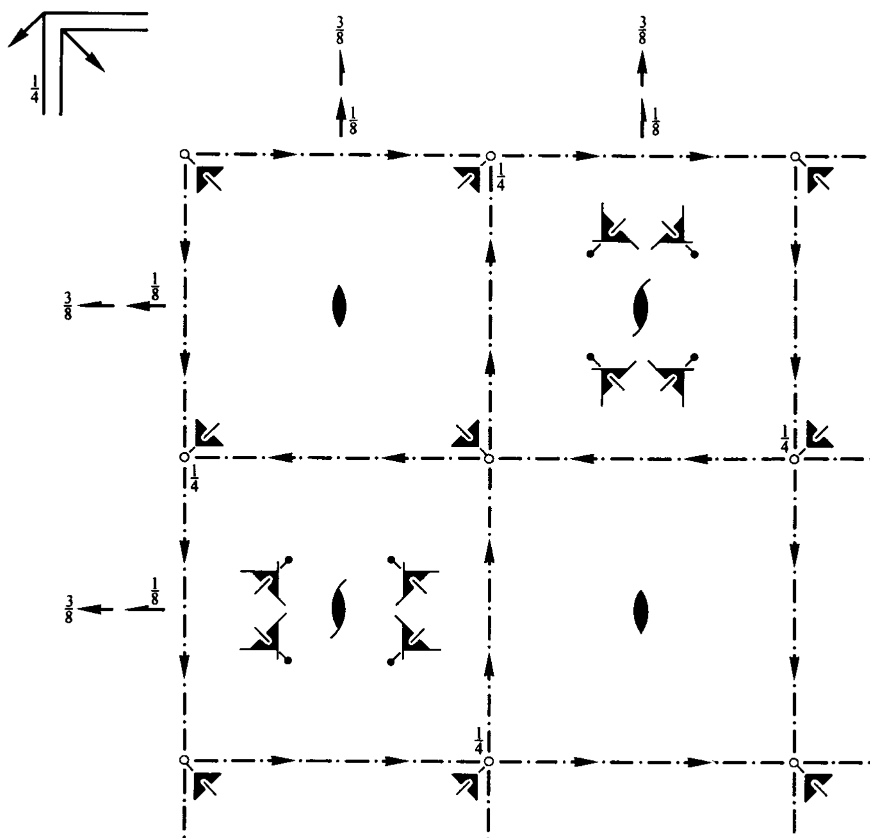
I [2] $Fd\bar{3}m$ (227); [2] $Fd\bar{3}c$ (228)

II [2] $Pn\bar{3}$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (201)

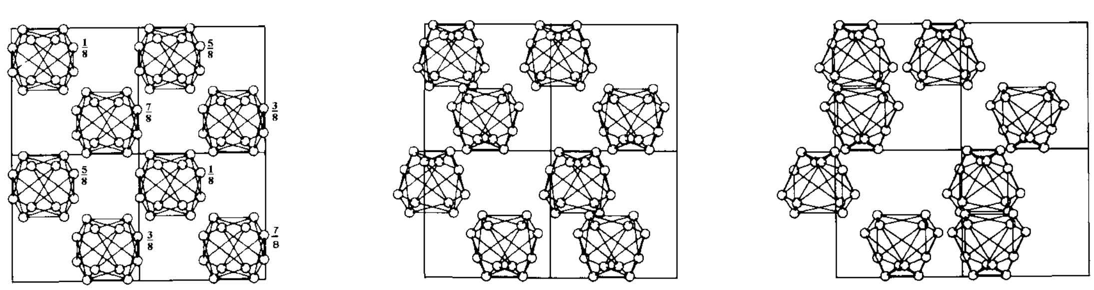
$F\,d\bar{3}$ $\quad T_h^4$ $\quad m\bar{3}$ $\quad$ Cubic

No. 203 $\quad F\,2/d\,\bar{3}$ $\quad$ Patterson symmetry $F\,m\,\bar{3}$

ORIGIN CHOICE 2



Upper left quadrant only



Origin at centre ($\bar{3}$), at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ from 23

Asymmetric unit $\quad -\frac{1}{8}\le x\le\frac{3}{8};\quad -\frac{1}{8}\le y\le\frac{1}{8};\quad -\frac{3}{8}\le z\le\frac{1}{8};\quad y\le \min(x,\frac{1}{4}-x);\quad -y-\frac{1}{4}\le z\le y$

Vertices $\quad -\frac{1}{8},-\frac{1}{8},-\frac{1}{8}\quad \frac{3}{8},-\frac{1}{8},-\frac{1}{8}\quad \frac{1}{8},\frac{1}{8},\frac{1}{8}\quad \frac{1}{8},\frac{1}{8},-\frac{3}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\ \ \frac{3}{8},\frac{3}{8},z$	(3) $2\ \ \frac{3}{8},y,\frac{3}{8}$	(4) $2\ \ x,\frac{3}{8},\frac{3}{8}$
(5) $3^+\ x,x,x$	(6) $3^+\ \bar{x},x+\frac{3}{4},\bar{x}$	(7) $3^+\ x+\frac{3}{4},\bar{x},\bar{x}$	(8) $3^+\ \bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},x$
(9) $3^-\ x,x,x$	(10) $3^-\ x+\frac{3}{4},\bar{x},\bar{x}$	(11) $3^-\ \bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},x$	(12) $3^-\ \bar{x},x+\frac{3}{4},\bar{x}$
(13) $\bar{1}\ \ 0,0,0$	(14) $d(\frac{1}{4},\frac{1}{4},0)\ \ x,y,0$	(15) $d(\frac{1}{4},0,\frac{1}{4})\ \ x,0,z$	(16) $d(0,\frac{1}{4},\frac{1}{4})\ \ 0,y,z$
(17) $\bar{3}^+\ x,x,x;\ 0,0,0$	(18) $\bar{3}^+\ \bar{x}-\frac{1}{2},x+\frac{1}{4},\bar{x};\ -\frac{1}{4},0,\frac{1}{4}$	(19) $\bar{3}^+\ x-\frac{1}{4},\bar{x}+\frac{1}{2},\bar{x};\ 0,\frac{1}{4},-\frac{1}{4}$	(20) $\bar{3}^+\ \bar{x}+\frac{1}{4},\bar{x}-\frac{1}{4},x;\ \frac{1}{4},-\frac{1}{4},0$
(21) $\bar{3}^-\ x,x,x;\ 0,0,0$	(22) $\bar{3}^-\ x+\frac{1}{4},\bar{x}-\frac{1}{2},\bar{x};\ 0,-\frac{1}{4},\frac{1}{4}$	(23) $\bar{3}^-\ \bar{x}-\frac{1}{4},\bar{x}+\frac{1}{4},x;\ -\frac{1}{4},\frac{1}{4},0$	(24) $\bar{3}^-\ \bar{x}+\frac{1}{2},x-\frac{1}{4},\bar{x};\ \frac{1}{4},0,-\frac{1}{4}$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\ \ \frac{3}{8},\frac{1}{8},z$	(3) $2(0,\frac{1}{2},0)\ \ \frac{3}{8},y,\frac{1}{8}$	(4) $2\ \ x,\frac{1}{8},\frac{1}{8}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x-\frac{1}{3},x-\frac{1}{6},x$	(6) $3^+\ \bar{x},x+\frac{1}{4},\bar{x}$	(7) $3^+\ x+\frac{3}{4},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\ \ \bar{x}+\frac{5}{12},\bar{x}+\frac{7}{12},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x-\frac{1}{6},x+\frac{1}{6},x$	(10) $3^-\ x+\frac{1}{4},\bar{x}+\frac{1}{2},\bar{x}$	(11) $3^-\ \bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\ \ \bar{x}-\frac{1}{6},x+\frac{7}{12},\bar{x}$
(13) $\bar{1}\ \ 0,\frac{1}{4},\frac{1}{4}$	(14) $d(\frac{1}{4},\frac{3}{4},0)\ \ x,y,\frac{1}{4}$	(15) $d(\frac{1}{4},0,\frac{3}{4})\ \ x,\frac{1}{4},z$	(16) $d(0,\frac{3}{4},\frac{3}{4})\ \ 0,y,z$
(17) $\bar{3}^+\ x,x+\frac{1}{2},x;\ 0,\frac{1}{2},0$	(18) $\bar{3}^+\ \bar{x}-\frac{3}{2},x+\frac{3}{4},\bar{x};\ -\frac{3}{4},0,\frac{3}{4}$	(19) $\bar{3}^+\ x-\frac{1}{4},\bar{x}+1,\bar{x};\ 0,\frac{3}{4},-\frac{1}{4}$	(20) $\bar{3}^+\ \bar{x}+\frac{5}{4},\bar{x}+\frac{1}{4},x;\ \frac{3}{4},-\frac{1}{4},\frac{1}{2}$
(21) $\bar{3}^-\ x-\frac{1}{2},x-\frac{1}{2},x;\ 0,0,\frac{1}{2}$	(22) $\bar{3}^-\ x+\frac{3}{4},\bar{x}-1,\bar{x};\ 0,-\frac{1}{4},\frac{3}{4}$	(23) $\bar{3}^-\ \bar{x}-\frac{3}{4},\bar{x}+\frac{3}{4},x;\ -\frac{3}{4},\frac{3}{4},0$	(24) $\bar{3}^-\ \bar{x}+1,x+\frac{1}{4},\bar{x};\ \frac{3}{4},\frac{1}{2},-\frac{1}{4}$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{8},\frac{3}{8},z$	(3) $2\ \ \frac{1}{8},y,\frac{1}{8}$	(4) $2(\frac{1}{2},0,0)\ \ x,\frac{3}{8},\frac{1}{8}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{6},x-\frac{1}{6},x$	(6) $3^+\ \bar{x}+\frac{1}{2},x+\frac{1}{4},\bar{x}$	(7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{7}{12},\bar{x}-\frac{1}{6},\bar{x}$	(8) $3^+\ \bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x-\frac{1}{6},x-\frac{1}{3},x$	(10) $3^-\ x+\frac{1}{4},\bar{x},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\ \ \bar{x}+\frac{7}{12},\bar{x}+\frac{5}{12},x$	(12) $3^-\ \bar{x}-\frac{1}{2},x+\frac{3}{4},\bar{x}$
(13) $\bar{1}\ \ \frac{1}{4},0,\frac{1}{4}$	(14) $d(\frac{3}{4},\frac{1}{4},0)\ \ x,y,\frac{1}{4}$	(15) $d(\frac{3}{4},0,\frac{3}{4})\ \ x,0,z$	(16) $d(0,\frac{1}{4},\frac{3}{4})\ \ \frac{1}{4},y,z$
(17) $\bar{3}^+\ x-\frac{1}{2},x-\frac{1}{2},x;\ 0,0,\frac{1}{2}$	(18) $\bar{3}^+\ \bar{x}-1,x+\frac{3}{4},\bar{x};\ -\frac{1}{4},0,\frac{3}{4}$	(19) $\bar{3}^+\ x+\frac{1}{4},\bar{x}+1,\bar{x};\ \frac{1}{2},\frac{3}{4},-\frac{1}{4}$	(20) $\bar{3}^+\ \bar{x}+\frac{3}{4},\bar{x}-\frac{3}{4},x;\ \frac{3}{4},-\frac{3}{4},0$
(21) $\bar{3}^-\ x+\frac{1}{2},x,x;\ \frac{1}{2},0,0$	(22) $\bar{3}^-\ x+\frac{3}{4},\bar{x}-\frac{3}{2},\bar{x};\ 0,-\frac{3}{4},\frac{3}{4}$	(23) $\bar{3}^-\ \bar{x}+\frac{1}{4},\bar{x}+\frac{5}{4},x;\ -\frac{1}{4},\frac{3}{4},\frac{1}{2}$	(24) $\bar{3}^-\ \bar{x}+1,x-\frac{1}{4},\bar{x};\ \frac{3}{4},0,-\frac{1}{4}$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\ \ \frac{1}{8},\frac{1}{8},z$	(3) $2(0,\frac{1}{2},0)\ \ \frac{1}{8},y,\frac{3}{8}$	(4) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{8},\frac{3}{8}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{6},x+\frac{1}{3},x$	(6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\ \ \bar{x}+\frac{1}{6},x+\frac{5}{12},\bar{x}$	(7) $3^+\ x+\frac{1}{4},\bar{x},\bar{x}$	(8) $3^+\ \bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{3},x+\frac{1}{6},x$	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{5}{12},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-\ \bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},x$	(12) $3^-\ \bar{x},x+\frac{1}{4},\bar{x}$
(13) $\bar{1}\ \ \frac{1}{4},\frac{1}{4},0$	(14) $d(\frac{3}{4},\frac{3}{4},0)\ \ x,y,0$	(15) $d(\frac{3}{4},0,\frac{1}{4})\ \ x,\frac{1}{4},z$	(16) $d(0,\frac{3}{4},\frac{1}{4})\ \ \frac{1}{4},y,z$
(17) $\bar{3}^+\ x+\frac{1}{2},x,x;\ \frac{1}{2},0,0$	(18) $\bar{3}^+\ \bar{x}-1,x+\frac{5}{4},\bar{x};\ -\frac{1}{4},\frac{1}{2},\frac{3}{4}$	(19) $\bar{3}^+\ x-\frac{3}{4},\bar{x}+\frac{3}{2},\bar{x};\ 0,\frac{3}{4},-\frac{3}{4}$	(20) $\bar{3}^+\ \bar{x}+\frac{3}{4},\bar{x}-\frac{1}{4},x;\ \frac{3}{4},-\frac{1}{4},0$
(21) $\bar{3}^-\ x,x+\frac{1}{2},x;\ 0,\frac{1}{2},0$	(22) $\bar{3}^-\ x+\frac{5}{4},\bar{x}-1,\bar{x};\ \frac{1}{2},-\frac{1}{4},\frac{3}{4}$	(23) $\bar{3}^-\ \bar{x}-\frac{1}{4},\bar{x}+\frac{3}{4},x;\ -\frac{1}{4},\frac{3}{4},0$	(24) $\bar{3}^-\ \bar{x}+\frac{3}{2},x-\frac{3}{4},\bar{x};\ \frac{3}{4},0,-\frac{3}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\ \ (0,\frac{1}{2},\frac{1}{2})+\ \ (\frac{1}{2},0,\frac{1}{2})+\ \ (\frac{1}{2},\frac{1}{2},0)+$						Reflection conditions h,k,l cyclically permutable General:
96	g	1	(1) x,y,z	(2) $\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4},z$	(3) $\bar{x}+\frac{3}{4},y,\bar{z}+\frac{3}{4}$	(4) $x,\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4}$			hkl : $h+k,h+l,k+l=2n$
			(5) z,x,y	(6) $z,\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(7) $\bar{z}+\frac{3}{4},\bar{x}+\frac{3}{4},y$	(8) $\bar{z}+\frac{3}{4},x,\bar{y}+\frac{3}{4}$			$0kl$: $k+l=4n,\ k,l=2n$
			(9) y,z,x	(10) $\bar{y}+\frac{3}{4},z,\bar{x}+\frac{3}{4}$	(11) $y,\bar{z}+\frac{3}{4},\bar{x}+\frac{3}{4}$	(12) $\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4},x$			hhl : $h+l=2n$
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x+\frac{1}{4},y+\frac{1}{4},\bar{z}$	(15) $x+\frac{1}{4},\bar{y},z+\frac{1}{4}$	(16) $\bar{x},y+\frac{1}{4},z+\frac{1}{4}$			$h00$: $h=4n$
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z},x+\frac{1}{4},y+\frac{1}{4}$	(19) $z+\frac{1}{4},x+\frac{1}{4},\bar{y}$	(20) $z+\frac{1}{4},\bar{x},y+\frac{1}{4}$			
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y+\frac{1}{4},\bar{z},x+\frac{1}{4}$	(23) $\bar{y},z+\frac{1}{4},x+\frac{1}{4}$	(24) $y+\frac{1}{4},z+\frac{1}{4},\bar{x}$			
									Special: as above, plus
48	f	$2\,.\,.$	$x,\frac{1}{8},\frac{1}{8}$	$\bar{x}+\frac{3}{4},\frac{5}{8},\frac{1}{8}$	$\frac{1}{8},x,\frac{1}{8}$	$\frac{1}{8},\bar{x}+\frac{3}{4},\frac{5}{8}$	$\frac{1}{8},\frac{1}{8},x$	$\frac{5}{8},\frac{1}{8},\bar{x}+\frac{3}{4}$	hkl : $h=2n+1$
			$\bar{x},\frac{7}{8},\frac{7}{8}$	$x+\frac{1}{4},\frac{3}{8},\frac{7}{8}$	$\frac{7}{8},\bar{x},\frac{7}{8}$	$\frac{7}{8},x+\frac{1}{4},\frac{3}{8}$	$\frac{7}{8},\frac{7}{8},\bar{x}$	$\frac{3}{8},\frac{7}{8},x+\frac{1}{4}$	or $h+k+l=4n$
32	e	$.\,3\,.$	x,x,x	$\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},x$	$\bar{x}+\frac{3}{4},x,\bar{x}+\frac{3}{4}$	$x,\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4}$			no extra conditions
			$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{4},x+\frac{1}{4},\bar{x}$	$x+\frac{1}{4},\bar{x},x+\frac{1}{4}$	$\bar{x},x+\frac{1}{4},x+\frac{1}{4}$			
16	d	$.\,\bar{3}\,.$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$			hkl : $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16	c	$.\,\bar{3}\,.$	$0,0,0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},0,\frac{3}{4}$	$0,\frac{3}{4},\frac{3}{4}$			
8	b	$2\,3\,.$	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{3}{8},\frac{3}{8},\frac{3}{8}$					hkl : $h=2n+1$ or $h+k+l=4n$
8	a	$2\,3\,.$	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$					

(*Continued on page 623*)

ORIGIN CHOICE 1

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [111] $p6$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,\frac{1}{8}$

ORIGIN CHOICE 2

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{8},\frac{1}{8},z$

Along [111] $p6$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

ORIGIN CHOICES 1 AND 2

Maximal non-isomorphic subgroups

I	[2] $F23$ (196)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
	[3] $Fd1$ ($Fddd$, 70)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[4] $F1\bar{3}$ ($R\bar{3}$, 148)	(1; 5; 9; 13; 17; 21)+
	[4] $F1\bar{3}$ ($R\bar{3}$, 148)	(1; 6; 12; 13; 18; 24)+
	[4] $F1\bar{3}$ ($R\bar{3}$, 148)	(1; 7; 10; 13; 19; 22)+
	[4] $F1\bar{3}$ ($R\bar{3}$, 148)	(1; 8; 11; 13; 20; 23)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $Fd\bar{3}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (203)

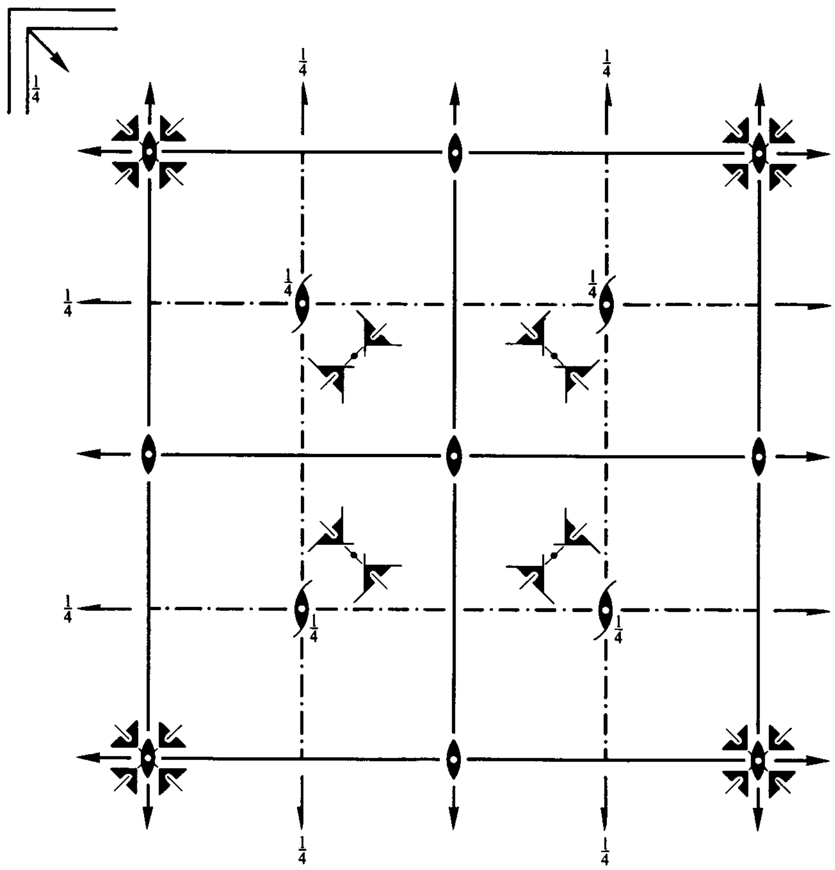
Minimal non-isomorphic supergroups

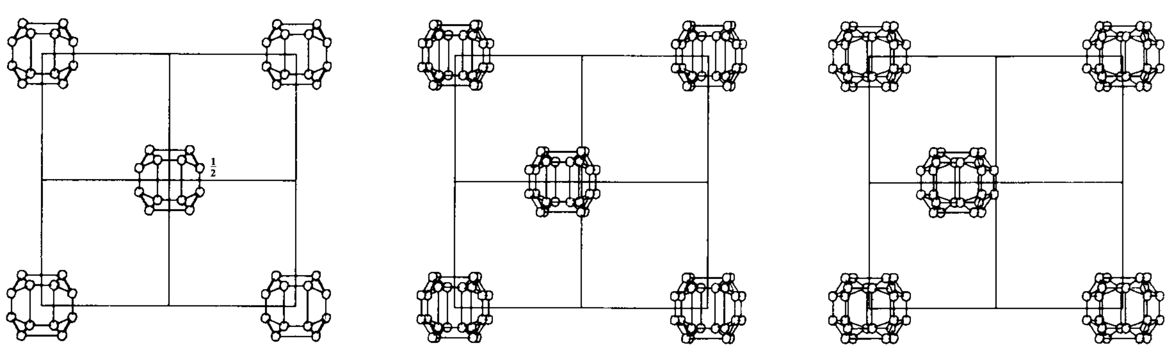
I [2] $Fd\bar{3}m$ (227); [2] $Fd\bar{3}c$ (228)

II [2] $Pn\bar{3}$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (201)

International Tables for Crystallography (2006). Vol. A, Space group 204, pp. 628–629.

$Im\bar{3}$	T_h^5	$m\bar{3}$	Cubic
No. 204	$I2/m\bar{3}$		Patterson symmetry $Im\bar{3}$





Origin at centre ($m\bar{3}$)

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le x$; $z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) $\bar{1}$ $0,0,0$	(14) m $x,y,0$	(15) m $x,0,z$	(16) m $0,y,z$
(17) $\bar{3}^+$ x,x,x; $0,0,0$	(18) $\bar{3}^+$ $\bar{x},x,\bar{x}$; $0,0,0$	(19) $\bar{3}^+$ $x,\bar{x},\bar{x}$; $0,0,0$	(20) $\bar{3}^+$ $\bar{x},\bar{x},x$; $0,0,0$
(21) $\bar{3}^-$ x,x,x; $0,0,0$	(22) $\bar{3}^-$ $x,\bar{x},\bar{x}$; $0,0,0$	(23) $\bar{3}^-$ $\bar{x},\bar{x},x$; $0,0,0$	(24) $\bar{3}^-$ $\bar{x},x,\bar{x}$; $0,0,0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}+\frac{1}{3},x+\frac{1}{3},\bar{x}$	(7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{2}{3},\bar{x}-\frac{1}{3},\bar{x}$	(8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{2}{3},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(10) $3^-(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{3},\bar{x}+\frac{1}{3},\bar{x}$	(11) $3^-(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{2}{3},\bar{x}+\frac{1}{3},x$	(12) $3^-(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}-\frac{1}{3},x+\frac{2}{3},\bar{x}$
(13) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(14) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(15) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(16) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$
(17) $\bar{3}^+$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(18) $\bar{3}^+$ $\bar{x}-1,x+1,\bar{x}$; $-\frac{1}{4},\frac{1}{4},\frac{3}{4}$	(19) $\bar{3}^+$ $x,\bar{x}+1,\bar{x}$; $\frac{1}{4},\frac{3}{4},-\frac{1}{4}$	(20) $\bar{3}^+$ $\bar{x}+1,\bar{x},x$; $\frac{3}{4},-\frac{1}{4},\frac{1}{4}$
(21) $\bar{3}^-$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(22) $\bar{3}^-$ $x+1,\bar{x}-1,\bar{x}$; $\frac{1}{4},-\frac{1}{4},\frac{3}{4}$	(23) $\bar{3}^-$ $\bar{x},\bar{x}+1,x$; $-\frac{1}{4},\frac{3}{4},\frac{1}{4}$	(24) $\bar{3}^-$ $\bar{x}+1,x,\bar{x}$; $\frac{3}{4},\frac{1}{4},-\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$						h,k,l cyclically permutable General:
48	h	1	(1) x,y,z (5) z,x,y (9) y,z,x (13) $\bar{x},\bar{y},\bar{z}$ (17) $\bar{z},\bar{x},\bar{y}$ (21) $\bar{y},\bar{z},\bar{x}$	(2) $\bar{x},\bar{y},z$ (6) $z,\bar{x},\bar{y}$ (10) $\bar{y},z,\bar{x}$ (14) $x,y,\bar{z}$ (18) $\bar{z},x,y$ (22) $y,\bar{z},x$	(3) $\bar{x},y,\bar{z}$ (7) $\bar{z},\bar{x},y$ (11) $y,\bar{z},\bar{x}$ (15) $x,\bar{y},z$ (19) $z,x,\bar{y}$ (23) $\bar{y},z,x$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{z},x,\bar{y}$ (12) $\bar{y},\bar{z},x$ (16) $\bar{x},y,z$ (20) $z,\bar{x},y$ (24) $y,z,\bar{x}$			hkl : $h+k+l=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $h00$: $h=2n$
									Special: as above, plus
24	g	$m\,.\,.$	$0,y,z$ $\bar{z},0,y$	$0,\bar{y},z$ $\bar{z},0,\bar{y}$	$0,y,\bar{z}$ $y,z,0$	$0,\bar{y},\bar{z}$ $\bar{y},z,0$	$z,0,y$ $y,\bar{z},0$	$z,0,\bar{y}$ $\bar{y},\bar{z},0$	no extra conditions
16	f	$.\,3\,.$	x,x,x $\bar{x},\bar{x},\bar{x}$	$\bar{x},\bar{x},x$ $x,x,\bar{x}$	$\bar{x},x,\bar{x}$ $x,\bar{x},x$	$x,\bar{x},\bar{x}$ $\bar{x},x,x$			no extra conditions
12	e	$m\,m\,2\,.\,.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$0,\frac{1}{2},x$	$0,\frac{1}{2},\bar{x}$	no extra conditions
12	d	$m\,m\,2\,.\,.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	no extra conditions
8	c	$.\,\bar{3}\,.$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$			hkl : $k,l=2n$
6	b	$m\,m\,m\,.\,.$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
2	a	$m\,\bar{3}\,.$	$0,0,0$						no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [111] $p6$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I23$ (197)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
	[3] $Im1$ ($Immm$, 71)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 5; 9; 13; 17; 21)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 6; 12; 13; 18; 24)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 7; 10; 13; 19; 22)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 8; 11; 13; 20; 23)+
IIa	[2] $Pn\bar{3}$ (201)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pm\bar{3}$ (200)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $Im\bar{3}$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (204)

Minimal non-isomorphic supergroups

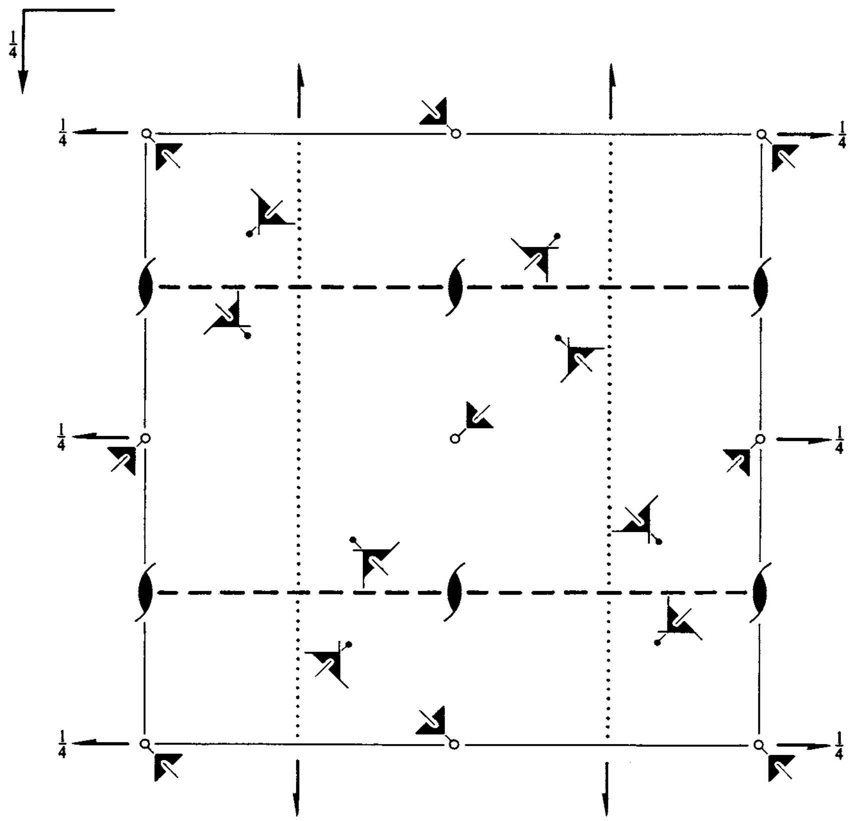
I [2] $Im\bar{3}m$ (229)

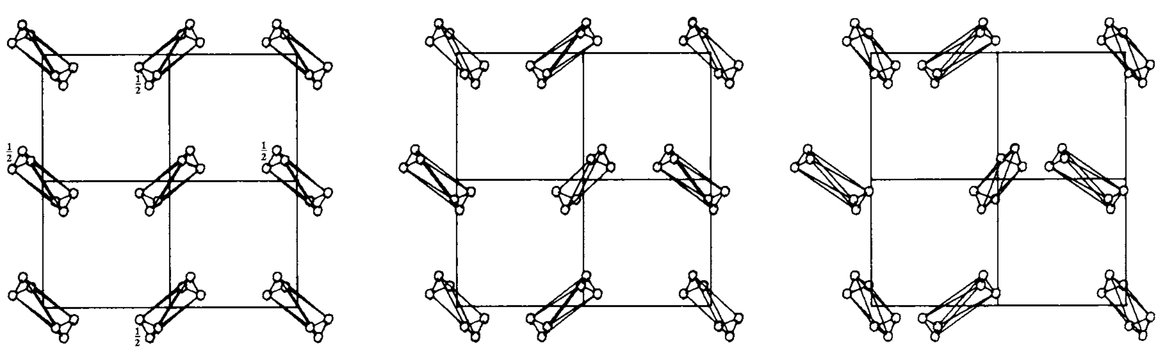
II [4] $Pm\bar{3}$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (200)

International Tables for Crystallography (2006). Vol. A, Space group 205, pp. 630–631.

$Pa\bar{3}$ T_h^6 $m\bar{3}$ Cubic

No. 205 $P2_1/a\bar{3}$ Patterson symmetry $Pm\bar{3}$





Origin at centre ($\bar{3}$)

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $z \le \min(x,y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$	(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) 3^- x,x,x	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $\bar{1}$ $0,0,0$	(14) a $x,y,\frac{1}{4}$	(15) c $x,\frac{1}{4},z$	(16) b $\frac{1}{4},y,z$
(17) $\bar{3}^+$ x,x,x; $0,0,0$	(18) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+1,\bar{x}$; $0,\frac{1}{2},\frac{1}{2}$	(19) $\bar{3}^+$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$; $\frac{1}{2},\frac{1}{2},0$	(20) $\bar{3}^+$ $\bar{x}+1,\bar{x}+\frac{1}{2},x$; $\frac{1}{2},0,\frac{1}{2}$
(21) $\bar{3}^-$ x,x,x; $0,0,0$	(22) $\bar{3}^-$ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$; $0,0,\frac{1}{2}$	(23) $\bar{3}^-$ $\bar{x},\bar{x}+\frac{1}{2},x$; $0,\frac{1}{2},0$	(24) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x,\bar{x}$; $\frac{1}{2},0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							h,k,l cyclically permutable
							General:
24	d	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$0kl$: $k=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	$h00$: $h=2n$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(15) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y$	(19) $z+\frac{1}{2},x,\bar{y}+\frac{1}{2}$	(20) $z,\bar{x}+\frac{1}{2},y+\frac{1}{2}$	
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x$	(24) $y+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	
							Special: as above, plus
8	c	$.3.$	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$	no extra conditions
			$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{2},x,\bar{x}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x$	
4	b	$.\bar{3}.$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	hkl : $h+k,h+l,k+l=2n$
4	a	$.\bar{3}.$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl : $h+k,h+l,k+l=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [111] $p6$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2gg$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P2_13$ (198) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
[3] $Pa1$ ($Pbca$, 61) 1; 2; 3; 4; 13; 14; 15; 16
[4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 5; 9; 13; 17; 21
[4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 6; 12; 13; 18; 24
[4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 7; 10; 13; 19; 22
[4] $P1\bar{3}$ ($R\bar{3}$, 148) 1; 8; 11; 13; 20; 23

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $Pa\bar{3}$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (205)

Minimal non-isomorphic supergroups

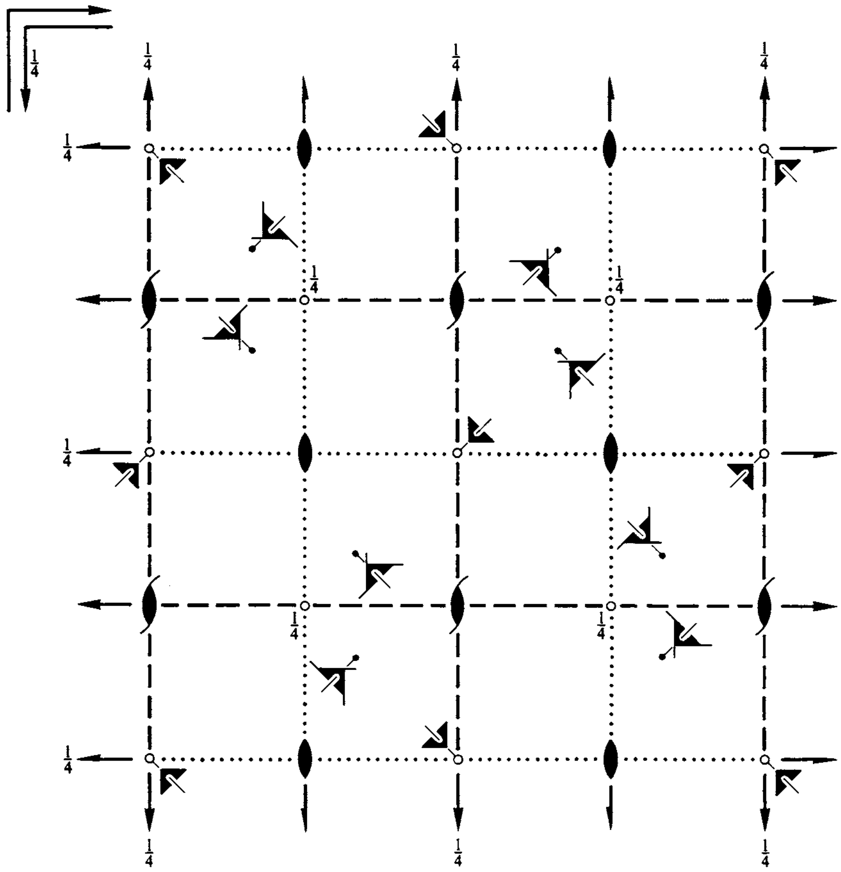
I none

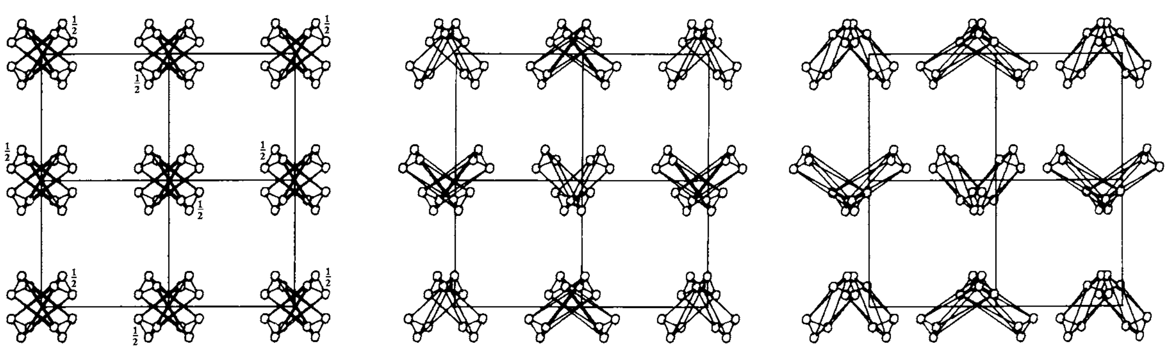
II [2] $Ia\bar{3}$ (206); [4] $Fm\bar{3}$ (202)

International Tables for Crystallography (2006). Vol. A, Space group 206, pp. 632–633.

$I\,a\,\bar{3}$ $\quad T_h^7$ $\quad m\bar{3}$ $\quad$ Cubic

No. 206 $\quad I\,2_1/a\,\bar{3}$ $\quad$ Patterson symmetry $I\,m\,\bar{3}$





Origin at centre ($\bar{3}$)

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}; \quad z \le \min(x, \frac{1}{2}-x, y, \frac{1}{2}-y)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad 0,\frac{1}{2},0 \quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $3^+\ x,x,x$	(6) $3^+\ \bar{x}+\frac{1}{2},x,\bar{x}$	(7) $3^+\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^+\ \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^-\ x,x,x$	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $\bar{1}\quad 0,0,0$	(14) $a\quad x,y,\frac{1}{4}$	(15) $c\quad x,\frac{1}{4},z$	(16) $b\quad \frac{1}{4},y,z$
(17) $\bar{3}^+\ x,x,x;\ 0,0,0$	(18) $\bar{3}^+\ \bar{x}-\frac{1}{2},x+1,\bar{x};\ 0,\frac{1}{2},\frac{1}{2}$	(19) $\bar{3}^+\ x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x};\ \frac{1}{2},\frac{1}{2},0$	(20) $\bar{3}^+\ \bar{x}+1,\bar{x}+\frac{1}{2},x;\ \frac{1}{2},0,\frac{1}{2}$
(21) $\bar{3}^-\ x,x,x;\ 0,0,0$	(22) $\bar{3}^-\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};\ 0,0,\frac{1}{2}$	(23) $\bar{3}^-\ \bar{x},\bar{x}+\frac{1}{2},x;\ 0,\frac{1}{2},0$	(24) $\bar{3}^-\ \bar{x}+\frac{1}{2},x,\bar{x};\ \frac{1}{2},0,0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\quad 0,\frac{1}{4},z$	(3) $2\quad \frac{1}{4},y,0$	(4) $2\quad x,0,\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,x$	(6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$	(7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,x$	(10) $3^-(\frac{1}{6},-\frac{1}{6},-\frac{1}{6})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-(-\frac{1}{6},-\frac{1}{6},\frac{1}{6})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^-(-\frac{1}{6},\frac{1}{6},-\frac{1}{6})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $\bar{1}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(14) $b\quad x,y,0$	(15) $a\quad x,0,z$	(16) $c\quad 0,y,z$
(17) $\bar{3}^+\ x,x,x;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(18) $\bar{3}^+\ \bar{x}-\frac{1}{2},x,\bar{x};\ -\frac{1}{4},-\frac{1}{4},\frac{1}{4}$	(19) $\bar{3}^+\ x-\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x};\ -\frac{1}{4},\frac{1}{4},-\frac{1}{4}$	(20) $\bar{3}^+\ \bar{x},\bar{x}-\frac{1}{2},x;\ \frac{1}{4},-\frac{1}{4},-\frac{1}{4}$
(21) $\bar{3}^-\ x,x,x;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(22) $\bar{3}^-\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};\ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$	(23) $\bar{3}^-\ \bar{x},\bar{x}+\frac{1}{2},x;\ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(24) $\bar{3}^-\ \bar{x}+\frac{1}{2},x,\bar{x};\ \frac{1}{4},\frac{1}{4},-\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
			$(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$						h,k,l cyclically permutable
									General:
48	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$			hkl : $h+k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$			$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$			hhl : $l=2n$
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(15) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$			$h00$: $h=2n$
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y$	(19) $z+\frac{1}{2},x,\bar{y}+\frac{1}{2}$	(20) $z,\bar{x}+\frac{1}{2},y+\frac{1}{2}$			
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x$	(24) $y+\frac{1}{2},z,\bar{x}+\frac{1}{2}$			
									Special: as above, plus
24	d	2 . .	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{4},x,0$	$\frac{3}{4},\bar{x}+\frac{1}{2},0$	$0,\frac{1}{4},x$	$0,\frac{3}{4},\bar{x}+\frac{1}{2}$	no extra conditions
			$\bar{x},0,\frac{3}{4}$	$x+\frac{1}{2},0,\frac{1}{4}$	$\frac{3}{4},\bar{x},0$	$\frac{1}{4},x+\frac{1}{2},0$	$0,\frac{3}{4},\bar{x}$	$0,\frac{1}{4},x+\frac{1}{2}$	
16	c	. 3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$			no extra conditions
			$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{2},x,\bar{x}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x$			
8	b	. $\bar{3}$.	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$			hkl : $k,l=2n$
8	a	. $\bar{3}$.	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $k,l=2n$

Symmetry of special projections

Along [001] $p2mm$	Along [111] $p6$	Along [110] $p2mg$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$	$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$	$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $0,0,z$	Origin at x,x,x	Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I2_13$ (199)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
	[3] $Ia1$ ($Ibca$, 73)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 5; 9; 13; 17; 21)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 6; 12; 13; 18; 24)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 7; 10; 13; 19; 22)+
	[4] $I1\bar{3}$ ($R\bar{3}$, 148)	(1; 8; 11; 13; 20; 23)+
IIa	[2] $Pa\bar{3}$ (205)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[2] $Pa\bar{3}$ (205)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $Ia\bar{3}$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (206)

Minimal non-isomorphic supergroups

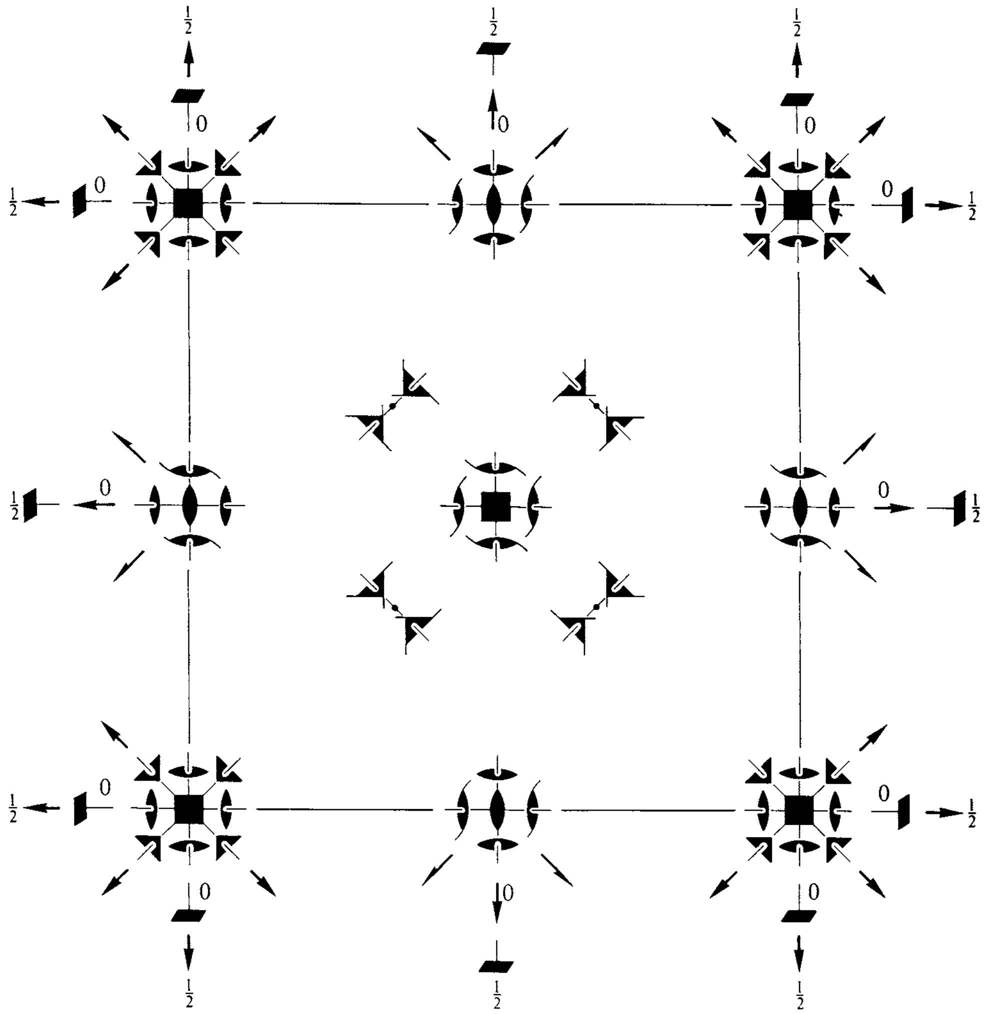
I [2] $Ia\bar{3}d$ (230)

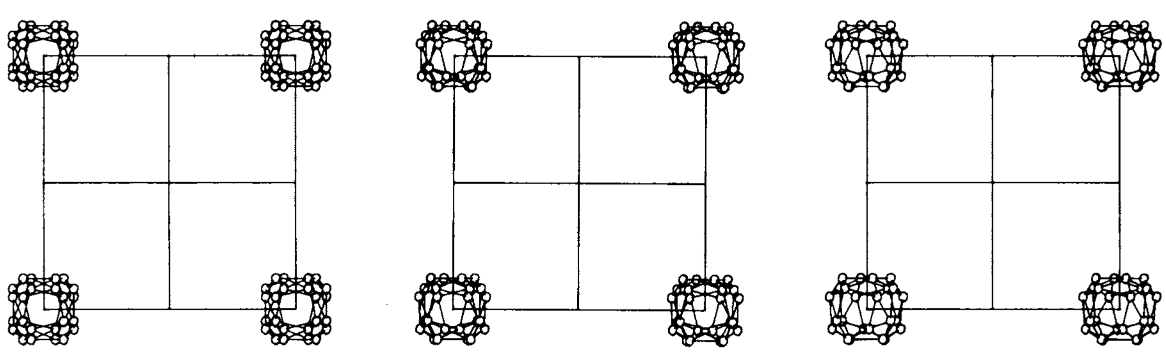
II [4] $Pm\bar{3}$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (200)

International Tables for Crystallography (2006). Vol. A, Space group 207, pp. 634–635.

$P432$ O^1 432 Cubic

No. 207 $P432$ Patterson symmetry $Pm\bar{3}m$





Origin at 432

Asymmetric unit $0 \le x \le 1$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le \min(x, 1-x)$; $z \le y$

Vertices $0,0,0$ $\quad 1,0,0$ $\quad \frac{1}{2},\frac{1}{2},0$ $\quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) $2\ \ 0,0,z$	(3) $2\ \ 0,y,0$	(4) $2\ \ x,0,0$
(5) $3^+\ \ x,x,x$	(6) $3^+\ \ \bar{x},x,\bar{x}$	(7) $3^+\ \ x,\bar{x},\bar{x}$	(8) $3^+\ \ \bar{x},\bar{x},x$
(9) $3^-\ \ x,x,x$	(10) $3^-\ \ x,\bar{x},\bar{x}$	(11) $3^-\ \ \bar{x},\bar{x},x$	(12) $3^-\ \ \bar{x},x,\bar{x}$
(13) $2\ \ x,x,0$	(14) $2\ \ x,\bar{x},0$	(15) $4^-\ \ 0,0,z$	(16) $4^+\ \ 0,0,z$
(17) $4^-\ \ x,0,0$	(18) $2\ \ 0,y,y$	(19) $2\ \ 0,y,\bar{y}$	(20) $4^+\ \ x,0,0$
(21) $4^+\ \ 0,y,0$	(22) $2\ \ x,0,x$	(23) $4^-\ \ 0,y,0$	(24) $2\ \ \bar{x},0,x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									h,k,l permutable General:
24	k	1	(1) x,y,z (5) z,x,y (9) y,z,x (13) $y,x,\bar{z}$ (17) $x,z,\bar{y}$ (21) $z,y,\bar{x}$	(2) $\bar{x},\bar{y},z$ (6) $z,\bar{x},\bar{y}$ (10) $\bar{y},z,\bar{x}$ (14) $\bar{y},\bar{x},\bar{z}$ (18) $\bar{x},z,y$ (22) $z,\bar{y},x$	(3) $\bar{x},y,\bar{z}$ (7) $\bar{z},\bar{x},y$ (11) $y,\bar{z},\bar{x}$ (15) $y,\bar{x},z$ (19) $\bar{x},\bar{z},\bar{y}$ (23) $\bar{z},y,x$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{z},x,\bar{y}$ (12) $\bar{y},\bar{z},x$ (16) $\bar{y},x,z$ (20) $x,\bar{z},y$ (24) $\bar{z},\bar{y},\bar{x}$			no conditions
									Special: no extra conditions
12	j	. . 2	$\frac{1}{2},y,y$ $\bar{y},\frac{1}{2},y$	$\frac{1}{2},\bar{y},y$ $\bar{y},\frac{1}{2},\bar{y}$	$\frac{1}{2},y,\bar{y}$ $y,y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\bar{y}$ $\bar{y},y,\frac{1}{2}$	$y,\frac{1}{2},y$ $y,\bar{y},\frac{1}{2}$	$y,\frac{1}{2},\bar{y}$ $\bar{y},\bar{y},\frac{1}{2}$	
12	i	. . 2	$0,y,y$ $\bar{y},0,y$	$0,\bar{y},y$ $\bar{y},0,\bar{y}$	$0,y,\bar{y}$ $y,y,0$	$0,\bar{y},\bar{y}$ $\bar{y},y,0$	$y,0,y$ $y,\bar{y},0$	$y,0,\bar{y}$ $\bar{y},\bar{y},0$	
12	h	2 . .	$x,\frac{1}{2},0$ $\frac{1}{2},x,0$	$\bar{x},\frac{1}{2},0$ $\frac{1}{2},\bar{x},0$	$0,x,\frac{1}{2}$ $x,0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$	$\frac{1}{2},0,x$ $0,\frac{1}{2},\bar{x}$	$\frac{1}{2},0,\bar{x}$ $0,\frac{1}{2},x$	
8	g	. 3 .	x,x,x $x,x,\bar{x}$	$\bar{x},\bar{x},x$ $\bar{x},\bar{x},\bar{x}$	$\bar{x},x,\bar{x}$ $x,\bar{x},x$	$x,\bar{x},\bar{x}$ $\bar{x},x,x$			
6	f	4 . .	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$	
6	e	4 . .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	
3	d	4 2 . 2	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$				
3	c	4 2 . 2	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$				
1	b	4 3 2	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						
1	a	4 3 2	$0,0,0$						

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [111] $p3m1$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P231$ ($P23$, 195)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[3] $P412$ ($P422$, 89)	1; 2; 3; 4; 13; 14; 15; 16
	[3] $P412$ ($P422$, 89)	1; 2; 3; 4; 17; 18; 19; 20
	[3] $P412$ ($P422$, 89)	1; 2; 3; 4; 21; 22; 23; 24
	[4] $P132$ ($R32$, 155)	1; 5; 9; 14; 19; 24
	[4] $P132$ ($R32$, 155)	1; 6; 12; 13; 18; 24
	[4] $P132$ ($R32$, 155)	1; 7; 10; 13; 19; 22
	[4] $P132$ ($R32$, 155)	1; 8; 11; 14; 18; 22

IIa none

IIb [2] $F432$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (209); [4] $I432$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (211)

Maximal isomorphic subgroups of lowest index

IIc [27] $P432$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (207)

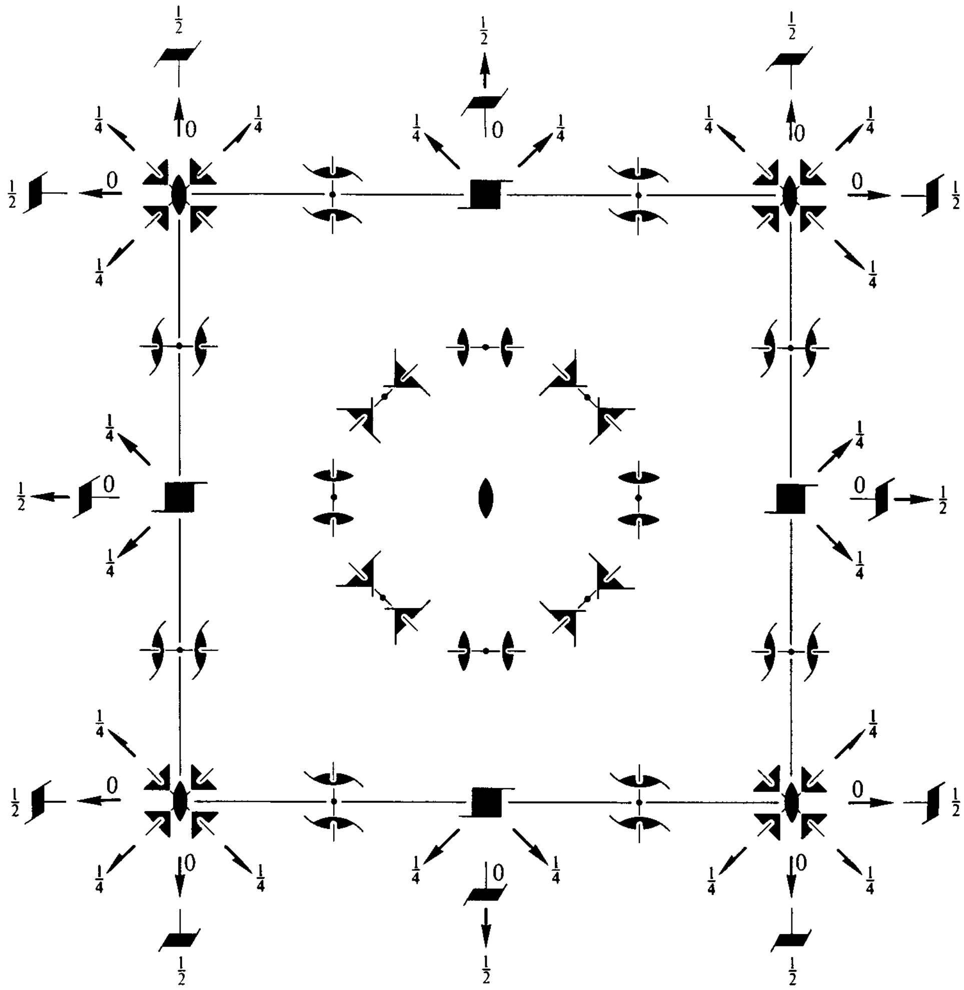
Minimal non-isomorphic supergroups

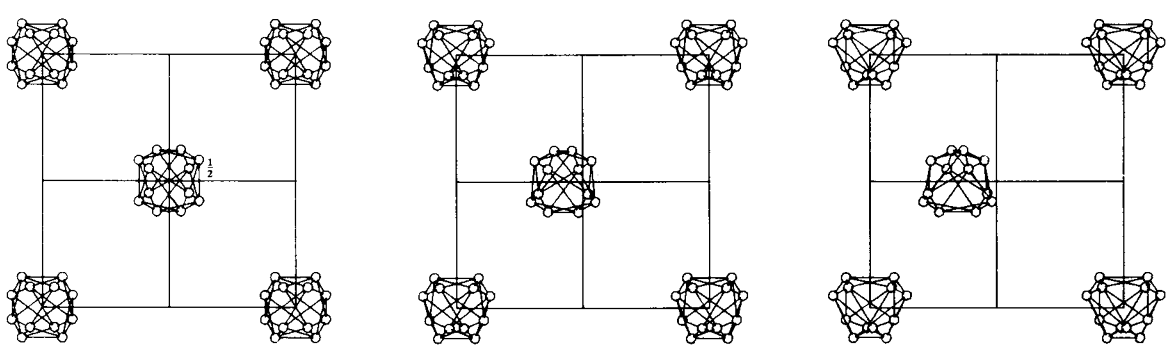
I [2] $Pm\bar{3}m$ (221); [2] $Pn\bar{3}n$ (222)

II [2] $I432$ (211); [4] $F432$ (209)

International Tables for Crystallography (2006). Vol. A, Space group 208, pp. 636–638.

$P4_232$	O^2	432	Cubic
No. 208	$P4_232$		Patterson symmetry $Pm\bar{3}m$





Origin at 23

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $-\frac{1}{4} \le z \le \frac{1}{4}$; $\max(-x, x-\frac{1}{2}, -y, y-\frac{1}{2}) \le z \le \min(x, \frac{1}{2}-x, y, \frac{1}{2}-y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\;\; 0,0,z$	(3) $2\;\; 0,y,0$	(4) $2\;\; x,0,0$
(5) $3^+\;\; x,x,x$	(6) $3^+\;\; \bar{x},x,\bar{x}$	(7) $3^+\;\; x,\bar{x},\bar{x}$	(8) $3^+\;\; \bar{x},\bar{x},x$
(9) $3^-\;\; x,x,x$	(10) $3^-\;\; x,\bar{x},\bar{x}$	(11) $3^-\;\; \bar{x},\bar{x},x$	(12) $3^-\;\; \bar{x},x,\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\;\; x,x,\frac{1}{4}$	(14) $2\;\; x,\bar{x}+\frac{1}{2},\frac{1}{4}$	(15) $4^-(0,0,\frac{1}{2})\;\; \frac{1}{2},0,z$	(16) $4^+(0,0,\frac{1}{2})\;\; 0,\frac{1}{2},z$
(17) $4^-(\frac{1}{2},0,0)\;\; x,\frac{1}{2},0$	(18) $2(0,\frac{1}{2},\frac{1}{2})\;\; \frac{1}{4},y,y$	(19) $2\;\; \frac{1}{4},y+\frac{1}{2},\bar{y}$	(20) $4^+(\frac{1}{2},0,0)\;\; x,0,\frac{1}{2}$
(21) $4^+(0,\frac{1}{2},0)\;\; \frac{1}{2},y,0$	(22) $2(\frac{1}{2},0,\frac{1}{2})\;\; x,\frac{1}{4},x$	(23) $4^-(0,\frac{1}{2},0)\;\; 0,y,\frac{1}{2}$	(24) $2\;\; \bar{x}+\frac{1}{2},\frac{1}{4},x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	Reflection conditions
				h,k,l permutable General:
24	m	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}$ (4) $x,\bar{y},\bar{z}$ (5) z,x,y (6) $z,\bar{x},\bar{y}$ (7) $\bar{z},\bar{x},y$ (8) $\bar{z},x,\bar{y}$ (9) y,z,x (10) $\bar{y},z,\bar{x}$ (11) $y,\bar{z},\bar{x}$ (12) $\bar{y},\bar{z},x$ (13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ (17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$ (18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$ (19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$ (20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$ (21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$ (22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$ (23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$ (24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$h00$: $h=2n$
				Special: as above, plus
12	l	..2	$\frac{1}{4},y,y+\frac{1}{2}$ $\frac{3}{4},\bar{y},y+\frac{1}{2}$ $\frac{3}{4},y,\bar{y}+\frac{1}{2}$ $\frac{1}{4},\bar{y},\bar{y}+\frac{1}{2}$ $y+\frac{1}{2},\frac{1}{4},y$ $y+\frac{1}{2},\frac{3}{4},\bar{y}$ $\bar{y}+\frac{1}{2},\frac{3}{4},y$ $\bar{y}+\frac{1}{2},\frac{1}{4},\bar{y}$ $y,y+\frac{1}{2},\frac{1}{4}$ $\bar{y},y+\frac{1}{2},\frac{3}{4}$ $y,\bar{y}+\frac{1}{2},\frac{3}{4}$ $\bar{y},\bar{y}+\frac{1}{2},\frac{1}{4}$	no extra conditions
12	k	..2	$\frac{1}{4},y,\bar{y}+\frac{1}{2}$ $\frac{3}{4},\bar{y},\bar{y}+\frac{1}{2}$ $\frac{3}{4},y,y+\frac{1}{2}$ $\frac{1}{4},\bar{y},y+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{1}{4},y$ $\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}$ $y+\frac{1}{2},\frac{3}{4},y$ $y+\frac{1}{2},\frac{1}{4},\bar{y}$ $y,\bar{y}+\frac{1}{2},\frac{1}{4}$ $\bar{y},\bar{y}+\frac{1}{2},\frac{3}{4}$ $y,y+\frac{1}{2},\frac{3}{4}$ $\bar{y},y+\frac{1}{2},\frac{1}{4}$	no extra conditions
12	j	2..	$x,\frac{1}{2},0$ $\bar{x},\frac{1}{2},0$ $0,x,\frac{1}{2}$ $0,\bar{x},\frac{1}{2}$ $\frac{1}{2},0,x$ $\frac{1}{2},0,\bar{x}$ $0,x+\frac{1}{2},\frac{1}{2}$ $0,\bar{x}+\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},\frac{1}{2},0$ $\bar{x}+\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},0,\bar{x}+\frac{1}{2}$ $\frac{1}{2},0,x+\frac{1}{2}$	hkl : $h=2n$ hhl : $l=2n$
12	i	2..	$x,0,\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$ $\frac{1}{2},x,0$ $\frac{1}{2},\bar{x},0$ $0,\frac{1}{2},x$ $0,\frac{1}{2},\bar{x}$ $\frac{1}{2},x+\frac{1}{2},0$ $\frac{1}{2},\bar{x}+\frac{1}{2},0$ $x+\frac{1}{2},0,\frac{1}{2}$ $\bar{x}+\frac{1}{2},0,\frac{1}{2}$ $0,\frac{1}{2},\bar{x}+\frac{1}{2}$ $0,\frac{1}{2},x+\frac{1}{2}$	hkl : $h=2n$ hhl : $l=2n$
12	h	2..	$x,0,0$ $\bar{x},0,0$ $0,x,0$ $0,\bar{x},0$ $0,0,x$ $0,0,\bar{x}$ $\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$	hkl : $h+k+l=2n$
8	g	.3.	x,x,x $\bar{x},\bar{x},x$ $\bar{x},x,\bar{x}$ $x,\bar{x},\bar{x}$ $x+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	$0kl$: $k+l=2n$
6	f	2.22	$\frac{1}{4},\frac{1}{2},0$ $\frac{3}{4},\frac{1}{2},0$ $0,\frac{1}{4},\frac{1}{2}$ $0,\frac{3}{4},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{4}$ $\frac{1}{2},0,\frac{3}{4}$	hkl : $h+k+l=2n$ or $h=2n+1, k=4n$ and $l=4n+2$
6	e	2.22	$\frac{1}{4},0,\frac{1}{2}$ $\frac{3}{4},0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{4},0$ $\frac{1}{2},\frac{3}{4},0$ $0,\frac{1}{2},\frac{1}{4}$ $0,\frac{1}{2},\frac{3}{4}$	
6	d	222..	$0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{2},0,0$ $0,0,\frac{1}{2}$	hkl : $h+k+l=2n$
4	c	.32	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$ $\frac{1}{4},\frac{1}{4},\frac{3}{4}$ $\frac{1}{4},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\frac{1}{4},\frac{1}{4}$	hkl : $h+k,h+l,k+l=2n$
4	b	.32	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\frac{1}{4},\frac{3}{4}$ $\frac{1}{4},\frac{3}{4},\frac{3}{4}$	hkl : $h+k,h+l,k+l=2n$
2	a	23.	$0,0,0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,\frac{1}{2},z$

Along [111] $p3m1$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{1}{4}$

Maximal non-isomorphic subgroups

I	[2] $P231$ ($P23$, 195)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[3] $P4_2 12$ ($P4_2 22$, 93)	1; 2; 3; 4; 13; 14; 15; 16
	[3] $P4_2 12$ ($P4_2 22$, 93)	1; 2; 3; 4; 17; 18; 19; 20
	[3] $P4_2 12$ ($P4_2 22$, 93)	1; 2; 3; 4; 21; 22; 23; 24
	[4] $P132$ ($R32$, 155)	1; 5; 9; 14; 19; 24
	[4] $P132$ ($R32$, 155)	1; 6; 12; 13; 18; 24
	[4] $P132$ ($R32$, 155)	1; 7; 10; 13; 19; 22
	[4] $P132$ ($R32$, 155)	1; 8; 11; 14; 18; 22

IIa none

IIb [2] $F4_1 32$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (210); [4] $I4_1 32$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (214)

Maximal isomorphic subgroups of lowest index

IIc [27] $P4_2 32$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (208)

Minimal non-isomorphic supergroups

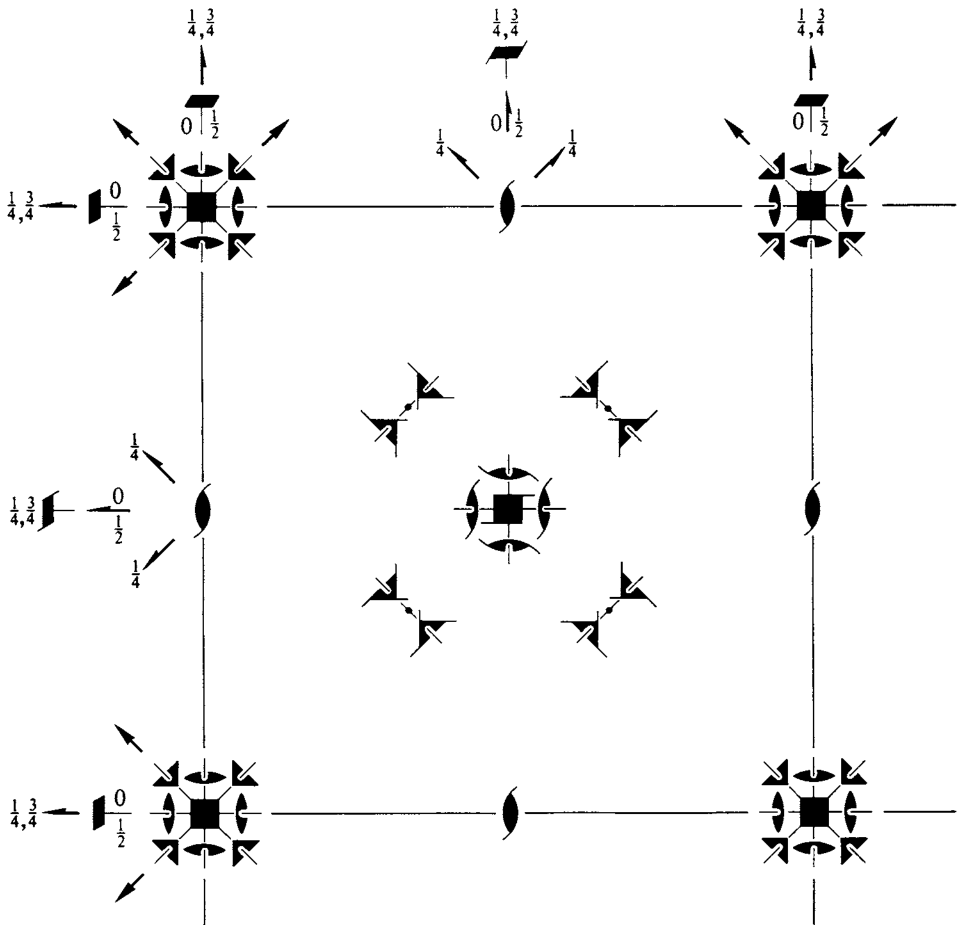
I [2] $Pm\bar{3}n$ (223); [2] $Pn\bar{3}m$ (224)

II [2] $I432$ (211); [4] $F432$ (209)

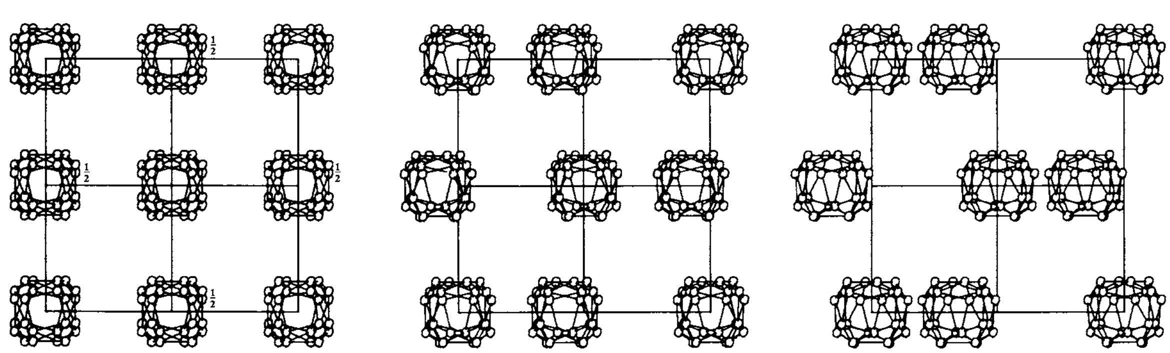
International Tables for Crystallography (2006). Vol. A, Space group 209, pp. 639–641.

$F432$ O^3 432   Cubic

No. 209 $F432$ Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Origin at 432

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{4};\quad -\frac{1}{4} \le z \le \frac{1}{4};\quad y \le \min(x, \frac{1}{2}-x);\quad -y \le z \le y$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{4},\frac{1}{4},\frac{1}{4} \quad \frac{1}{4},\frac{1}{4},-\frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $3^+\quad x,x,x$	(6) $3^+\quad \bar{x},x,\bar{x}$	(7) $3^+\quad x,\bar{x},\bar{x}$	(8) $3^+\quad \bar{x},\bar{x},x$
(9) $3^-\quad x,x,x$	(10) $3^-\quad x,\bar{x},\bar{x}$	(11) $3^-\quad \bar{x},\bar{x},x$	(12) $3^-\quad \bar{x},x,\bar{x}$
(13) $2\quad x,x,0$	(14) $2\quad x,\bar{x},0$	(15) $4^-\quad 0,0,z$	(16) $4^+\quad 0,0,z$
(17) $4^-\quad x,0,0$	(18) $2\quad 0,y,y$	(19) $2\quad 0,y,\bar{y}$	(20) $4^+\quad x,0,0$
(21) $4^+\quad 0,y,0$	(22) $2\quad x,0,x$	(23) $4^-\quad 0,y,0$	(24) $2\quad \bar{x},0,x$

Symmetry operations *(continued)*

For $(0,\frac12,\frac12)+$ set

(1) $t(0,\frac12,\frac12)$	(2) $2(0,0,\frac12)\quad 0,\frac14,z$	(3) $2(0,\frac12,0)\quad 0,y,\frac14$	(4) $2\quad x,\frac14,\frac14$
(5) $3^{+}(\frac13,\frac13,\frac13)\quad x-\frac13,x-\frac16,x$	(6) $3^{+}\quad \bar{x},x+\frac12,\bar{x}$	(7) $3^{+}(-\frac13,\frac13,\frac13)\quad x+\frac13,\bar{x}-\frac16,\bar{x}$	(8) $3^{+}\quad \bar{x},\bar{x}+\frac12,x$
(9) $3^{-}(\frac13,\frac13,\frac13)\quad x-\frac16,x+\frac16,x$	(10) $3^{-}(-\frac13,\frac13,\frac13)\quad x+\frac16,\bar{x}+\frac16,\bar{x}$	(11) $3^{-}\quad \bar{x}+\frac12,\bar{x}+\frac12,x$	(12) $3^{-}\quad \bar{x}-\frac12,x+\frac12,\bar{x}$
(13) $2(\frac14,\frac14,0)\quad x,x+\frac14,\frac14$	(14) $2(-\frac14,\frac14,0)\quad x,\bar{x}+\frac14,\frac14$	(15) $4^{-}(0,0,\frac12)\quad \frac14,\frac14,z$	(16) $4^{+}(0,0,\frac12)\quad -\frac14,\frac14,z$
(17) $4^{-}\quad x,\frac12,0$	(18) $2(0,\frac12,\frac12)\quad 0,y,y$	(19) $2\quad 0,y+\frac12,\bar{y}$	(20) $4^{+}\quad x,0,\frac12$
(21) $4^{+}(0,\frac12,0)\quad \frac14,y,\frac14$	(22) $2(\frac14,0,\frac14)\quad x-\frac14,\frac14,x$	(23) $4^{-}(0,\frac12,0)\quad -\frac14,y,\frac14$	(24) $2(-\frac14,0,\frac14)\quad \bar{x}+\frac14,\frac14,x$

For $(\frac12,0,\frac12)+$ set

(1) $t(\frac12,0,\frac12)$	(2) $2(0,0,\frac12)\quad \frac14,0,z$	(3) $2\quad \frac14,y,\frac14$	(4) $2(\frac12,0,0)\quad x,0,\frac14$
(5) $3^{+}(\frac13,\frac13,\frac13)\quad x+\frac16,x-\frac16,x$	(6) $3^{+}(\frac13,-\frac13,\frac13)\quad \bar{x}+\frac16,x+\frac16,\bar{x}$	(7) $3^{+}\quad x+\frac12,\bar{x}-\frac12,\bar{x}$	(8) $3^{+}\quad \bar{x}+\frac12,\bar{x}+\frac12,x$
(9) $3^{-}(\frac13,\frac13,\frac13)\quad x-\frac16,x-\frac13,x$	(10) $3^{-}\quad x+\frac12,\bar{x},\bar{x}$	(11) $3^{-}\quad \bar{x}+\frac12,\bar{x},x$	(12) $3^{-}(\frac13,-\frac13,\frac13)\quad \bar{x}-\frac16,x+\frac13,\bar{x}$
(13) $2(\frac14,\frac14,0)\quad x,x-\frac14,\frac14$	(14) $2(\frac14,-\frac14,0)\quad x,\bar{x}+\frac14,\frac14$	(15) $4^{-}(0,0,\frac12)\quad \frac14,-\frac14,z$	(16) $4^{+}(0,0,\frac12)\quad \frac14,\frac14,z$
(17) $4^{-}(\frac12,0,0)\quad x,\frac14,\frac14$	(18) $2(0,\frac14,\frac14)\quad \frac14,y-\frac14,y$	(19) $2(0,-\frac14,\frac14)\quad \frac14,y+\frac14,\bar{y}$	(20) $4^{+}(\frac12,0,0)\quad x,-\frac14,\frac14$
(21) $4^{+}\quad \frac12,y,0$	(22) $2(\frac12,0,\frac12)\quad x,0,x$	(23) $4^{-}\quad 0,y,\frac12$	(24) $2\quad \bar{x}+\frac12,0,x$

For $(\frac12,\frac12,0)+$ set

(1) $t(\frac12,\frac12,0)$	(2) $2\quad \frac14,\frac14,z$	(3) $2(0,\frac12,0)\quad \frac14,y,0$	(4) $2(\frac12,0,0)\quad x,\frac14,0$
(5) $3^{+}(\frac13,\frac13,\frac13)\quad x+\frac16,x+\frac13,x$	(6) $3^{+}\quad \bar{x}+\frac12,x,\bar{x}$	(7) $3^{+}\quad x+\frac12,\bar{x},\bar{x}$	(8) $3^{+}(\frac13,\frac13,-\frac13)\quad \bar{x}+\frac16,\bar{x}+\frac13,x$
(9) $3^{-}(\frac13,\frac13,\frac13)\quad x+\frac13,x+\frac16,x$	(10) $3^{-}\quad x,\bar{x}+\frac12,\bar{x}$	(11) $3^{-}(\frac13,\frac13,-\frac13)\quad \bar{x}+\frac13,\bar{x}+\frac16,x$	(12) $3^{-}\quad \bar{x},x+\frac12,\bar{x}$
(13) $2(\frac12,\frac12,0)\quad x,x,0$	(14) $2\quad x,\bar{x}+\frac12,0$	(15) $4^{-}\quad \frac12,0,z$	(16) $4^{+}\quad 0,\frac12,z$
(17) $4^{-}(\frac12,0,0)\quad x,\frac14,-\frac14$	(18) $2(0,\frac14,\frac14)\quad \frac14,y+\frac14,y$	(19) $2(0,\frac14,-\frac14)\quad \frac14,y+\frac14,\bar{y}$	(20) $4^{+}(\frac12,0,0)\quad x,\frac14,\frac14$
(21) $4^{+}(0,\frac12,0)\quad \frac14,y,-\frac14$	(22) $2(\frac14,0,\frac14)\quad x+\frac14,\frac14,x$	(23) $4^{-}(0,\frac12,0)\quad \frac14,y,\frac14$	(24) $2(\frac14,0,-\frac14)\quad \bar{x}+\frac14,\frac14,x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac12,\frac12)$; $t(\frac12,0,\frac12)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(0,\frac12,\frac12)+\quad(\frac12,0,\frac12)+\quad(\frac12,\frac12,0)+$						Reflection conditions h,k,l permutable
									General:
96	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			hkl : $h+k,h+l,k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			hhl : $h+l=2n$
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$			$h00$: $h=2n$
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$			
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$			
									Special: as above, plus
48	i	2 . .	$x,\frac14,\frac14$	$\bar{x},\frac34,\frac14$	$\frac14,x,\frac14$	$\frac14,\bar{x},\frac34$	$\frac14,\frac14,x$	$\frac34,\frac14,\bar{x}$	hkl : $h=2n$
			$\frac14,x,\frac34$	$\frac34,\bar{x},\frac34$	$x,\frac14,\frac34$	$\bar{x},\frac14,\frac14$	$\frac14,\frac14,\bar{x}$	$\frac14,\frac34,x$	
48	h	. . 2	$\frac12,y,y$	$\frac12,\bar{y},y$	$\frac12,y,\bar{y}$	$\frac12,\bar{y},\bar{y}$	$y,\frac12,y$	$y,\frac12,\bar{y}$	no extra conditions
			$\bar{y},\frac12,y$	$\bar{y},\frac12,\bar{y}$	$y,y,\frac12$	$\bar{y},y,\frac12$	$y,\bar{y},\frac12$	$\bar{y},\bar{y},\frac12$	
48	g	. . 2	$0,y,y$	$0,\bar{y},y$	$0,y,\bar{y}$	$0,\bar{y},\bar{y}$	$y,0,y$	$y,0,\bar{y}$	no extra conditions
			$\bar{y},0,y$	$\bar{y},0,\bar{y}$	$y,y,0$	$\bar{y},y,0$	$y,\bar{y},0$	$\bar{y},\bar{y},0$	
32	f	. 3 .	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			no extra conditions
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$			
24	e	4 . .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	no extra conditions
24	d	2 . 22	$0,\frac14,\frac14$	$0,\frac34,\frac14$	$\frac14,0,\frac14$	$\frac14,0,\frac34$	$\frac14,\frac14,0$	$\frac34,\frac14,0$	hkl : $h=2n$
8	c	2 3 .	$\frac14,\frac14,\frac14$	$\frac14,\frac14,\frac34$					hkl : $h=2n$
4	b	4 3 2	$\frac12,\frac12,\frac12$						no extra conditions
4	a	4 3 2	$0,0,0$						no extra conditions

(*Continued on page 639*)

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(*from page* 641)

Symmetry of special projections

Along [001] $p\,4\,m\,m$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [111] $p\,3\,m\,1$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c\,2\,m\,m$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $F\,2\,3\,1$ ($F\,2\,3$, 196) (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
[3] $F\,4\,1\,2$ ($I\,4\,2\,2$, 97) (1; 2; 3; 4; 13; 14; 15; 16)+
[3] $F\,4\,1\,2$ ($I\,4\,2\,2$, 97) (1; 2; 3; 4; 17; 18; 19; 20)+
[3] $F\,4\,1\,2$ ($I\,4\,2\,2$, 97) (1; 2; 3; 4; 21; 22; 23; 24)+
[4] $F\,1\,3\,2$ ($R\,3\,2$, 155) (1; 5; 9; 14; 19; 24)+
[4] $F\,1\,3\,2$ ($R\,3\,2$, 155) (1; 6; 12; 13; 18; 24)+
[4] $F\,1\,3\,2$ ($R\,3\,2$, 155) (1; 7; 10; 13; 19; 22)+
[4] $F\,1\,3\,2$ ($R\,3\,2$, 155) (1; 8; 11; 14; 18; 22)+

IIa [4] $P\,4_2\,3\,2$ (208) 1; 5; 9; 14; 19; 24; (4; 6; 11; 16; 18; 23) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 8; 10; 15; 20; 22) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 7; 12; 13; 17; 21) + $(\frac{1}{2},\frac{1}{2},0)$
[4] $P\,4_2\,3\,2$ (208) 1; 6; 12; 13; 18; 24; (4; 5; 10; 15; 19; 23) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 7; 11; 16; 17; 22) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 8; 9; 14; 20; 21) + $(\frac{1}{2},\frac{1}{2},0)$
[4] $P\,4_2\,3\,2$ (208) 1; 7; 10; 13; 19; 22; (4; 8; 12; 15; 18; 21) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 6; 9; 16; 20; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 5; 11; 14; 17; 23) + $(\frac{1}{2},\frac{1}{2},0)$
[4] $P\,4_2\,3\,2$ (208) 1; 8; 11; 14; 18; 22; (4; 7; 9; 16; 19; 21) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 5; 12; 15; 17; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 6; 10; 13; 20; 23) + $(\frac{1}{2},\frac{1}{2},0)$
[4] $P\,4\,3\,2$ (207) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
[4] $P\,4\,3\,2$ (207) 1; 2; 3; 4; 13; 14; 15; 16; (9; 10; 11; 12; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (5; 6; 7; 8; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$
[4] $P\,4\,3\,2$ (207) 1; 2; 3; 4; 17; 18; 19; 20; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$
[4] $P\,4\,3\,2$ (207) 1; 2; 3; 4; 21; 22; 23; 24; (5; 6; 7; 8; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $F\,4\,3\,2$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (209)

Minimal non-isomorphic supergroups

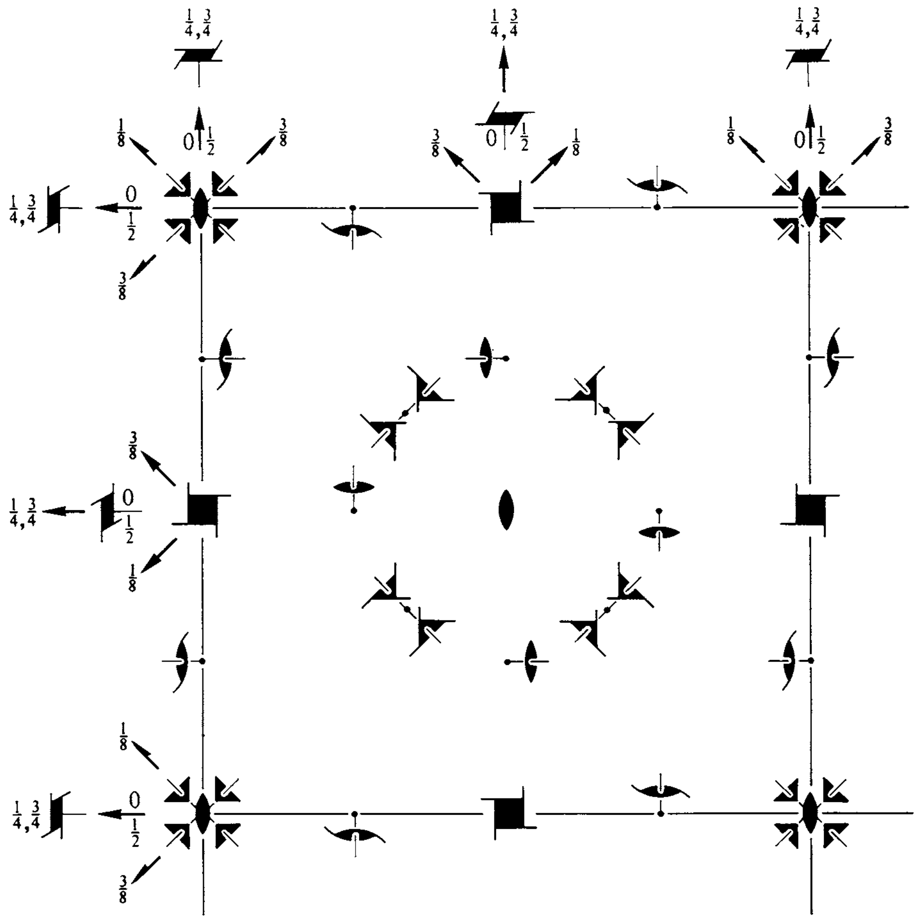
I [2] $F\,m\,\bar{3}\,m$ (225); [2] $F\,m\,\bar{3}\,c$ (226)

II [2] $P\,4\,3\,2$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (207)

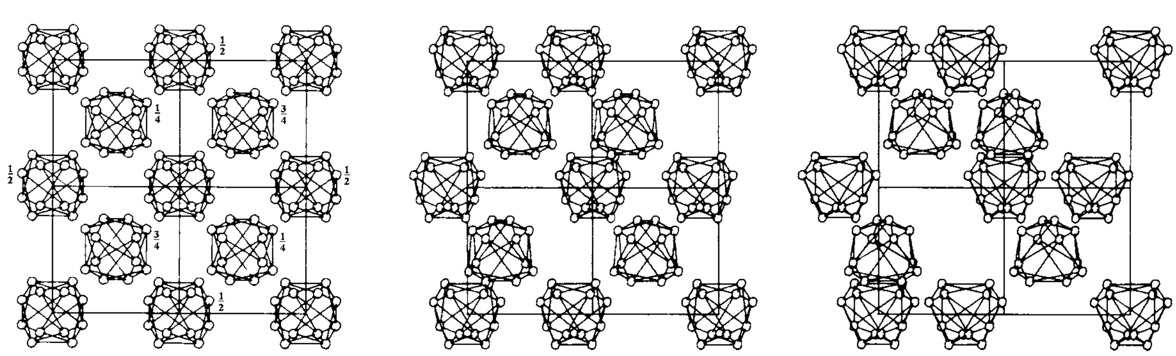
International Tables for Crystallography (2006). Vol. A, Space group 210, pp. 642–644.

$F4_132$ O^4 432 Cubic

No. 210 $F4_132$ Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Origin at 23

Asymmetric unit $0 \le x \le \frac{1}{2}$; $-\frac{1}{8} \le y \le \frac{1}{8}$; $-\frac{1}{8} \le z \le \frac{1}{8}$; $y \le \min(x, \frac{1}{2}-x)$; $-y \le z \le \min(x, \frac{1}{2}-x)$

Vertices $0,0,0$ $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $\frac{1}{8},\frac{1}{8},-\frac{1}{8}$ $\frac{1}{8},-\frac{1}{8},\frac{1}{8}$

$\frac{1}{2},0,0$ $\frac{3}{8},\frac{1}{8},\frac{1}{8}$ $\frac{3}{8},\frac{1}{8},-\frac{1}{8}$ $\frac{3}{8},-\frac{1}{8},\frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$
(5) 3^+ x,x,x	(6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$	(7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$	(8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x}+\frac{1}{2},\bar{x}$	(11) 3^- $\bar{x}+\frac{1}{2},\bar{x},x$	(12) 3^- $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{3}{8}$	(14) 2 $x,\bar{x}+\frac{1}{4},\frac{1}{8}$	(15) $4^-(0,0,\frac{3}{4})$ $\frac{1}{2},\frac{1}{4},z$	(16) $4^+(0,0,\frac{1}{4})$ $0,\frac{3}{4},z$
(17) $4^-(\frac{3}{4},0,0)$ $x,\frac{1}{2},\frac{1}{4}$	(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{3}{8},y+\frac{1}{4},y$	(19) 2 $\frac{1}{8},y+\frac{1}{4},\bar{y}$	(20) $4^+(\frac{1}{4},0,0)$ $x,0,\frac{3}{4}$
(21) $4^+(0,\frac{1}{4},0)$ $\frac{3}{4},y,0$	(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x-\frac{1}{4},\frac{3}{8},x$	(23) $4^-(0,\frac{3}{4},0)$ $\frac{1}{4},y,\frac{1}{2}$	(24) 2 $\bar{x}+\frac{1}{4},\frac{1}{8},x$

Symmetry operations *(continued)*

For $(0,\frac12,\frac12)+$ set

(1) $t(0,\frac12,\frac12)$	(2) $2\ \ 0,0,z$	(3) $2\ \ \frac14,y,\frac14$	(4) $2(\frac12,0,0)\ \ x,\frac14,0$
(5) $3^+(\frac13,\frac13,\frac13)\ \ x-\frac13,x-\frac16,x$	(6) $3^+\ \ \bar{x}+\frac12,x,\bar{x}$	(7) $3^+\ \ x,\bar{x},\bar{x}$	(8) $3^+\ \ \bar{x}+\frac12,\bar{x}+\frac12,x$
(9) $3^-(\frac13,\frac13,\frac13)\ \ x-\frac16,x+\frac16,x$	(10) $3^-\ \ x+\frac12,\bar{x},\bar{x}$	(11) $3^-(\frac13,\frac13,-\frac13)\ \ \bar{x}+\frac13,\bar{x}+\frac16,x$	(12) $3^-\ \ \bar{x},x,\bar{x}$
(13) $2(\frac34,\frac34,0)\ \ x,x,\frac18$	(14) $2(-\frac14,\frac14,0)\ \ x,\bar{x}+\frac12,\frac38$	(15) $4^-(0,0,\frac14)\ \ \frac14,0,z$	(16) $4^+(0,0,\frac34)\ \ \frac14,\frac12,z$
(17) $4^-(\frac34,0,0)\ \ x,\frac12,-\frac14$	(18) $2(0,\frac12,\frac12)\ \ \frac38,y-\frac14,y$	(19) $2\ \ \frac18,y+\frac34,\bar{y}$	(20) $4^+(\frac14,0,0)\ \ x,0,\frac14$
(21) $4^+(0,\frac34,0)\ \ \frac12,y,-\frac14$	(22) $2(\frac14,0,\frac14)\ \ x,\frac18,x$	(23) $4^-(0,\frac14,0)\ \ 0,y,\frac34$	(24) $2(-\frac14,0,\frac14)\ \ \bar{x}+\frac12,\frac38,x$

For $(\frac12,0,\frac12)+$ set

(1) $t(\frac12,0,\frac12)$	(2) $2\ \ \frac14,\frac14,z$	(3) $2(0,\frac12,0)\ \ 0,y,\frac14$	(4) $2\ \ x,0,0$
(5) $3^+(\frac13,\frac13,\frac13)\ \ x+\frac16,x-\frac16,x$	(6) $3^+\ \ \bar{x},x,\bar{x}$	(7) $3^+\ \ x+\frac12,\bar{x},\bar{x}$	(8) $3^+\ \ \bar{x},\bar{x}+\frac12,x$
(9) $3^-(\frac13,\frac13,\frac13)\ \ x-\frac16,x-\frac13,x$	(10) $3^-(-\frac13,\frac13,\frac13)\ \ x+\frac16,\bar{x}+\frac16,\bar{x}$	(11) $3^-\ \ \bar{x},\bar{x},x$	(12) $3^-\ \ \bar{x},x+\frac12,\bar{x}$
(13) $2(\frac14,\frac14,0)\ \ x,x,\frac18$	(14) $2(\frac14,-\frac14,0)\ \ x,\bar{x}+\frac12,\frac38$	(15) $4^-(0,0,\frac14)\ \ \frac34,0,z$	(16) $4^+(0,0,\frac34)\ \ -\frac14,\frac12,z$
(17) $4^-(\frac14,0,0)\ \ x,\frac14,0$	(18) $2(0,\frac34,\frac34)\ \ \frac18,y,y$	(19) $2(0,-\frac14,\frac14)\ \ \frac38,y+\frac12,\bar{y}$	(20) $4^+(\frac34,0,0)\ \ x,\frac14,\frac12$
(21) $4^+(0,\frac14,0)\ \ \frac14,y,0$	(22) $2(\frac12,0,\frac12)\ \ x+\frac14,\frac38,x$	(23) $4^-(0,\frac34,0)\ \ -\frac14,y,\frac12$	(24) $2\ \ \bar{x}+\frac34,\frac18,x$

For $(\frac12,\frac12,0)+$ set

(1) $t(\frac12,\frac12,0)$	(2) $2(0,0,\frac12)\ \ \frac14,0,z$	(3) $2\ \ 0,y,0$	(4) $2\ \ x,\frac14,\frac14$
(5) $3^+(\frac13,\frac13,\frac13)\ \ x+\frac16,x+\frac13,x$	(6) $3^+\ \ \bar{x},x+\frac12,\bar{x}$	(7) $3^+\ \ x+\frac12,\bar{x}-\frac12,\bar{x}$	(8) $3^+\ \ \bar{x},\bar{x},x$
(9) $3^-(\frac13,\frac13,\frac13)\ \ x+\frac13,x+\frac16,x$	(10) $3^-\ \ x,\bar{x},\bar{x}$	(11) $3^-\ \ \bar{x}+\frac12,\bar{x}+\frac12,x$	(12) $3^-(\frac13,-\frac13,\frac13)\ \ \bar{x}-\frac16,x+\frac13,\bar{x}$
(13) $2(\frac12,\frac12,0)\ \ x,x+\frac14,\frac38$	(14) $2\ \ x,\bar{x}+\frac34,\frac18$	(15) $4^-(0,0,\frac34)\ \ \frac12,-\frac14,z$	(16) $4^+(0,0,\frac14)\ \ 0,\frac14,z$
(17) $4^-(\frac14,0,0)\ \ x,\frac34,0$	(18) $2(0,\frac14,\frac14)\ \ \frac18,y,y$	(19) $2(0,\frac14,-\frac14)\ \ \frac38,y+\frac12,\bar{y}$	(20) $4^+(\frac34,0,0)\ \ x,-\frac14,\frac12$
(21) $4^+(0,\frac34,0)\ \ \frac12,y,\frac14$	(22) $2(\frac34,0,\frac34)\ \ x,\frac18,x$	(23) $4^-(0,\frac14,0)\ \ 0,y,\frac14$	(24) $2(\frac14,0,-\frac14)\ \ \bar{x}+\frac12,\frac38,x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac12,\frac12)$; $t(\frac12,0,\frac12)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(0,\frac12,\frac12)+\quad(\frac12,0,\frac12)+\quad(\frac12,\frac12,0)+$						Reflection conditions h,k,l permutable
									General:
96	h	1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac12,z+\frac12$	(3) $\bar{x}+\frac12,y+\frac12,\bar{z}$	(4) $x+\frac12,\bar{y},\bar{z}+\frac12$			hkl : $h+k=2n$ and $h+l,k+l=2n$
			(5) z,x,y	(6) $z+\frac12,\bar{x},\bar{y}+\frac12$	(7) $\bar{z},\bar{x}+\frac12,y+\frac12$	(8) $\bar{z}+\frac12,x+\frac12,\bar{y}$			$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y}+\frac12,z+\frac12,\bar{x}$	(11) $y+\frac12,\bar{z},\bar{x}+\frac12$	(12) $\bar{y},\bar{z}+\frac12,x+\frac12$			hhl : $h+l=2n$
			(13) $y+\frac34,x+\frac14,\bar{z}+\frac34$	(14) $\bar{y}+\frac14,\bar{x}+\frac14,\bar{z}+\frac14$	(15) $y+\frac14,\bar{x}+\frac34,z+\frac34$	(16) $\bar{y}+\frac34,x+\frac34,z+\frac14$			$h00$: $h=4n$
			(17) $x+\frac34,z+\frac14,\bar{y}+\frac34$	(18) $\bar{x}+\frac34,z+\frac34,y+\frac14$	(19) $\bar{x}+\frac14,\bar{z}+\frac14,\bar{y}+\frac14$	(20) $x+\frac14,\bar{z}+\frac34,y+\frac34$			
			(21) $z+\frac34,y+\frac14,\bar{x}+\frac34$	(22) $z+\frac14,\bar{y}+\frac34,x+\frac34$	(23) $\bar{z}+\frac34,y+\frac34,x+\frac14$	(24) $\bar{z}+\frac14,\bar{y}+\frac14,\bar{x}+\frac14$			
									Special: as above, plus
48	g	..2	$\frac18,y,\bar{y}+\frac14$	$\frac78,\bar{y}+\frac12,\bar{y}+\frac34$	$\frac38,y+\frac12,y+\frac34$	$\frac58,\bar{y},y+\frac14$			no extra conditions
			$\bar{y}+\frac14,\frac18,y$	$\bar{y}+\frac34,\frac78,\bar{y}+\frac12$	$y+\frac34,\frac38,y+\frac12$	$y+\frac14,\frac58,\bar{y}$			
			$y,\bar{y}+\frac14,\frac18$	$\bar{y}+\frac12,\bar{y}+\frac34,\frac78$	$y+\frac12,y+\frac34,\frac38$	$\bar{y},y+\frac14,\frac58$			
48	f	2..	$x,0,0$	$\bar{x},\frac12,\frac12$	$0,x,0$	$\frac12,\bar{x},\frac12$	$0,0,x$	$\frac12,\frac12,\bar{x}$	hkl : $h=2n+1$ or $h+k+l=4n$
			$\frac34,x+\frac14,\frac34$	$\frac14,\bar{x}+\frac14,\frac14$	$x+\frac34,\frac14,\frac34$	$\bar{x}+\frac34,\frac34,\frac14$	$\frac34,\frac14,\bar{x}+\frac34$	$\frac14,\frac34,x+\frac34$	
32	e	.3.	x,x,x	$\bar{x},\bar{x}+\frac12,x+\frac12$	$\bar{x}+\frac12,x+\frac12,\bar{x}$	$x+\frac12,\bar{x},\bar{x}+\frac12$			$0kl$: $k+l=4n$
			$x+\frac34,x+\frac14,\bar{x}+\frac34$	$\bar{x}+\frac14,\bar{x}+\frac14,\bar{x}+\frac14$	$x+\frac14,\bar{x}+\frac34,x+\frac34$	$\bar{x}+\frac34,x+\frac34,x+\frac14$			
16	d	.32	$\frac58,\frac58,\frac58$	$\frac38,\frac78,\frac18$	$\frac78,\frac18,\frac38$	$\frac18,\frac38,\frac78$			hkl : $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16	c	.32	$\frac18,\frac18,\frac18$	$\frac78,\frac38,\frac58$	$\frac38,\frac58,\frac78$	$\frac58,\frac78,\frac38$			
8	b	23.	$\frac12,\frac12,\frac12$	$\frac14,\frac34,\frac14$					hkl : $h=2n+1$ or $h+k+l=4n$
8	a	23.	$0,0,0$	$\frac34,\frac14,\frac34$					

Symmetry of special projections

Along [001] $p4mm$	Along [111] $p3m1$	Along [110] $c2mm$
$\mathbf{a}'=\frac12\mathbf{a}\quad \mathbf{b}'=\frac12\mathbf{b}$	$\mathbf{a}'=\frac16(2\mathbf{a}-\mathbf{b}-\mathbf{c})\quad \mathbf{b}'=\frac16(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$	$\mathbf{a}'=\frac12(-\mathbf{a}+\mathbf{b})\quad \mathbf{b}'=\mathbf{c}$
Origin at $\frac14,0,z$	Origin at x,x,x	Origin at $x,x,\frac18$

Maximal non-isomorphic subgroups

I [2] $F\,2\,3\,1$ ($F\,2\,3$, 196) (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+

[3] $F\,4_1\,1\,2$ ($I\,4_1\,2\,2$, 98) (1; 2; 3; 4; 13; 14; 15; 16)+
[3] $F\,4_1\,1\,2$ ($I\,4_1\,2\,2$, 98) (1; 2; 3; 4; 17; 18; 19; 20)+
[3] $F\,4_1\,1\,2$ ($I\,4_1\,2\,2$, 98) (1; 2; 3; 4; 21; 22; 23; 24)+

[4] $F\,1\,3\,2$ ($R\,3\,2$, 155) (1; 5; 9; 14; 19; 24)+
[4] $F\,1\,3\,2$ ($R\,3\,2$, 155) (1; 6; 12; 13; 18; 24)+
[4] $F\,1\,3\,2$ ($R\,3\,2$, 155) (1; 7; 10; 13; 19; 22)+
[4] $F\,1\,3\,2$ ($R\,3\,2$, 155) (1; 8; 11; 14; 18; 22)+

IIa [4] $P\,4_1\,3\,2$ (213) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24

[4] $P\,4_1\,3\,2$ (213) 1; 2; 3; 4; 13; 14; 15; 16; (9; 10; 11; 12; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (5; 6; 7; 8; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$

[4] $P\,4_1\,3\,2$ (213) 1; 2; 3; 4; 17; 18; 19; 20; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$

[4] $P\,4_1\,3\,2$ (213) 1; 2; 3; 4; 21; 22; 23; 24; (5; 6; 7; 8; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$

[4] $P\,4_3\,3\,2$ (212) 1; 5; 9; 14; 19; 24; (4; 6; 11; 16; 18; 23) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 8; 10; 15; 20; 22) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 7; 12; 13; 17; 21) + $(\frac{1}{2},\frac{1}{2},0)$

[4] $P\,4_3\,3\,2$ (212) 1; 6; 12; 13; 18; 24; (4; 5; 10; 15; 19; 23) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 7; 11; 16; 17; 22) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 8; 9; 14; 20; 21) + $(\frac{1}{2},\frac{1}{2},0)$

[4] $P\,4_3\,3\,2$ (212) 1; 7; 10; 13; 19; 22; (4; 8; 12; 15; 18; 21) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 6; 9; 16; 20; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 5; 11; 14; 17; 23) + $(\frac{1}{2},\frac{1}{2},0)$

[4] $P\,4_3\,3\,2$ (212) 1; 8; 11; 14; 18; 22; (4; 7; 9; 16; 19; 21) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 5; 12; 15; 17; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 6; 10; 13; 20; 23) + $(\frac{1}{2},\frac{1}{2},0)$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $F\,4_1\,3\,2$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (210)

Minimal non-isomorphic supergroups

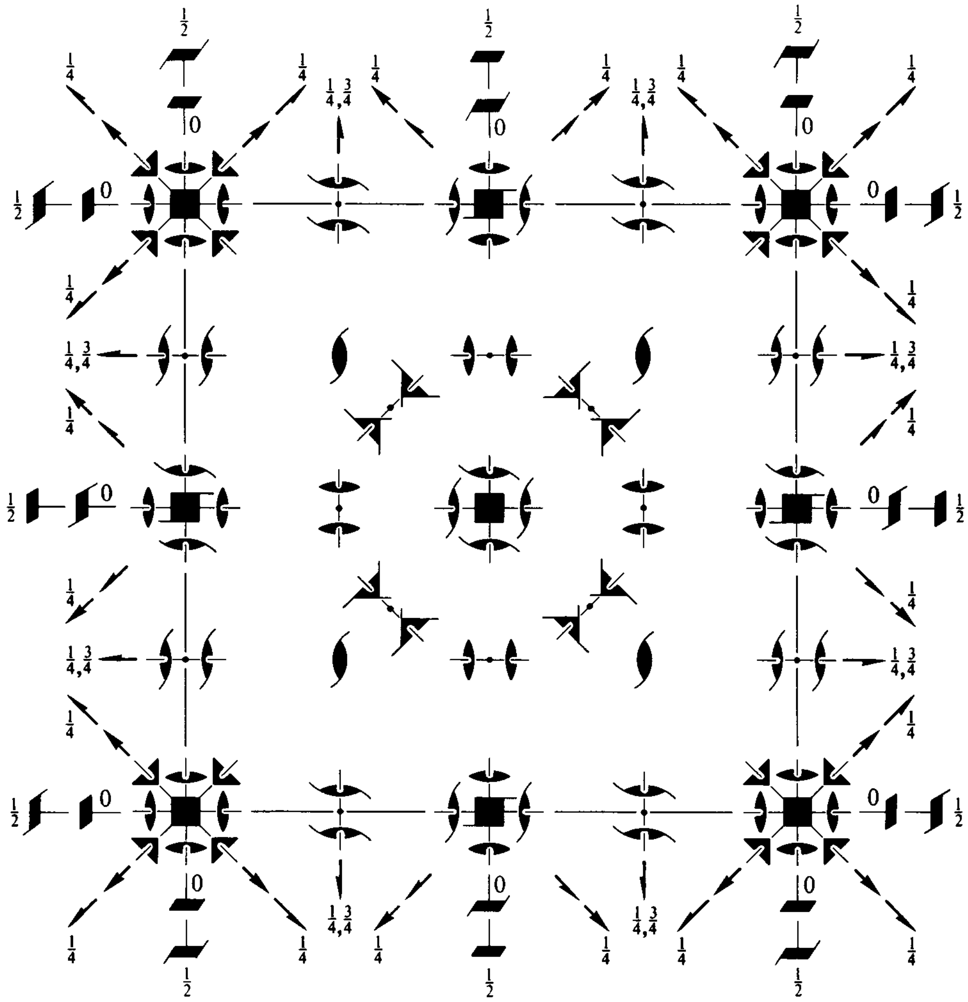
I [2] $F\,d\,\bar{3}\,m$ (227); [2] $F\,d\,\bar{3}\,c$ (228)

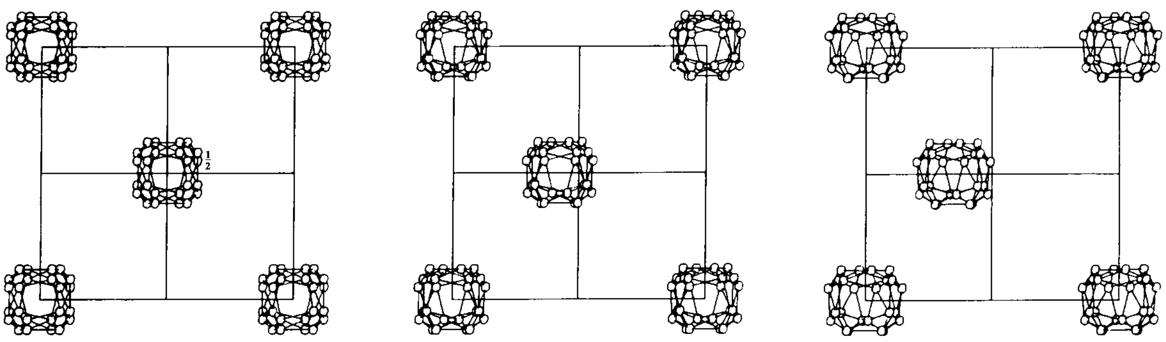
II [2] $P\,4_2\,3\,2$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (208)

International Tables for Crystallography (2006). Vol. A, Space group 211, pp. 645–647.

$I432$ O^5 432 Cubic

No. 211 $I432$ Patterson symmetry $Im\bar{3}m$





Origin at 432

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$; $z \le \min(x, \frac{1}{2}-x, y, \frac{1}{2}-y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) $2\ \ 0,0,z$	(3) $2\ \ 0,y,0$	(4) $2\ \ x,0,0$
(5) $3^+\ x,x,x$	(6) $3^+\ \bar{x},x,\bar{x}$	(7) $3^+\ x,\bar{x},\bar{x}$	(8) $3^+\ \bar{x},\bar{x},x$
(9) $3^-\ x,x,x$	(10) $3^-\ x,\bar{x},\bar{x}$	(11) $3^-\ \bar{x},\bar{x},x$	(12) $3^-\ \bar{x},x,\bar{x}$
(13) $2\ \ x,x,0$	(14) $2\ \ x,\bar{x},0$	(15) $4^-\ 0,0,z$	(16) $4^+\ 0,0,z$
(17) $4^-\ x,0,0$	(18) $2\ \ 0,y,y$	(19) $2\ \ 0,y,\bar{y}$	(20) $4^+\ x,0,0$
(21) $4^+\ 0,y,0$	(22) $2\ \ x,0,x$	(23) $4^-\ 0,y,0$	(24) $2\ \ \bar{x},0,x$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\ \ \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,x,x$	(6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})\ \ \bar{x}+\frac{1}{3},x+\frac{1}{3},\bar{x}$	(7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\ \ x+\frac{2}{3},\bar{x}-\frac{1}{3},\bar{x}$	(8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})\ \ \bar{x}+\frac{1}{3},\bar{x}+\frac{2}{3},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,x,x$	(10) $3^-(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\ \ x+\frac{1}{3},\bar{x}+\frac{1}{3},\bar{x}$	(11) $3^-(\frac{1}{6},\frac{1}{6},-\frac{1}{6})\ \ \bar{x}+\frac{2}{3},\bar{x}+\frac{1}{3},x$	(12) $3^-(\frac{1}{6},-\frac{1}{6},\frac{1}{6})\ \ \bar{x}-\frac{1}{3},x+\frac{2}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x,\frac{1}{4}$	(14) $2\ \ x,\bar{x}+\frac{1}{2},\frac{1}{4}$	(15) $4^-(0,0,\frac{1}{2})\ \ \frac{1}{2},0,z$	(16) $4^+(0,0,\frac{1}{2})\ \ 0,\frac{1}{2},z$
(17) $4^-(\frac{1}{2},0,0)\ \ x,\frac{1}{2},0$	(18) $2(0,\frac{1}{2},\frac{1}{2})\ \ \frac{1}{4},y,y$	(19) $2\ \ \frac{1}{4},y+\frac{1}{2},\bar{y}$	(20) $4^+(\frac{1}{2},0,0)\ \ x,0,\frac{1}{2}$
(21) $4^+(0,\frac{1}{2},0)\ \ \frac{1}{2},y,0$	(22) $2(\frac{1}{2},0,\frac{1}{2})\ \ x,\frac{1}{4},x$	(23) $4^-(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{2}$	(24) $2\ \ \bar{x}+\frac{1}{2},\frac{1}{4},x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\ \ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Reflection conditions
				h,k,l permutable General:
48	j	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}$ (4) $x,\bar{y},\bar{z}$ (5) z,x,y (6) $z,\bar{x},\bar{y}$ (7) $\bar{z},\bar{x},y$ (8) $\bar{z},x,\bar{y}$ (9) y,z,x (10) $\bar{y},z,\bar{x}$ (11) $y,\bar{z},\bar{x}$ (12) $\bar{y},\bar{z},x$ (13) $y,x,\bar{z}$ (14) $\bar{y},\bar{x},\bar{z}$ (15) $y,\bar{x},z$ (16) $\bar{y},x,z$ (17) $x,z,\bar{y}$ (18) $\bar{x},z,y$ (19) $\bar{x},\bar{z},\bar{y}$ (20) $x,\bar{z},y$ (21) $z,y,\bar{x}$ (22) $z,\bar{y},x$ (23) $\bar{z},y,x$ (24) $\bar{z},\bar{y},\bar{x}$	$hkl: h+k+l=2n$ $0kl: k+l=2n$ $hhl: l=2n$ $h00: h=2n$
				Special: as above, plus
24	i	. . 2	$\frac{1}{4},y,\bar{y}+\frac{1}{2}$ $\frac{3}{4},\bar{y},\bar{y}+\frac{1}{2}$ $\frac{3}{4},y,y+\frac{1}{2}$ $\frac{1}{4},\bar{y},y+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{1}{4},y$ $\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}$ $y+\frac{1}{2},\frac{3}{4},y$ $y+\frac{1}{2},\frac{1}{4},\bar{y}$ $y,\bar{y}+\frac{1}{2},\frac{1}{4}$ $\bar{y},\bar{y}+\frac{1}{2},\frac{3}{4}$ $y,y+\frac{1}{2},\frac{3}{4}$ $\bar{y},y+\frac{1}{2},\frac{1}{4}$	no extra conditions
24	h	. . 2	$0,y,y$ $0,\bar{y},y$ $0,y,\bar{y}$ $0,\bar{y},\bar{y}$ $y,0,y$ $y,0,\bar{y}$ $\bar{y},0,y$ $\bar{y},0,\bar{y}$ $y,y,0$ $\bar{y},y,0$ $y,\bar{y},0$ $\bar{y},\bar{y},0$	no extra conditions
24	g	2 . .	$x,\frac{1}{2},0$ $\bar{x},\frac{1}{2},0$ $0,x,\frac{1}{2}$ $0,\bar{x},\frac{1}{2}$ $\frac{1}{2},0,x$ $\frac{1}{2},0,\bar{x}$ $\frac{1}{2},x,0$ $\frac{1}{2},\bar{x},0$ $x,0,\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$ $0,\frac{1}{2},\bar{x}$ $0,\frac{1}{2},x$	no extra conditions
16	f	. 3 .	x,x,x $\bar{x},\bar{x},x$ $\bar{x},x,\bar{x}$ $x,\bar{x},\bar{x}$ $x,x,\bar{x}$ $\bar{x},\bar{x},\bar{x}$ $x,\bar{x},x$ $\bar{x},x,x$	no extra conditions
12	e	4 . .	$x,0,0$ $\bar{x},0,0$ $0,x,0$ $0,\bar{x},0$ $0,0,x$ $0,0,\bar{x}$	no extra conditions
12	d	2 . 2 2	$\frac{1}{4},\frac{1}{2},0$ $\frac{3}{4},\frac{1}{2},0$ $0,\frac{1}{4},\frac{1}{2}$ $0,\frac{3}{4},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{4}$ $\frac{1}{2},0,\frac{3}{4}$	no extra conditions
8	c	. 3 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\frac{1}{4},\frac{3}{4}$ $\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$hkl: k,l=2n$
6	b	4 2 . 2	$0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},0$	no extra conditions
2	a	4 3 2	$0,0,0$	no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [111] $p3m1$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

(*Continued on page 645*)

Maximal non-isomorphic subgroups

I	[2] $I231$ ($I23$, 197)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
	[3] $I412$ ($I422$, 97)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[3] $I412$ ($I422$, 97)	(1; 2; 3; 4; 17; 18; 19; 20)+
	[3] $I412$ ($I422$, 97)	(1; 2; 3; 4; 21; 22; 23; 24)+
	[4] $I132$ ($R32$, 155)	(1; 5; 9; 14; 19; 24)+
	[4] $I132$ ($R32$, 155)	(1; 6; 12; 13; 18; 24)+
	[4] $I132$ ($R32$, 155)	(1; 7; 10; 13; 19; 22)+
	[4] $I132$ ($R32$, 155)	(1; 8; 11; 14; 18; 22)+
IIa	[2] $P4_232$ (208)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P432$ (207)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $I432$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (211)

Minimal non-isomorphic supergroups

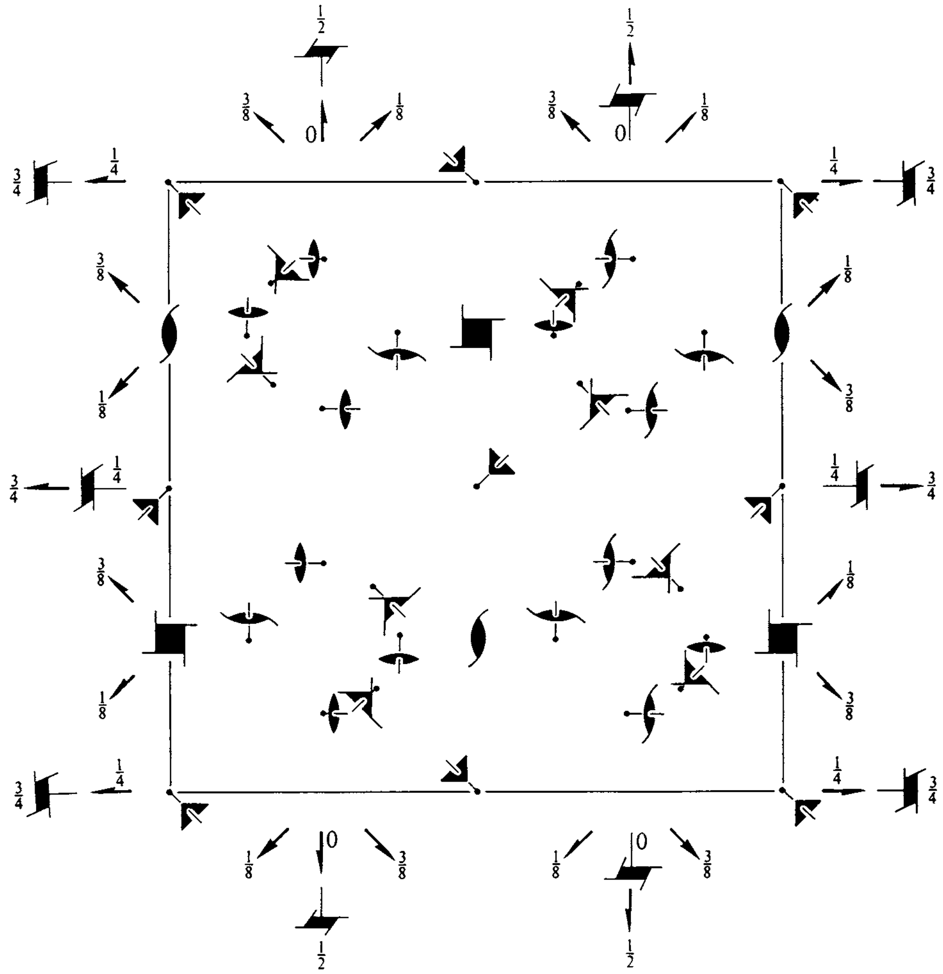
I [2] $Im\bar{3}m$ (229)

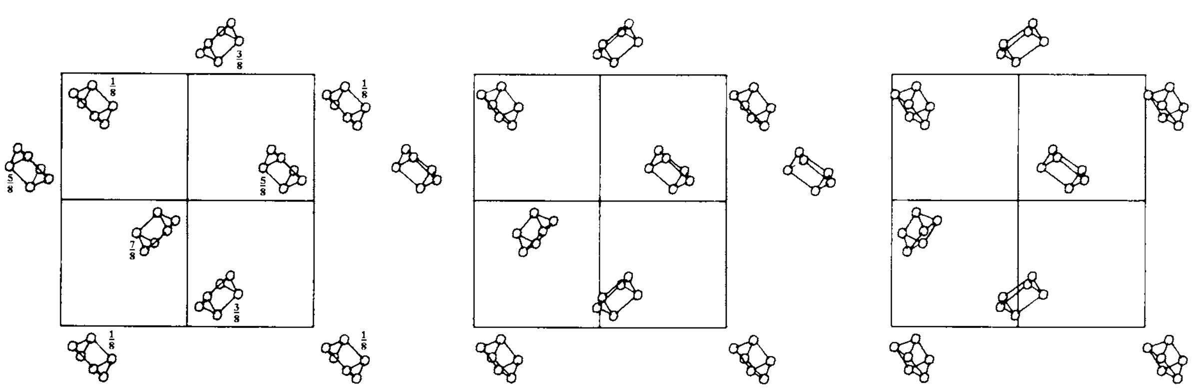
II [4] $P432$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (207)

International Tables for Crystallography (2006). Vol. A, Space group 212, pp. 648–649.

$P4_332$ O^6 432 Cubic

No. 212 $P4_332$ Patterson symmetry $Pm\bar{3}m$





Origin on 3[111] at midpoint of three non-intersecting pairs of parallel screw axes 4_3 and 2_1

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{3}{4}$; $-\frac{1}{2} \le z \le \frac{1}{4}$; $\max(-y, x-\frac{1}{2}) \le z \le \min(-y+\frac{1}{2}, 2x-y, 2y-x, y-2x+\frac{1}{2})$

Vertices $0,0,0$ $\frac{3}{8},\frac{1}{8},-\frac{1}{8}$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{4},\frac{3}{4},-\frac{1}{4}$ $0,\frac{1}{2},-\frac{1}{2}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$	(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) 3^- x,x,x	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{3}{8}$	(14) 2 $x,\bar{x}+\frac{1}{4},\frac{1}{8}$	(15) $4^-(0,0,\frac{1}{4})$ $\frac{3}{4},0,z$	(16) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{2},z$
(17) $4^-(\frac{1}{4},0,0)$ $x,\frac{3}{4},0$	(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{3}{8},y-\frac{1}{4},y$	(19) 2 $\frac{1}{8},y+\frac{1}{4},\bar{y}$	(20) $4^+(\frac{3}{4},0,0)$ $x,\frac{1}{4},\frac{1}{2}$
(21) $4^+(0,\frac{3}{4},0)$ $\frac{1}{2},y,\frac{1}{4}$	(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x+\frac{1}{4},\frac{3}{8},x$	(23) $4^-(0,\frac{1}{4},0)$ $0,y,\frac{3}{4}$	(24) 2 $\bar{x}+\frac{1}{4},\frac{1}{8},x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							h,k,l permutable General:
24	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$h00:\ h=4n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	
			(13) $y+\frac{1}{4},x+\frac{3}{4},\bar{z}+\frac{3}{4}$	(14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(15) $y+\frac{3}{4},\bar{x}+\frac{3}{4},z+\frac{1}{4}$	(16) $\bar{y}+\frac{3}{4},x+\frac{1}{4},z+\frac{3}{4}$	
			(17) $x+\frac{1}{4},z+\frac{3}{4},\bar{y}+\frac{3}{4}$	(18) $\bar{x}+\frac{3}{4},z+\frac{1}{4},y+\frac{3}{4}$	(19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(20) $x+\frac{3}{4},\bar{z}+\frac{3}{4},y+\frac{1}{4}$	
			(21) $z+\frac{1}{4},y+\frac{3}{4},\bar{x}+\frac{3}{4}$	(22) $z+\frac{3}{4},\bar{y}+\frac{3}{4},x+\frac{1}{4}$	(23) $\bar{z}+\frac{3}{4},y+\frac{1}{4},x+\frac{3}{4}$	(24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4}$	
							Special: as above, plus
12	d	..2	$\frac{1}{8},y,\bar{y}+\frac{1}{4}$	$\frac{3}{8},\bar{y},\bar{y}+\frac{3}{4}$	$\frac{7}{8},y+\frac{1}{2},y+\frac{1}{4}$	$\frac{5}{8},\bar{y}+\frac{1}{2},y+\frac{3}{4}$	no extra conditions
			$\bar{y}+\frac{1}{4},\frac{1}{8},y$	$\bar{y}+\frac{3}{4},\frac{3}{8},\bar{y}$	$y+\frac{1}{4},\frac{7}{8},y+\frac{1}{2}$	$y+\frac{3}{4},\frac{5}{8},\bar{y}+\frac{1}{2}$	
			$y,\bar{y}+\frac{1}{4},\frac{1}{8}$	$\bar{y},\bar{y}+\frac{3}{4},\frac{3}{8}$	$y+\frac{1}{2},y+\frac{1}{4},\frac{7}{8}$	$\bar{y}+\frac{1}{2},y+\frac{3}{4},\frac{5}{8}$	
8	c	.3.	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$	$0kl:\ k=2n+1$ or $l=2n+1$ or $k+l=4n$
			$x+\frac{1}{4},x+\frac{3}{4},\bar{x}+\frac{3}{4}$	$\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4}$	$x+\frac{3}{4},\bar{x}+\frac{3}{4},x+\frac{1}{4}$	$\bar{x}+\frac{3}{4},x+\frac{1}{4},x+\frac{3}{4}$	
4	b	.32	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{7}{8},\frac{3}{8},\frac{1}{8}$	$\frac{3}{8},\frac{1}{8},\frac{7}{8}$	$\frac{1}{8},\frac{7}{8},\frac{3}{8}$	$hkl:\ h,k=2n+1$ or $h=2n+1,\ k=4n$ and $l=4n+2$ or $h,k,l=4n+2$ or $h,k,l=4n$
4	a	.32	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{3}{8},\frac{7}{8},\frac{5}{8}$	$\frac{7}{8},\frac{5}{8},\frac{3}{8}$	$\frac{5}{8},\frac{3}{8},\frac{7}{8}$	

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{2},z$

Along [111] $p3m1$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2gm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x+\frac{1}{4},\frac{3}{8}$

Maximal non-isomorphic subgroups

I [2] $P2_131$ ($P2_13$, 198) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
[3] $P4_312$ ($P4_32_12$, 96) 1; 2; 3; 4; 13; 14; 15; 16
[3] $P4_312$ ($P4_32_12$, 96) 1; 2; 3; 4; 17; 18; 19; 20
[3] $P4_312$ ($P4_32_12$, 96) 1; 2; 3; 4; 21; 22; 23; 24
[4] $P132$ ($R32$, 155) 1; 5; 9; 14; 19; 24
[4] $P132$ ($R32$, 155) 1; 6; 12; 13; 18; 24
[4] $P132$ ($R32$, 155) 1; 7; 10; 13; 19; 22
[4] $P132$ ($R32$, 155) 1; 8; 11; 14; 18; 22

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $P4_132$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (213); [125] $P4_332$ ($\mathbf{a}'=5\mathbf{a},\mathbf{b}'=5\mathbf{b},\mathbf{c}'=5\mathbf{c}$) (212)

Minimal non-isomorphic supergroups

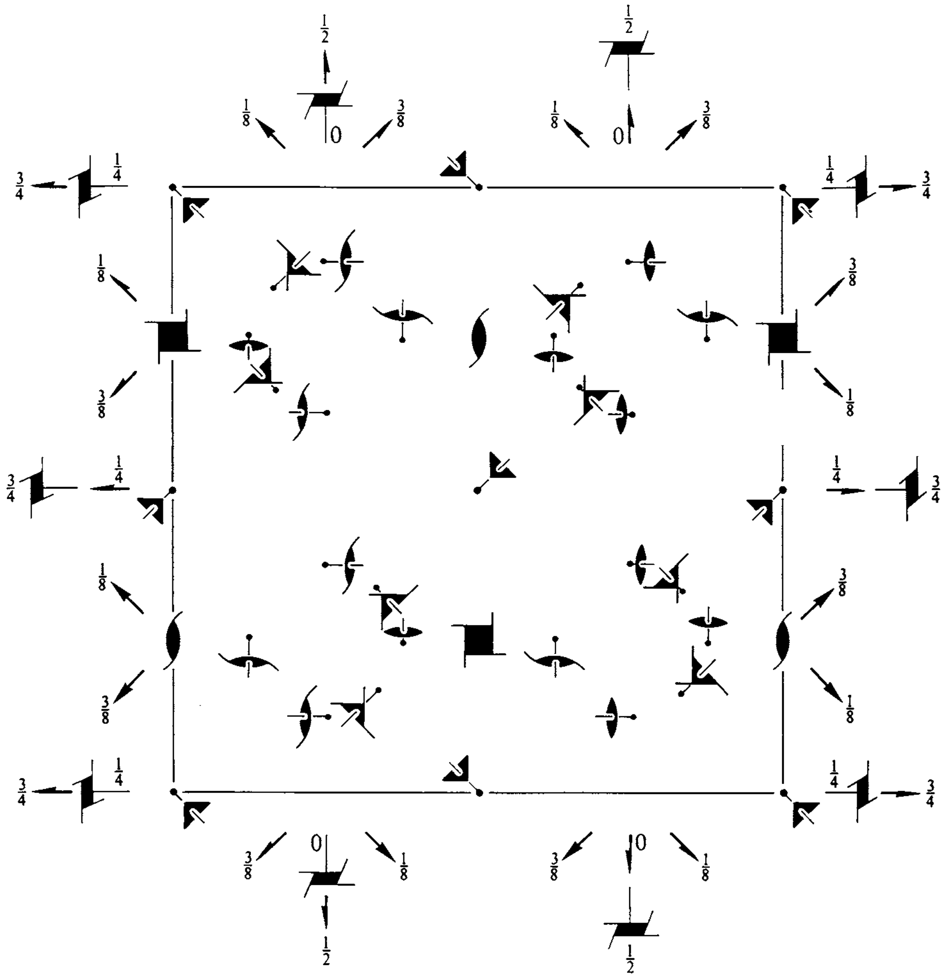
I none

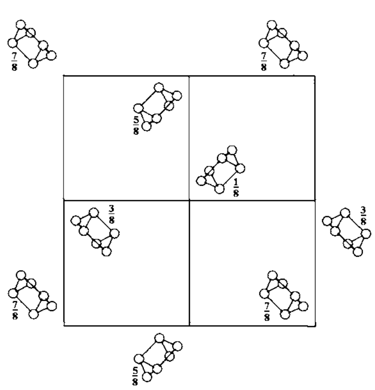
II [2] $I4_132$ (214); [4] $F4_132$ (210)

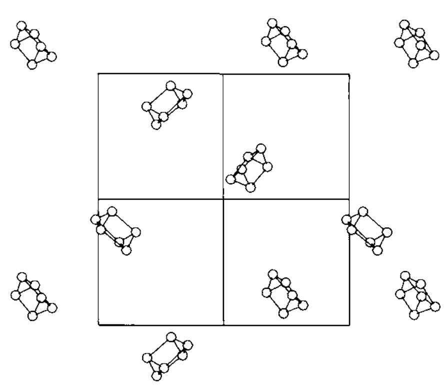
International Tables for Crystallography (2006). Vol. A, Space group 213, pp. 650–651.

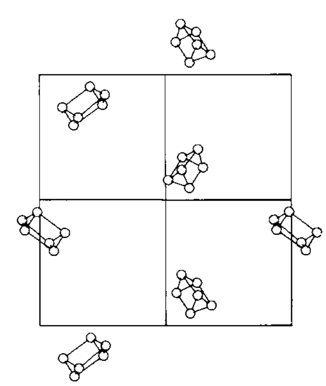
$P4_132$ O^7 432 Cubic

No. 213 $P4_132$ Patterson symmetry $Pm\bar{3}m$









Origin on 3[111] at midpoint of three non-intersecting pairs of parallel screw axes 4_1 and 2_1

Asymmetric unit $-\frac14 \le x \le \frac12;\quad 0 \le y \le \frac34;\quad 0 \le z \le \frac12;\quad x \le y \le x+\frac12;\quad (y-x)/2 \le z \le \min(y,(-4x-2y+3)/2,(3-2x-2y)/4)$

Vertices $0,0,0\quad \frac12,\frac12,0\quad \frac14,\frac34,\frac14\quad -\frac14,\frac14,\frac14\quad 0,\frac12,\frac12\quad \frac38,\frac38,\frac38$

Symmetry operations

(1) 1	(2) $2(0,0,\frac12)$ $\frac14,0,z$	(3) $2(0,\frac12,0)$ $0,y,\frac14$	(4) $2(\frac12,0,0)$ $x,\frac14,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x}+\frac12,x,\bar{x}$	(7) 3^+ $x+\frac12,\bar{x}-\frac12,\bar{x}$	(8) 3^+ $\bar{x},\bar{x}+\frac12,x$
(9) 3^- x,x,x	(10) $3^-(-\frac13,\frac13,\frac13)$ $x+\frac16,\bar{x}+\frac16,\bar{x}$	(11) $3^-(\frac13,\frac13,-\frac13)$ $\bar{x}+\frac13,\bar{x}+\frac16,x$	(12) $3^-(\frac13,-\frac13,\frac13)$ $\bar{x}-\frac16,x+\frac13,\bar{x}$
(13) $2(\frac12,\frac12,0)$ $x,x-\frac14,\frac18$	(14) 2 $x,\bar{x}+\frac34,\frac38$	(15) $4^-(0,0,\frac34)$ $\frac14,0,z$	(16) $4^+(0,0,\frac14)$ $-\frac14,\frac12,z$
(17) $4^-(\frac34,0,0)$ $x,\frac14,0$	(18) $2(0,\frac12,\frac12)$ $\frac18,y+\frac14,y$	(19) 2 $\frac38,y+\frac34,\bar{y}$	(20) $4^+(\frac14,0,0)$ $x,-\frac14,\frac12$
(21) $4^+(0,\frac14,0)$ $\frac12,y,-\frac14$	(22) $2(\frac12,0,\frac12)$ $x-\frac14,\frac18,x$	(23) $4^-(0,\frac34,0)$ $0,y,\frac14$	(24) 2 $\bar{x}+\frac34,\frac38,x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							h,k,l permutable
							General:
24	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$h00:\ h=4n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{4}$	(14) $\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$	
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{4}$	(18) $\bar{x}+\frac{1}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{1}{4},y+\frac{3}{4}$	
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{1}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{1}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4}$	
							Special: as above, plus
12	d	..2	$\frac{1}{8},y,y+\frac{1}{4}$	$\frac{3}{8},\bar{y},y+\frac{3}{4}$	$\frac{7}{8},y+\frac{1}{2},\bar{y}+\frac{1}{4}$	$\frac{5}{8},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$	no extra conditions
			$y+\frac{1}{4},\frac{1}{8},y$	$y+\frac{3}{4},\frac{3}{8},\bar{y}$	$\bar{y}+\frac{1}{4},\frac{7}{8},y+\frac{1}{2}$	$\bar{y}+\frac{3}{4},\frac{5}{8},\bar{y}+\frac{1}{2}$	
			$y,y+\frac{1}{4},\frac{1}{8}$	$\bar{y},y+\frac{3}{4},\frac{3}{8}$	$y+\frac{1}{2},\bar{y}+\frac{1}{4},\frac{7}{8}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{5}{8}$	
8	c	.3.	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$	$0kl:\ k=2n+1$ or $l=2n+1$ or $k+l=4n$
			$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{4}$	$\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4}$	$x+\frac{1}{4},\bar{x}+\frac{1}{4},x+\frac{3}{4}$	$\bar{x}+\frac{1}{4},x+\frac{3}{4},x+\frac{1}{4}$	
4	b	.32	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$	$\frac{5}{8},\frac{1}{8},\frac{3}{8}$	$\frac{1}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{1}{8}$	$hkl:\ h,k=2n+1$ or $h=2n+1,\ k=4n$ and $l=4n+2$ or $h,k,l=4n+2$ or $h,k,l=4n$
4	a	.32	$\frac{3}{8},\frac{3}{8},\frac{3}{8}$	$\frac{1}{8},\frac{5}{8},\frac{7}{8}$	$\frac{5}{8},\frac{7}{8},\frac{1}{8}$	$\frac{7}{8},\frac{1}{8},\frac{5}{8}$	(as for b)

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},0,z$

Along [111] $p3m1$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2gm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x+\frac{1}{4},\frac{1}{8}$

Maximal non-isomorphic subgroups

I [2] $P2_131$ ($P2_13$, 198) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
{ [3] $P4_112$ ($P4_12_12$, 92) 1; 2; 3; 4; 13; 14; 15; 16
{ [3] $P4_112$ ($P4_12_12$, 92) 1; 2; 3; 4; 17; 18; 19; 20
{ [3] $P4_112$ ($P4_12_12$, 92) 1; 2; 3; 4; 21; 22; 23; 24
{ [4] $P132$ ($R32$, 155) 1; 5; 9; 14; 19; 24
{ [4] $P132$ ($R32$, 155) 1; 6; 12; 13; 18; 24
{ [4] $P132$ ($R32$, 155) 1; 7; 10; 13; 19; 22
{ [4] $P132$ ($R32$, 155) 1; 8; 11; 14; 18; 22

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $P4_332$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (212); [125] $P4_132$ ($\mathbf{a}'=5\mathbf{a},\mathbf{b}'=5\mathbf{b},\mathbf{c}'=5\mathbf{c}$) (213)

Minimal non-isomorphic supergroups

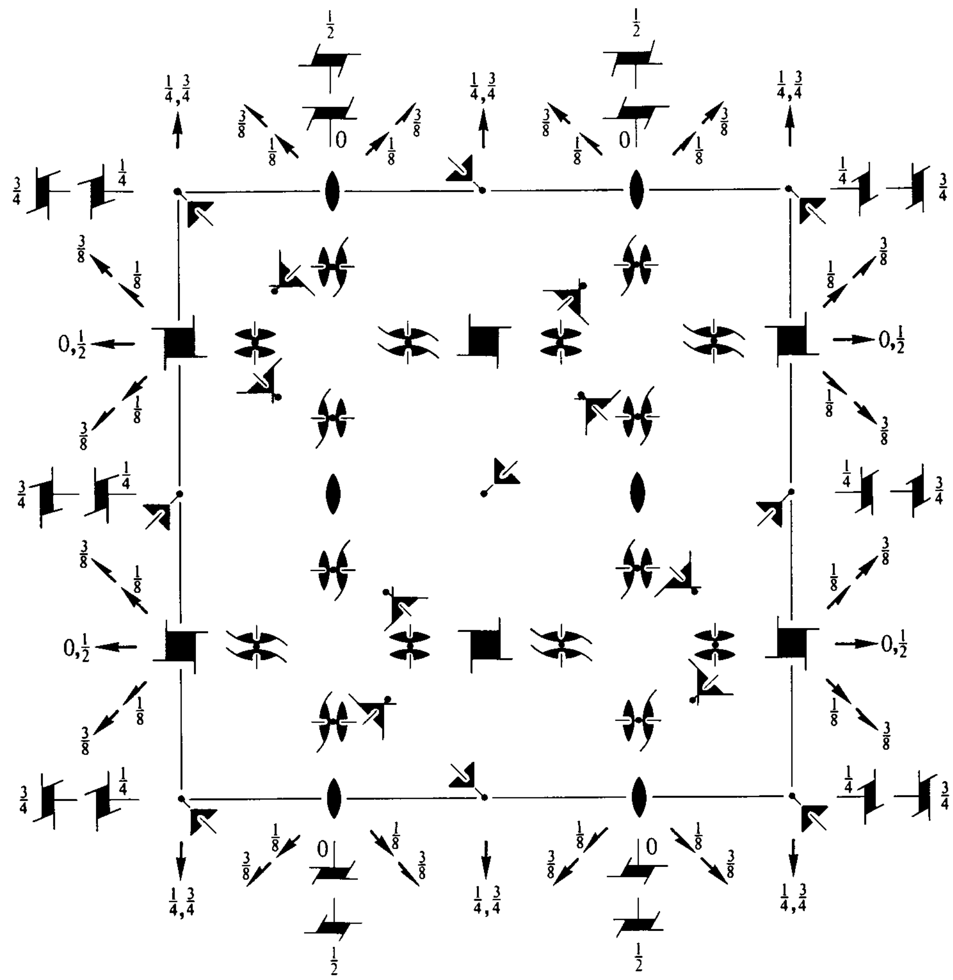
I none

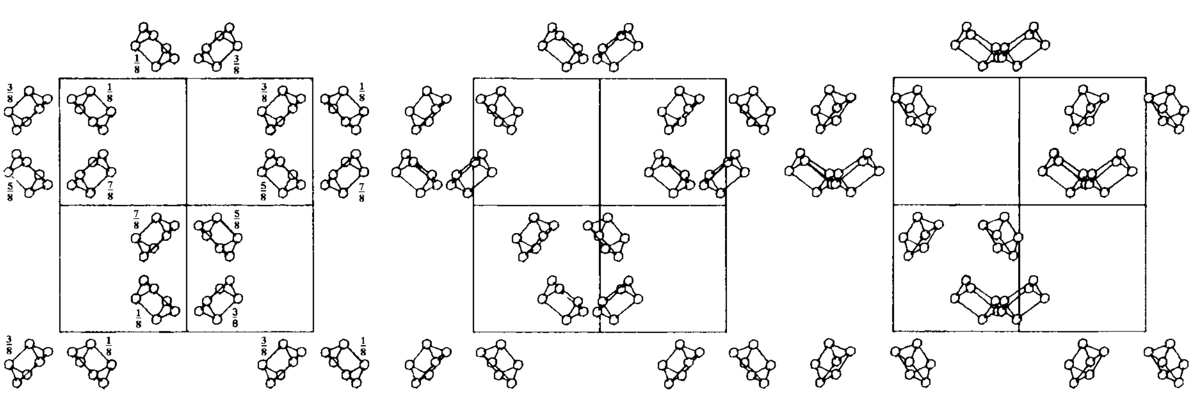
II [2] $I4_132$ (214); [4] $F4_132$ (210)

International Tables for Crystallography (2006). Vol. A, Space group 214, pp. 652–654.

$I4_132$ O^8 432 Cubic

No. 214 $I4_132$ Patterson symmetry $Im\bar{3}m$





Origin on 3[111] at midpoint of three non-intersecting pairs of parallel screw axes 4_1 and 4_3 and of three non-intersecting pairs of parallel 2 axes

Asymmetric unit $-\frac{3}{8} \le x \le \frac{1}{8};\quad -\frac{1}{8} \le y \le \frac{1}{8};\quad -\frac{1}{8} \le z \le \frac{3}{8};\quad \max(x, y, y-x-\frac{1}{8}) \le z \le y+\frac{1}{4}$

Vertices $\frac{1}{8},\frac{1}{8},\frac{1}{8}\quad \frac{1}{8},\frac{1}{8},\frac{3}{8}\quad \frac{1}{8},-\frac{1}{8},\frac{1}{8}\quad -\frac{1}{8},\frac{1}{8},\frac{1}{8}\quad -\frac{1}{8},-\frac{1}{8},-\frac{1}{8}\quad -\frac{3}{8},\frac{1}{8},\frac{3}{8}\quad -\frac{3}{8},-\frac{1}{8},\frac{1}{8}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $3^{+}\quad x,x,x$	(6) $3^{+}\quad \bar{x}+\frac{1}{2},x,\bar{x}$	(7) $3^{+}\quad x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^{+}\quad \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^{-}\quad x,x,x$	(10) $3^{-}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^{-}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^{-}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x-\frac{1}{4},\frac{1}{8}$	(14) $2\quad x,\bar{x}+\frac{3}{4},\frac{3}{8}$	(15) $4^{-}(0,0,\frac{3}{4})\quad \frac{1}{4},0,z$	(16) $4^{+}(0,0,\frac{1}{4})\quad -\frac{1}{4},\frac{1}{2},z$
(17) $4^{-}(\frac{3}{4},0,0)\quad x,\frac{1}{4},0$	(18) $2(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{8},y+\frac{1}{4},y$	(19) $2\quad \frac{3}{8},y+\frac{3}{4},\bar{y}$	(20) $4^{+}(\frac{1}{4},0,0)\quad x,-\frac{1}{4},\frac{1}{2}$
(21) $4^{+}(0,\frac{1}{4},0)\quad \frac{1}{2},y,-\frac{1}{4}$	(22) $2(\frac{1}{2},0,\frac{1}{2})\quad x-\frac{1}{4},\frac{1}{8},x$	(23) $4^{-}(0,\frac{3}{4},0)\quad 0,y,\frac{1}{4}$	(24) $2\quad \bar{x}+\frac{3}{4},\frac{3}{8},x$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\quad 0,\frac{1}{4},z$	(3) $2\quad \frac{1}{4},y,0$	(4) $2\quad x,0,\frac{1}{4}$
(5) $3^{+}(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,x$	(6) $3^{+}(\frac{1}{6},-\frac{1}{6},\frac{1}{6})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$	(7) $3^{+}(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(8) $3^{+}(\frac{1}{6},\frac{1}{6},-\frac{1}{6})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(9) $3^{-}(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,x$	(10) $3^{-}(\frac{1}{6},-\frac{1}{6},-\frac{1}{6})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^{-}(-\frac{1}{6},-\frac{1}{6},\frac{1}{6})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^{-}(-\frac{1}{6},\frac{1}{6},-\frac{1}{6})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x+\frac{1}{4},\frac{3}{8}$	(14) $2\quad x,\bar{x}+\frac{1}{4},\frac{1}{8}$	(15) $4^{-}(0,0,\frac{1}{4})\quad \frac{3}{4},0,z$	(16) $4^{+}(0,0,\frac{3}{4})\quad \frac{1}{4},\frac{1}{2},z$
(17) $4^{-}(\frac{1}{4},0,0)\quad x,\frac{3}{4},0$	(18) $2(0,\frac{1}{2},\frac{1}{2})\quad \frac{3}{8},y-\frac{1}{4},y$	(19) $2\quad \frac{1}{8},y+\frac{1}{4},\bar{y}$	(20) $4^{+}(\frac{3}{4},0,0)\quad x,\frac{1}{4},\frac{1}{2}$
(21) $4^{+}(0,\frac{3}{4},0)\quad \frac{1}{2},y,\frac{1}{4}$	(22) $2(\frac{1}{2},0,\frac{1}{2})\quad x+\frac{1}{4},\frac{3}{8},x$	(23) $4^{-}(0,\frac{1}{4},0)\quad 0,y,\frac{3}{4}$	(24) $2\quad \bar{x}+\frac{1}{4},\frac{1}{8},x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
			$(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$						h,k,l permutable General:
48	i	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$			hkl : $h+k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$			$0kl$: $k+l=2n$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$			hhl : $l=2n$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{4}$	(14) $\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$			$h00$: $h=4n$
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{4}$	(18) $\bar{x}+\frac{1}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{1}{4},y+\frac{3}{4}$			
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{1}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{1}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4}$			
									Special: as above, plus
24	h	..2	$\frac{1}{8},y,\bar{y}+\frac{1}{4}$	$\frac{3}{8},\bar{y},\bar{y}+\frac{3}{4}$	$\frac{7}{8},y+\frac{1}{2},y+\frac{1}{4}$	$\frac{5}{8},\bar{y}+\frac{1}{2},y+\frac{3}{4}$			no extra conditions
			$\bar{y}+\frac{1}{4},\frac{1}{8},y$	$\bar{y}+\frac{3}{4},\frac{3}{8},\bar{y}$	$y+\frac{1}{4},\frac{7}{8},y+\frac{1}{2}$	$y+\frac{3}{4},\frac{5}{8},\bar{y}+\frac{1}{2}$			
			$y,\bar{y}+\frac{1}{4},\frac{1}{8}$	$\bar{y},\bar{y}+\frac{3}{4},\frac{3}{8}$	$y+\frac{1}{2},y+\frac{1}{4},\frac{7}{8}$	$\bar{y}+\frac{1}{2},y+\frac{3}{4},\frac{5}{8}$			
24	g	..2	$\frac{1}{8},y,y+\frac{1}{4}$	$\frac{3}{8},\bar{y},y+\frac{3}{4}$	$\frac{7}{8},y+\frac{1}{2},\bar{y}+\frac{1}{4}$	$\frac{5}{8},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$			no extra conditions
			$y+\frac{1}{4},\frac{1}{8},y$	$y+\frac{3}{4},\frac{3}{8},\bar{y}$	$\bar{y}+\frac{1}{4},\frac{7}{8},y+\frac{1}{2}$	$\bar{y}+\frac{3}{4},\frac{5}{8},\bar{y}+\frac{1}{2}$			
			$y,y+\frac{1}{4},\frac{1}{8}$	$\bar{y},y+\frac{3}{4},\frac{3}{8}$	$y+\frac{1}{2},\bar{y}+\frac{1}{4},\frac{7}{8}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{5}{8}$			
24	f	2..	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{4},x,0$	$\frac{3}{4},\bar{x}+\frac{1}{2},0$	$0,\frac{1}{4},x$	$0,\frac{3}{4},\bar{x}+\frac{1}{2}$	hkl : $h=2n+1$
			$\frac{3}{4},x+\frac{1}{4},0$	$\frac{3}{4},\bar{x}+\frac{3}{4},\frac{1}{2}$	$x+\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{4},0,\frac{1}{4}$	$0,\frac{1}{4},\bar{x}+\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},x+\frac{3}{4}$	or $h=4n$
									hhl : $h=2n+1$
									or $h+k+l=4n$
16	e	.3.	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$			$0kl$: $k=2n+1$
			$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{4}$	$\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4}$	$x+\frac{1}{4},\bar{x}+\frac{1}{4},x+\frac{3}{4}$	$\bar{x}+\frac{1}{4},x+\frac{3}{4},x+\frac{1}{4}$			or $k+l=4n$
12	d	2.22	$\frac{5}{8},0,\frac{1}{4}$	$\frac{7}{8},0,\frac{3}{4}$	$\frac{1}{4},\frac{5}{8},0$	$\frac{3}{4},\frac{7}{8},0$	$0,\frac{1}{4},\frac{5}{8}$	$0,\frac{3}{4},\frac{7}{8}$	hkl : $h,k=2n,\ h+k+l=4n$
									or $h,k=2n+1,\ l=4n+2$
12	c	2.22	$\frac{1}{8},0,\frac{1}{4}$	$\frac{3}{8},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{8},0$	$\frac{3}{4},\frac{3}{8},0$	$0,\frac{1}{4},\frac{1}{8}$	$0,\frac{3}{4},\frac{3}{8}$	or $h=8n,\ k=8n+4$ and $h+k+l=4n+2$
									or $h,k=8n+1,\ l=4n$
									or $h=8n+1$ and $k=8n-1,\ l=4n$
									or $h,k=8n+3,\ l=4n$
									or $h=8n+3$ and $k=8n-3,\ l=4n$
8	b	.32	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$	$\frac{5}{8},\frac{1}{8},\frac{3}{8}$	$\frac{1}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{1}{8}$			hkl : $h=2n+1$
									or $h,k,l=4n+2$
8	a	.32	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{3}{8},\frac{7}{8},\frac{5}{8}$	$\frac{7}{8},\frac{5}{8},\frac{3}{8}$	$\frac{5}{8},\frac{3}{8},\frac{7}{8}$			or $h,k,l=4n$

Symmetry of special projections

Along [001] $p4mm$	Along [111] $p3m1$	Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$	$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$	$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $\frac{1}{4},0,z$	Origin at x,x,x	Origin at $x,x+\frac{1}{4},\frac{1}{8}$

Maximal non-isomorphic subgroups

I [2] $I2_131$ ($I2_13$, 199) (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+

[3] $I4_112$ ($I4_122$, 98) (1; 2; 3; 4; 13; 14; 15; 16)+
[3] $I4_112$ ($I4_122$, 98) (1; 2; 3; 4; 17; 18; 19; 20)+
[3] $I4_112$ ($I4_122$, 98) (1; 2; 3; 4; 21; 22; 23; 24)+

[4] $I132$ ($R32$, 155) (1; 5; 9; 14; 19; 24)+
[4] $I132$ ($R32$, 155) (1; 6; 12; 13; 18; 24)+
[4] $I132$ ($R32$, 155) (1; 7; 10; 13; 19; 22)+
[4] $I132$ ($R32$, 155) (1; 8; 11; 14; 18; 22)+

IIa [2] $P4_132$ (213) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
[2] $P4_332$ (212) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $I4_132$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (214)

Minimal non-isomorphic supergroups

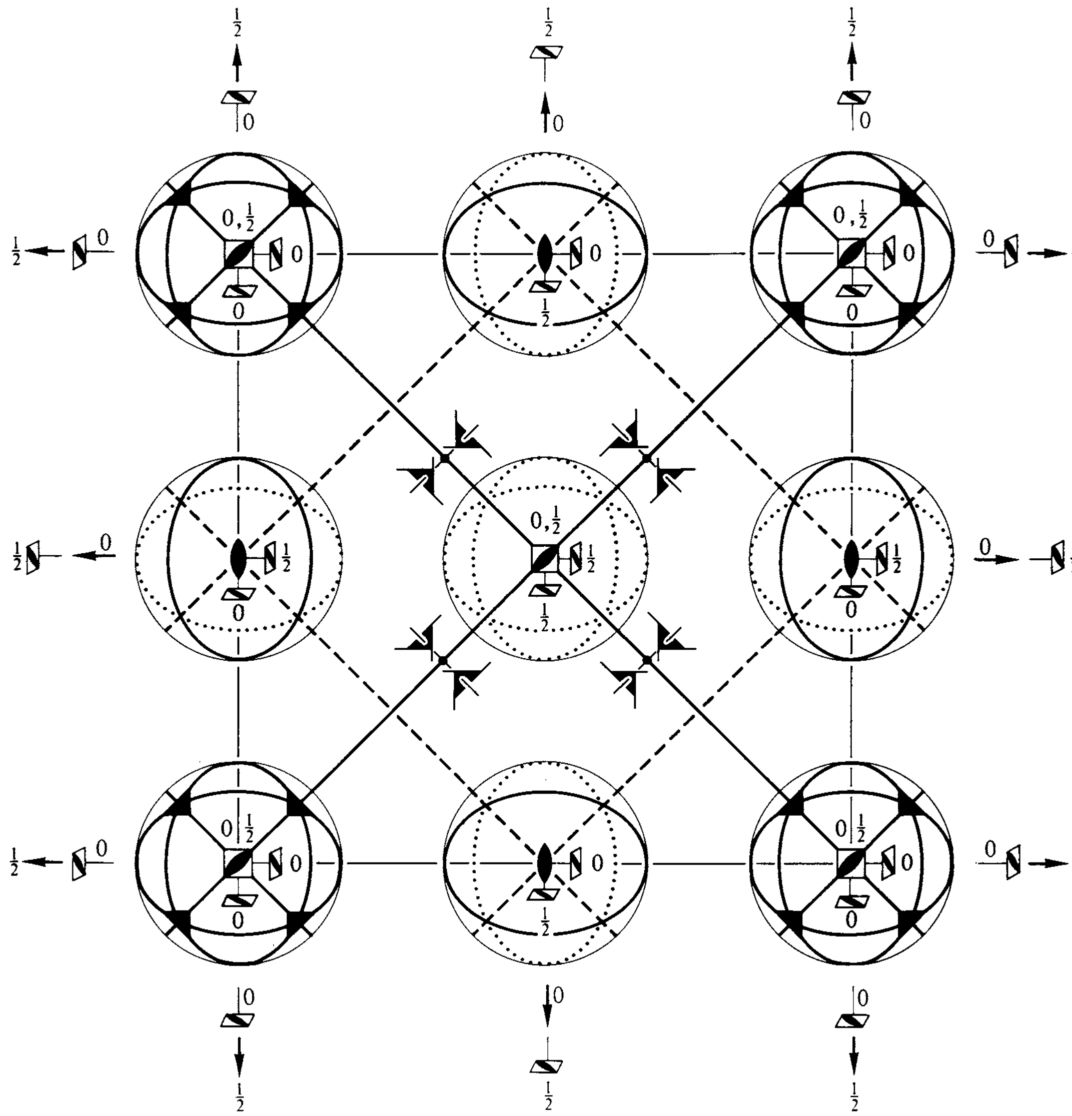
I [2] $Ia\bar{3}d$ (230)

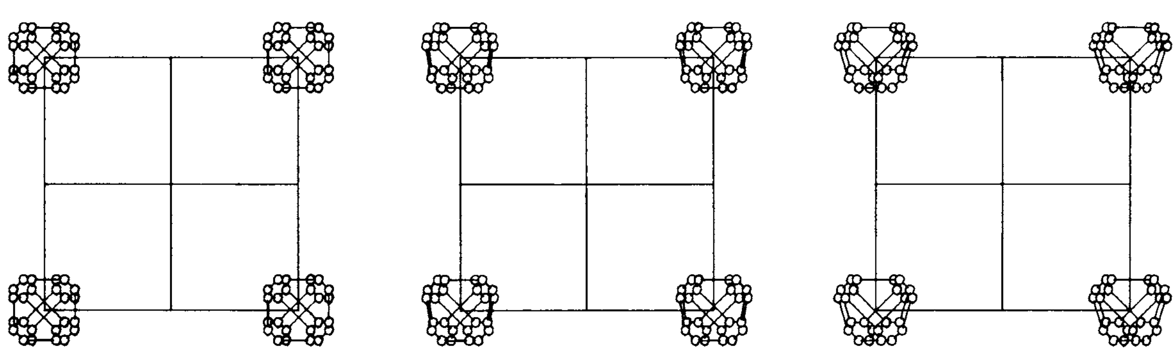
II [4] $P4_232$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (208)

International Tables for Crystallography (2006). Vol. A, Space group 215, pp. 656–657.

$P\bar{4}3m$ | T_d^1 | $\bar{4}3m$ | Cubic

No. 215 | $P\bar{4}3m$ | Patterson symmetry $Pm\bar{3}m$





Origin at $\bar{4}3m$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2};\quad y \le \min(x, 1-x);\quad z \le y$

Vertices $0,0,0 \quad 1,0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) $2 \quad 0,0,z$	(3) $2 \quad 0,y,0$	(4) $2 \quad x,0,0$
(5) $3^+ \quad x,x,x$	(6) $3^+ \quad \bar{x},x,\bar{x}$	(7) $3^+ \quad x,\bar{x},\bar{x}$	(8) $3^+ \quad \bar{x},\bar{x},x$
(9) $3^- \quad x,x,x$	(10) $3^- \quad x,\bar{x},\bar{x}$	(11) $3^- \quad \bar{x},\bar{x},x$	(12) $3^- \quad \bar{x},x,\bar{x}$
(13) $m \quad x,x,z$	(14) $m \quad x,\bar{x},z$	(15) $\bar{4}^+ \quad 0,0,z;\ \ 0,0,0$	(16) $\bar{4}^- \quad 0,0,z;\ \ 0,0,0$
(17) $m \quad x,y,y$	(18) $\bar{4}^+ \quad x,0,0;\ \ 0,0,0$	(19) $\bar{4}^- \quad x,0,0;\ \ 0,0,0$	(20) $m \quad x,y,\bar{y}$
(21) $m \quad x,y,x$	(22) $\bar{4}^- \quad 0,y,0;\ \ 0,0,0$	(23) $m \quad \bar{x},y,x$	(24) $\bar{4}^+ \quad 0,y,0;\ \ 0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									h,k,l permutable General:
24	j	1	(1) x,y,z (5) z,x,y (9) y,z,x (13) y,x,z (17) x,z,y (21) z,y,x	(2) $\bar{x},\bar{y},z$ (6) $z,\bar{x},\bar{y}$ (10) $\bar{y},z,\bar{x}$ (14) $\bar{y},\bar{x},z$ (18) $\bar{x},z,\bar{y}$ (22) $z,\bar{y},\bar{x}$	(3) $\bar{x},y,\bar{z}$ (7) $\bar{z},\bar{x},y$ (11) $y,\bar{z},\bar{x}$ (15) $y,\bar{x},\bar{z}$ (19) $\bar{x},\bar{z},y$ (23) $\bar{z},y,\bar{x}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{z},x,\bar{y}$ (12) $\bar{y},\bar{z},x$ (16) $\bar{y},x,\bar{z}$ (20) $x,\bar{z},\bar{y}$ (24) $\bar{z},\bar{y},x$			no conditions
									Special: no extra conditions
12	i	$..m$	x,x,z $\bar{z},\bar{x},x$	$\bar{x},\bar{x},z$ $\bar{z},x,\bar{x}$	$\bar{x},x,\bar{z}$ x,z,x	$x,\bar{x},\bar{z}$ $\bar{x},z,\bar{x}$	z,x,x $x,\bar{z},\bar{x}$	$z,\bar{x},\bar{x}$ $\bar{x},\bar{z},x$	
12	h	$2..$	$x,\frac{1}{2},0$ $\frac{1}{2},x,0$	$\bar{x},\frac{1}{2},0$ $\frac{1}{2},\bar{x},0$	$0,x,\frac{1}{2}$ $x,0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$	$\frac{1}{2},0,x$ $0,\frac{1}{2},x$	$\frac{1}{2},0,\bar{x}$ $0,\frac{1}{2},\bar{x}$	
6	g	$2.mm$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$	
6	f	$2.mm$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	
4	e	$.3m$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			
3	d	$\bar{4}2.m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$				
3	c	$\bar{4}2.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$				
1	b	$\bar{4}3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						
1	a	$\bar{4}3m$	$0,0,0$						

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [111] $p31m$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P231$ ($P23$, 195) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
{ [3] $P\bar{4}1m$ ($P\bar{4}2m$, 111) 1; 2; 3; 4; 13; 14; 15; 16
{ [3] $P\bar{4}1m$ ($P\bar{4}2m$, 111) 1; 2; 3; 4; 17; 18; 19; 20
{ [3] $P\bar{4}1m$ ($P\bar{4}2m$, 111) 1; 2; 3; 4; 21; 22; 23; 24
{ [4] $P13m$ ($R3m$, 160) 1; 5; 9; 13; 17; 21
{ [4] $P13m$ ($R3m$, 160) 1; 6; 12; 14; 20; 21
{ [4] $P13m$ ($R3m$, 160) 1; 7; 10; 14; 17; 23
{ [4] $P13m$ ($R3m$, 160) 1; 8; 11; 13; 20; 23

IIa none

IIb [2] $F\bar{4}3c$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (219); [2] $F\bar{4}3m$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (216); [4] $I\bar{4}3m$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (217)

Maximal isomorphic subgroups of lowest index

IIc [27] $P\bar{4}3m$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (215)

Minimal non-isomorphic supergroups

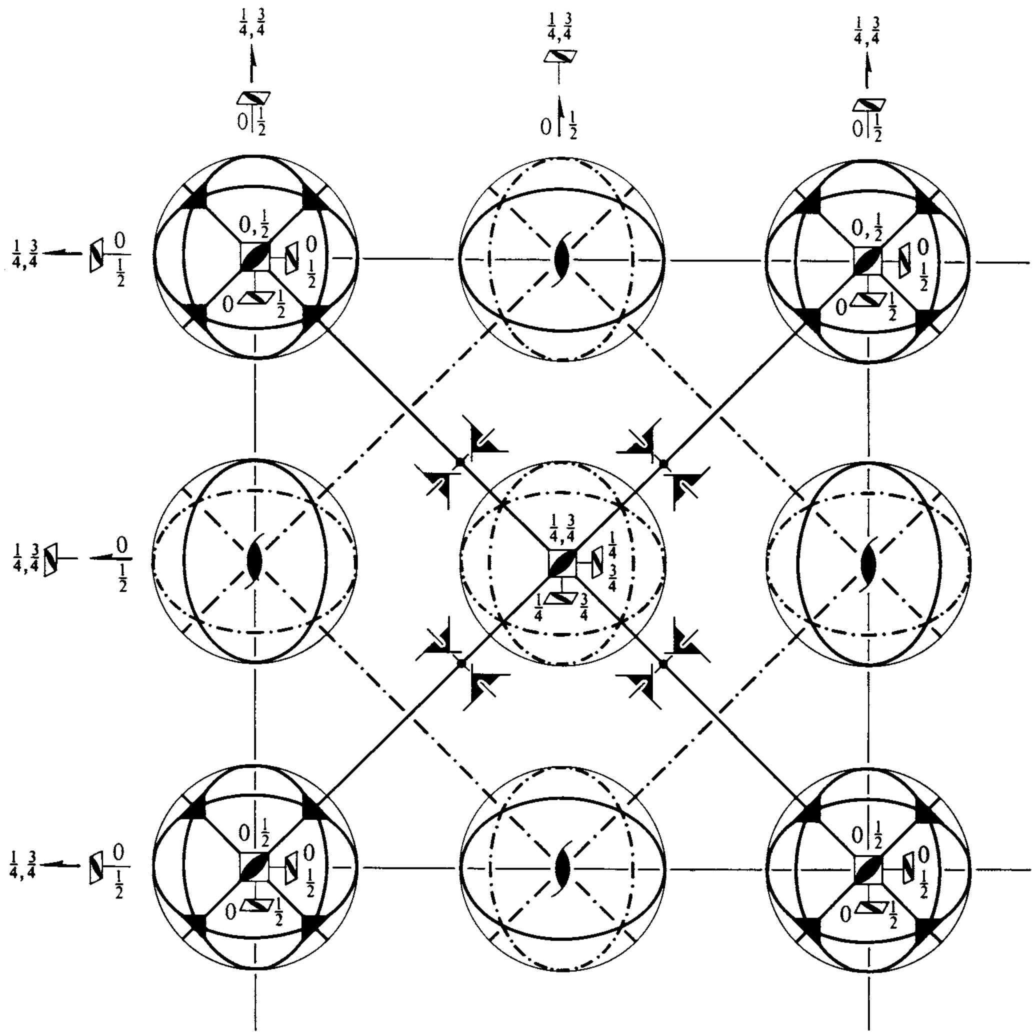
I [2] $Pm\bar{3}m$ (221); [2] $Pn\bar{3}m$ (224)

II [2] $I\bar{4}3m$ (217); [4] $F\bar{4}3m$ (216)

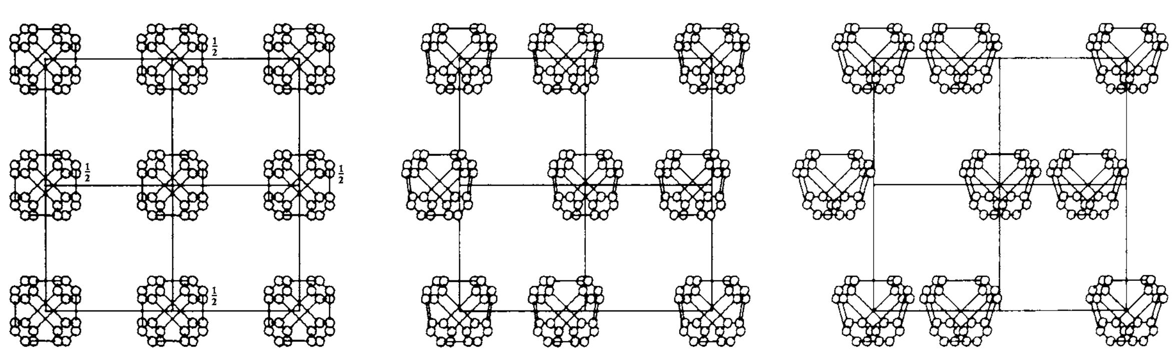
International Tables for Crystallography (2006). Vol. A, Space group 216, pp. 658–660.

$F\bar{4}3m$ $\quad T_d^2$ $\quad \bar{4}3m$ $\quad$ Cubic

No. 216 $\quad F\bar{4}3m$ $\quad$ Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Origin at $\bar{4}3m$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{4};\quad -\frac{1}{4} \le z \le \frac{1}{4};\quad y \le \min(x, \frac{1}{2}-x);\quad -y \le z \le y$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{4},\frac{1}{4},\frac{1}{4} \quad \frac{1}{4},\frac{1}{4},-\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $3^{+}\ x,x,x$	(6) $3^{+}\ \bar{x},x,\bar{x}$	(7) $3^{+}\ x,\bar{x},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x},x$
(9) $3^{-}\ x,x,x$	(10) $3^{-}\ x,\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x},\bar{x},x$	(12) $3^{-}\ \bar{x},x,\bar{x}$
(13) $m\ \ x,x,z$	(14) $m\ \ x,\bar{x},z$	(15) $\bar{4}^{+}\ 0,0,z;\ 0,0,0$	(16) $\bar{4}^{-}\ 0,0,z;\ 0,0,0$
(17) $m\ \ x,y,y$	(18) $\bar{4}^{+}\ x,0,0;\ 0,0,0$	(19) $\bar{4}^{-}\ x,0,0;\ 0,0,0$	(20) $m\ \ x,y,\bar{y}$
(21) $m\ \ x,y,x$	(22) $\bar{4}^{-}\ 0,y,0;\ 0,0,0$	(23) $m\ \ \bar{x},y,x$	(24) $\bar{4}^{+}\ 0,y,0;\ 0,0,0$

For $(0,\frac{1}{2},\frac{1}{2})$+ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2\quad x,\frac{1}{4},\frac{1}{4}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{3},x-\frac{1}{6},x$	(6) $3^{+}\ \bar{x},x+\frac{1}{2},\bar{x}$	(7) $3^{+}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x+\frac{1}{6},x$	(10) $3^{-}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) $3^{-}\ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})\quad x-\frac{1}{4},x,z$	(14) $g(-\frac{1}{4},\frac{1}{4},\frac{1}{2})\quad x+\frac{1}{4},\bar{x},z$	(15) $\bar{4}^{+}\ \frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(16) $\bar{4}^{-}\ -\frac{1}{4},\frac{1}{4},z;\ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(17) $g(0,\frac{1}{2},\frac{1}{2})\quad x,y,y$	(18) $\bar{4}^{+}\ x,\frac{1}{2},0;\ 0,\frac{1}{2},0$	(19) $\bar{4}^{-}\ x,0,\frac{1}{2};\ 0,0,\frac{1}{2}$	(20) $m\ \ x,y+\frac{1}{2},\bar{y}$
(21) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})\quad x-\frac{1}{4},y,x$	(22) $\bar{4}^{-}\ \frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(23) $g(-\frac{1}{4},\frac{1}{2},\frac{1}{4})\quad \bar{x}+\frac{1}{4},y,x$	(24) $\bar{4}^{+}\ -\frac{1}{4},y,\frac{1}{4};\ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$

For $(\frac{1}{2},0,\frac{1}{2})$+ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,0,\frac{1}{4}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x-\frac{1}{6},x$	(6) $3^{+}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^{+}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x-\frac{1}{3},x$	(10) $3^{-}\ x+\frac{1}{2},\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{1}{2},\bar{x},x$	(12) $3^{-}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})\quad x+\frac{1}{4},x,z$	(14) $g(\frac{1}{4},-\frac{1}{4},\frac{1}{2})\quad x+\frac{1}{4},\bar{x},z$	(15) $\bar{4}^{+}\ \frac{1}{4},-\frac{1}{4},z;\ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$	(16) $\bar{4}^{-}\ \frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(17) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})\quad x,y-\frac{1}{4},y$	(18) $\bar{4}^{+}\ x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(19) $\bar{4}^{-}\ x,-\frac{1}{4},\frac{1}{4};\ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$	(20) $g(\frac{1}{2},-\frac{1}{4},\frac{1}{4})\quad x,y+\frac{1}{4},\bar{y}$
(21) $g(\frac{1}{2},0,\frac{1}{2})\quad x,y,x$	(22) $\bar{4}^{-}\ \frac{1}{2},y,0;\ \frac{1}{2},0,0$	(23) $m\ \ \bar{x}+\frac{1}{2},y,x$	(24) $\bar{4}^{+}\ 0,y,\frac{1}{2};\ 0,0,\frac{1}{2}$

For $(\frac{1}{2},\frac{1}{2},0)$+ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x+\frac{1}{3},x$	(6) $3^{+}\ \bar{x}+\frac{1}{2},x,\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x},\bar{x}$	(8) $3^{+}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{3},x+\frac{1}{6},x$	(10) $3^{-}\ x,\bar{x}+\frac{1}{2},\bar{x}$	(11) $3^{-}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^{-}\ \bar{x},x+\frac{1}{2},\bar{x}$
(13) $g(\frac{1}{2},\frac{1}{2},0)\quad x,x,z$	(14) $m\ \ x+\frac{1}{2},\bar{x},z$	(15) $\bar{4}^{+}\ \frac{1}{2},0,z;\ \frac{1}{2},0,0$	(16) $\bar{4}^{-}\ 0,\frac{1}{2},z;\ 0,\frac{1}{2},0$
(17) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})\quad x,y+\frac{1}{4},y$	(18) $\bar{4}^{+}\ x,\frac{1}{4},-\frac{1}{4};\ \frac{1}{4},\frac{1}{4},-\frac{1}{4}$	(19) $\bar{4}^{-}\ x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(20) $g(\frac{1}{2},\frac{1}{4},-\frac{1}{4})\quad x,y+\frac{1}{4},\bar{y}$
(21) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})\quad x+\frac{1}{4},y,x$	(22) $\bar{4}^{-}\ \frac{1}{4},y,-\frac{1}{4};\ \frac{1}{4},\frac{1}{4},-\frac{1}{4}$	(23) $g(\frac{1}{4},\frac{1}{2},-\frac{1}{4})\quad \bar{x}+\frac{1}{4},y,x$	(24) $\bar{4}^{+}\ \frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad (0,\frac{1}{2},\frac{1}{2})+\quad (\frac{1}{2},0,\frac{1}{2})+\quad (\frac{1}{2},\frac{1}{2},0)+$						Reflection conditions
									h,k,l permutable General:
96	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			hkl : $h+k,h+l,k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			hhl : $h+l=2n$
			(13) y,x,z	(14) $\bar{y},\bar{x},z$	(15) $y,\bar{x},\bar{z}$	(16) $\bar{y},x,\bar{z}$			$h00$: $h=2n$
			(17) x,z,y	(18) $\bar{x},z,\bar{y}$	(19) $\bar{x},\bar{z},y$	(20) $x,\bar{z},\bar{y}$			
			(21) z,y,x	(22) $z,\bar{y},\bar{x}$	(23) $\bar{z},y,\bar{x}$	(24) $\bar{z},\bar{y},x$			
									Special: no extra conditions
48	h	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x	$z,\bar{x},\bar{x}$	
			$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$	
24	g	$2.mm$	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}$	
24	f	$2.mm$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	
16	e	$.3m$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			
4	d	$\bar{4}3m$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$						
4	c	$\bar{4}3m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$						
4	b	$\bar{4}3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						
4	a	$\bar{4}3m$	$0,0,0$						

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [111] $p31m$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $F231$ ($F23$, 196)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
	[3] $F\bar{4}1m$ ($I\bar{4}m2$, 119)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[3] $F\bar{4}1m$ ($I\bar{4}m2$, 119)	(1; 2; 3; 4; 17; 18; 19; 20)+
	[3] $F\bar{4}1m$ ($I\bar{4}m2$, 119)	(1; 2; 3; 4; 21; 22; 23; 24)+
	[4] $F13m$ ($R3m$, 160)	(1; 5; 9; 13; 17; 21)+
	[4] $F13m$ ($R3m$, 160)	(1; 6; 12; 14; 20; 21)+
	[4] $F13m$ ($R3m$, 160)	(1; 7; 10; 14; 17; 23)+
	[4] $F13m$ ($R3m$, 160)	(1; 8; 11; 13; 20; 23)+
IIa	[4] $P\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[4] $P\bar{4}3m$ (215)	1; 2; 3; 4; 13; 14; 15; 16; (9; 10; 11; 12; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (5; 6; 7; 8; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$
	[4] $P\bar{4}3m$ (215)	1; 2; 3; 4; 17; 18; 19; 20; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\bar{4}3m$ (215)	1; 2; 3; 4; 21; 22; 23; 24; (5; 6; 7; 8; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\bar{4}3m$ (215)	1; 5; 9; 13; 17; 21; (4; 6; 11; 15; 20; 22) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 8; 10; 16; 18; 23) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 7; 12; 14; 19; 24) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\bar{4}3m$ (215)	1; 6; 12; 14; 20; 21; (4; 5; 10; 16; 17; 22) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 7; 11; 15; 19; 23) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 8; 9; 13; 18; 24) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\bar{4}3m$ (215)	1; 7; 10; 14; 17; 23; (4; 8; 12; 16; 20; 24) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 6; 9; 15; 18; 21) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 5; 11; 13; 19; 22) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $P\bar{4}3m$ (215)	1; 8; 11; 13; 20; 23; (4; 7; 9; 15; 17; 24) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 5; 12; 16; 19; 21) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 6; 10; 14; 18; 22) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $F\bar{4}3m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (216)

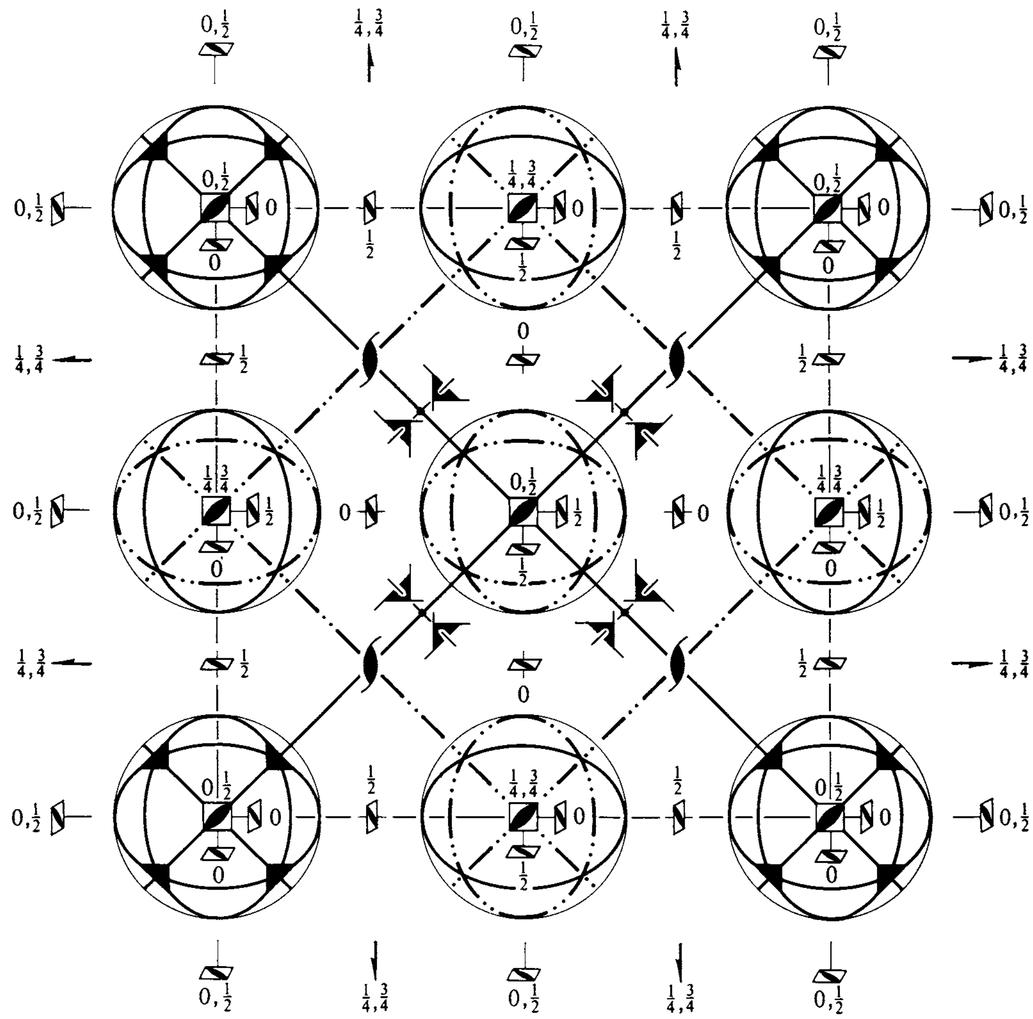
Minimal non-isomorphic supergroups

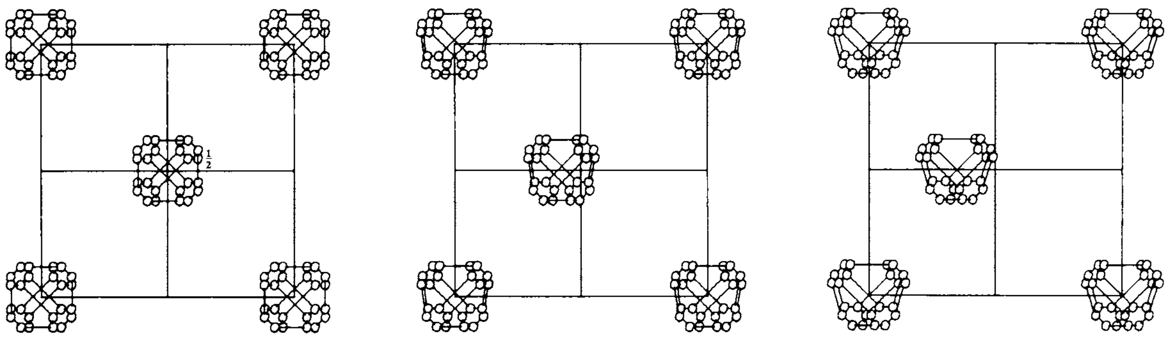
I [2] $Fm\bar{3}m$ (225); [2] $Fd\bar{3}m$ (227)

II [2] $P\bar{4}3m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (215)

$I\bar{4}3m$ T_d^3 $\bar{4}3m$ Cubic

No. 217 $I\bar{4}3m$ Patterson symmetry $Im\bar{3}m$





Origin at $\bar{4}3m$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le x$; $z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $3^{+}\ x,x,x$	(6) $3^{+}\ \bar{x},x,\bar{x}$	(7) $3^{+}\ x,\bar{x},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x},x$
(9) $3^{-}\ x,x,x$	(10) $3^{-}\ x,\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x},\bar{x},x$	(12) $3^{-}\ \bar{x},x,\bar{x}$
(13) $m\ \ x,x,z$	(14) $m\ \ x,\bar{x},z$	(15) $\bar{4}^{+}\ 0,0,z;\ 0,0,0$	(16) $\bar{4}^{-}\ 0,0,z;\ 0,0,0$
(17) $m\ \ x,y,y$	(18) $\bar{4}^{+}\ x,0,0;\ 0,0,0$	(19) $\bar{4}^{-}\ x,0,0;\ 0,0,0$	(20) $m\ \ x,y,\bar{y}$
(21) $m\ \ x,y,x$	(22) $\bar{4}^{-}\ 0,y,0;\ 0,0,0$	(23) $m\ \ \bar{x},y,x$	(24) $\bar{4}^{+}\ 0,y,0;\ 0,0,0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{1}{4}$
(5) $3^{+}(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,x$	(6) $3^{+}(\frac{1}{6},-\frac{1}{6},\frac{1}{6})\quad \bar{x}+\frac{1}{3},x+\frac{1}{3},\bar{x}$	(7) $3^{+}(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\quad x+\frac{2}{3},\bar{x}-\frac{1}{3},\bar{x}$	(8) $3^{+}(\frac{1}{6},\frac{1}{6},-\frac{1}{6})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{2}{3},x$
(9) $3^{-}(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,x$	(10) $3^{-}(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\quad x+\frac{1}{3},\bar{x}+\frac{1}{3},\bar{x}$	(11) $3^{-}(\frac{1}{6},\frac{1}{6},-\frac{1}{6})\quad \bar{x}+\frac{2}{3},\bar{x}+\frac{1}{3},x$	(12) $3^{-}(\frac{1}{6},-\frac{1}{6},\frac{1}{6})\quad \bar{x}-\frac{1}{3},x+\frac{2}{3},\bar{x}$
(13) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,z$	(14) $c\quad x+\frac{1}{2},\bar{x},z$	(15) $\bar{4}^{+}\ \frac{1}{2},0,z;\ \frac{1}{2},0,\frac{1}{4}$	(16) $\bar{4}^{-}\ 0,\frac{1}{2},z;\ 0,\frac{1}{2},\frac{1}{4}$
(17) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,y,y$	(18) $\bar{4}^{+}\ x,\frac{1}{2},0;\ \frac{1}{4},\frac{1}{2},0$	(19) $\bar{4}^{-}\ x,0,\frac{1}{2};\ \frac{1}{4},0,\frac{1}{2}$	(20) $a\quad x,y+\frac{1}{2},\bar{y}$
(21) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,y,x$	(22) $\bar{4}^{-}\ \frac{1}{2},y,0;\ \frac{1}{2},\frac{1}{4},0$	(23) $b\quad \bar{x}+\frac{1}{2},y,x$	(24) $\bar{4}^{+}\ 0,y,\frac{1}{2};\ 0,\frac{1}{4},\frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates: $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ — Reflection conditions

Reflection conditions: h,k,l permutable

General:

$hkl:\ h+k+l=2n$
$0kl:\ k+l=2n$
$hhl:\ l=2n$
$h00:\ h=2n$

48 h 1

(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
(13) y,x,z	(14) $\bar{y},\bar{x},z$	(15) $y,\bar{x},\bar{z}$	(16) $\bar{y},x,\bar{z}$
(17) x,z,y	(18) $\bar{x},z,\bar{y}$	(19) $\bar{x},\bar{z},y$	(20) $x,\bar{z},\bar{y}$
(21) z,y,x	(22) $z,\bar{y},\bar{x}$	(23) $\bar{z},y,\bar{x}$	(24) $\bar{z},\bar{y},x$

Special: no extra conditions

24	g	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x	$z,\bar{x},\bar{x}$
			$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$
24	f	$2..$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$
			$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\frac{1}{2},x$	$0,\frac{1}{2},\bar{x}$
12	e	$2.mm$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
12	d	$\bar{4}..$	$\frac{1}{4},\frac{1}{2},0$	$\frac{3}{4},\frac{1}{2},0$	$0,\frac{1}{4},\frac{1}{2}$	$0,\frac{3}{4},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$
8	c	$.3m$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$		
6	b	$\bar{4}2.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			
2	a	$\bar{4}3m$	$0,0,0$					

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})\qquad \mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [111] $p31m$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})\qquad \mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})\qquad \mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

(*Continued on page 661*)

Maximal non-isomorphic subgroups

I	[2] $I231$ ($I23$, 197)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
	[3] $I\bar{4}1m$ ($I\bar{4}2m$, 121)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[3] $I\bar{4}1m$ ($I\bar{4}2m$, 121)	(1; 2; 3; 4; 17; 18; 19; 20)+
	[3] $I\bar{4}1m$ ($I\bar{4}2m$, 121)	(1; 2; 3; 4; 21; 22; 23; 24)+
	[4] $I13m$ ($R3m$, 160)	(1; 5; 9; 13; 17; 21)+
	[4] $I13m$ ($R3m$, 160)	(1; 6; 12; 14; 20; 21)+
	[4] $I13m$ ($R3m$, 160)	(1; 7; 10; 14; 17; 23)+
	[4] $I13m$ ($R3m$, 160)	(1; 8; 11; 13; 20; 23)+
IIa	[2] $P\bar{4}3n$ (218)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $I\bar{4}3m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (217)

Minimal non-isomorphic supergroups

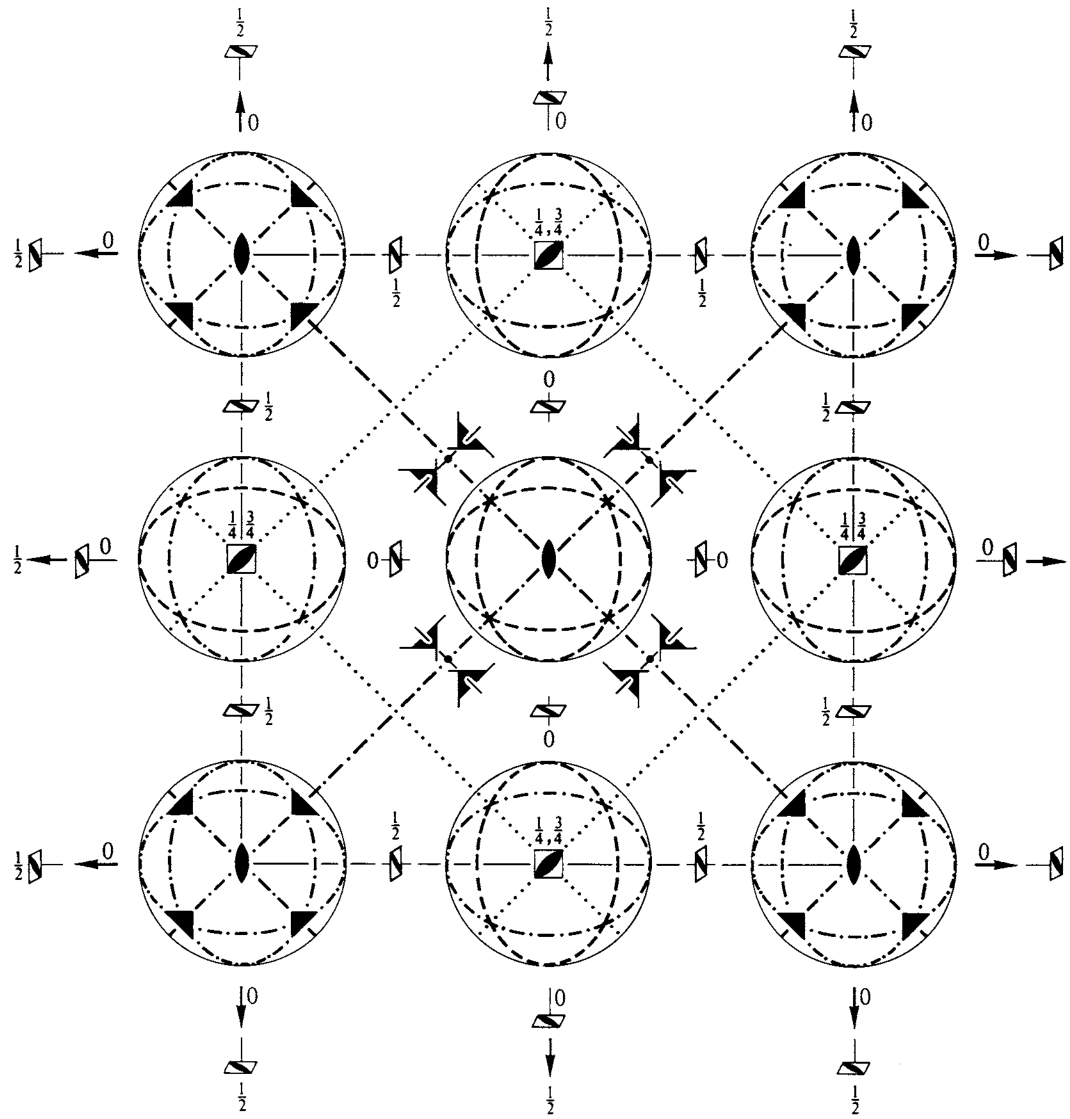
I [2] $Im\bar{3}m$ (229)

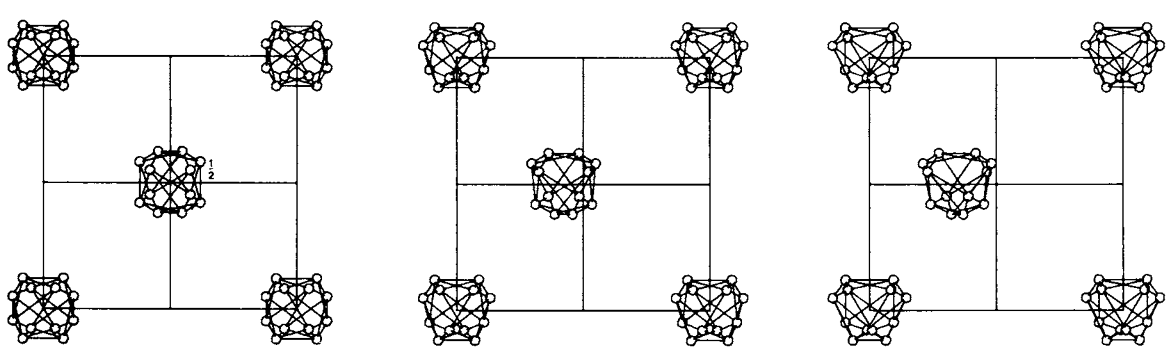
II [4] $P\bar{4}3m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (215)

International Tables for Crystallography (2006). Vol. A, Space group 218, pp. 664–665.

$P\bar{4}3n$ $\quad T_d^4$ $\quad \bar{4}3m$ $\quad$ Cubic

No. 218 $\quad P\bar{4}3n$ $\quad$ Patterson symmetry $Pm\bar{3}m$





Origin at 23

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2};\quad z \le \min(x,y)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad 0,\frac{1}{2},0 \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $3^{+}\quad x,x,x$	(6) $3^{+}\quad \bar{x},x,\bar{x}$	(7) $3^{+}\quad x,\bar{x},\bar{x}$	(8) $3^{+}\quad \bar{x},\bar{x},x$
(9) $3^{-}\quad x,x,x$	(10) $3^{-}\quad x,\bar{x},\bar{x}$	(11) $3^{-}\quad \bar{x},\bar{x},x$	(12) $3^{-}\quad \bar{x},x,\bar{x}$
(13) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,z$	(14) $c\quad x+\frac{1}{2},\bar{x},z$	(15) $\bar{4}^{+}\quad \frac{1}{2},0,z;\quad \frac{1}{2},0,\frac{1}{4}$	(16) $\bar{4}^{-}\quad 0,\frac{1}{2},z;\quad 0,\frac{1}{2},\frac{1}{4}$
(17) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,y,y$	(18) $\bar{4}^{+}\quad x,\frac{1}{2},0;\quad \frac{1}{4},\frac{1}{2},0$	(19) $\bar{4}^{-}\quad x,0,\frac{1}{2};\quad \frac{1}{4},0,\frac{1}{2}$	(20) $a\quad x,y+\frac{1}{2},\bar{y}$
(21) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,y,x$	(22) $\bar{4}^{-}\quad \frac{1}{2},y,0;\quad \frac{1}{2},\frac{1}{4},0$	(23) $b\quad \bar{x}+\frac{1}{2},y,x$	(24) $\bar{4}^{+}\quad 0,y,\frac{1}{2};\quad 0,\frac{1}{4},\frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									h,k,l permutable General:
24	i	1	(1) x,y,z (5) z,x,y (9) y,z,x (13) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ (17) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$ (21) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $z,\bar{x},\bar{y}$ (10) $\bar{y},z,\bar{x}$ (14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$ (22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}$ (7) $\bar{z},\bar{x},y$ (11) $y,\bar{z},\bar{x}$ (15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$ (23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{z},x,\bar{y}$ (12) $\bar{y},\bar{z},x$ (16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$ (24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$			hhl : $l=2n$ $h00$: $h=2n$
									Special: as above, plus
12	h	$2\,.\,.$	$x,0,\frac{1}{2}$ $\frac{1}{2},x+\frac{1}{2},0$	$\bar{x},0,\frac{1}{2}$ $\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\frac{1}{2},x,0$ $x+\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\bar{x},0$ $\bar{x}+\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},x$ $0,\frac{1}{2},x+\frac{1}{2}$	$0,\frac{1}{2},\bar{x}$ $0,\frac{1}{2},\bar{x}+\frac{1}{2}$	hkl : $h=2n$
12	g	$2\,.\,.$	$x,\frac{1}{2},0$ $0,x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},0$ $0,\bar{x}+\frac{1}{2},\frac{1}{2}$	$0,x,\frac{1}{2}$ $x+\frac{1}{2},\frac{1}{2},0$	$0,\bar{x},\frac{1}{2}$ $\bar{x}+\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,x$ $\frac{1}{2},0,x+\frac{1}{2}$	$\frac{1}{2},0,\bar{x}$ $\frac{1}{2},0,\bar{x}+\frac{1}{2}$	hkl : $h=2n$
12	f	$2\,.\,.$	$x,0,0$ $\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x},0,0$ $\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$0,x,0$ $x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\bar{x},0$ $\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,x$ $\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$	$0,0,\bar{x}$ $\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	hkl : $h+k+l=2n$
8	e	$.\,3\,.$	x,x,x $x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{x},\bar{x},x$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x},x,\bar{x}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x,\bar{x},\bar{x}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$			hkl : $h+k+l=2n$
6	d	$\bar{4}\,.\,.$	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},0$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	hkl : $h+k+l=2n$ or $h=2n+1$, $k=4n$ and $l=4n+2$ (for d and c)
6	c	$\bar{4}\,.\,.$	$\frac{1}{4},\frac{1}{2},0$	$\frac{3}{4},\frac{1}{2},0$	$0,\frac{1}{4},\frac{1}{2}$	$0,\frac{3}{4},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	
6	b	$2\,2\,2\,.\,.$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	hkl : $h+k+l=2n$
2	a	$2\,3\,.$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{2},0,z$

Along [111] $p31m$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P231$ ($P23$, 195) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
[3] $P\bar{4}1n$ ($P\bar{4}2c$, 112) 1; 2; 3; 4; 13; 14; 15; 16
[3] $P\bar{4}1n$ ($P\bar{4}2c$, 112) 1; 2; 3; 4; 17; 18; 19; 20
[3] $P\bar{4}1n$ ($P\bar{4}2c$, 112) 1; 2; 3; 4; 21; 22; 23; 24
[4] $P13n$ ($R3c$, 161) 1; 5; 9; 13; 17; 21
[4] $P13n$ ($R3c$, 161) 1; 6; 12; 14; 20; 21
[4] $P13n$ ($R3c$, 161) 1; 7; 10; 14; 17; 23
[4] $P13n$ ($R3c$, 161) 1; 8; 11; 13; 20; 23

IIa none

IIb [4] $I\bar{4}3d$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (220)

Maximal isomorphic subgroups of lowest index

IIc [27] $P\bar{4}3n$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (218)

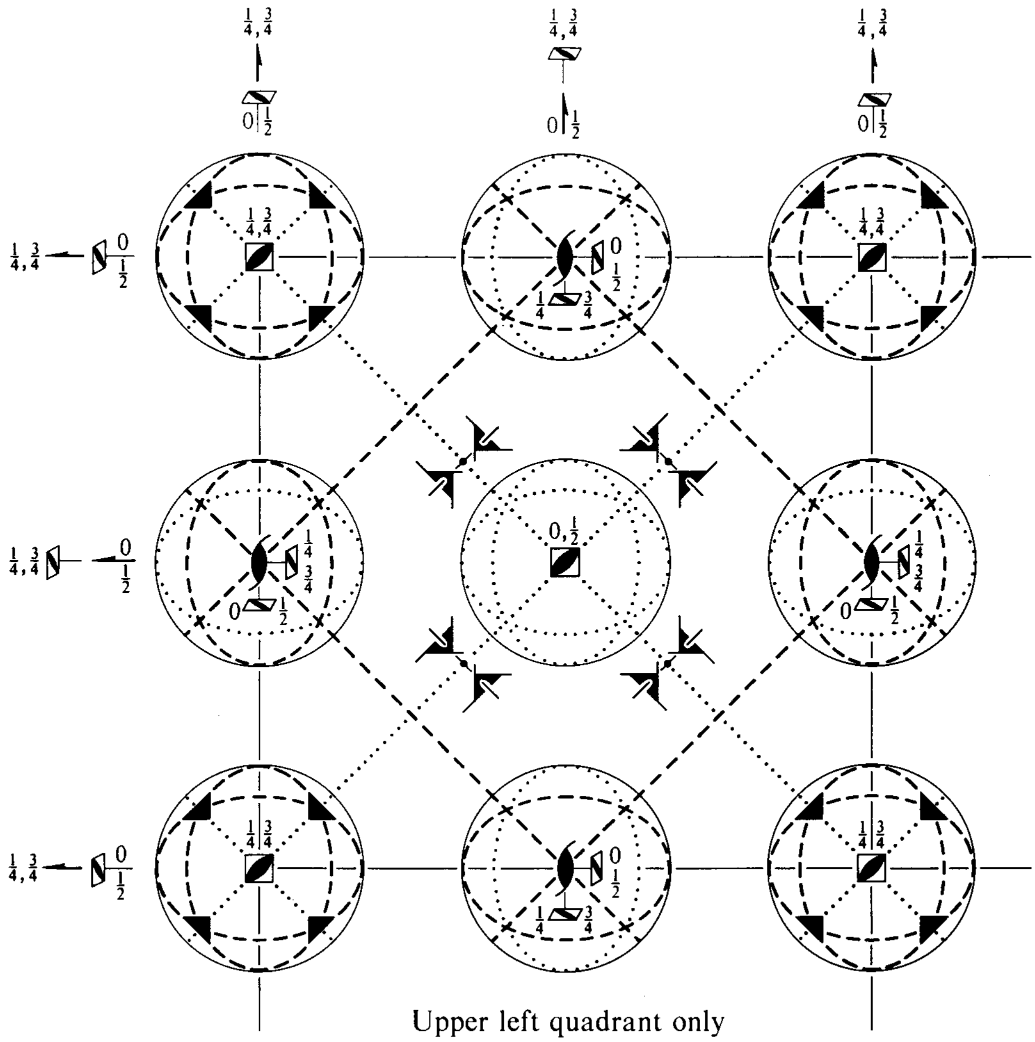
Minimal non-isomorphic supergroups

I [2] $Pn\bar{3}n$ (222); [2] $Pm\bar{3}n$ (223)

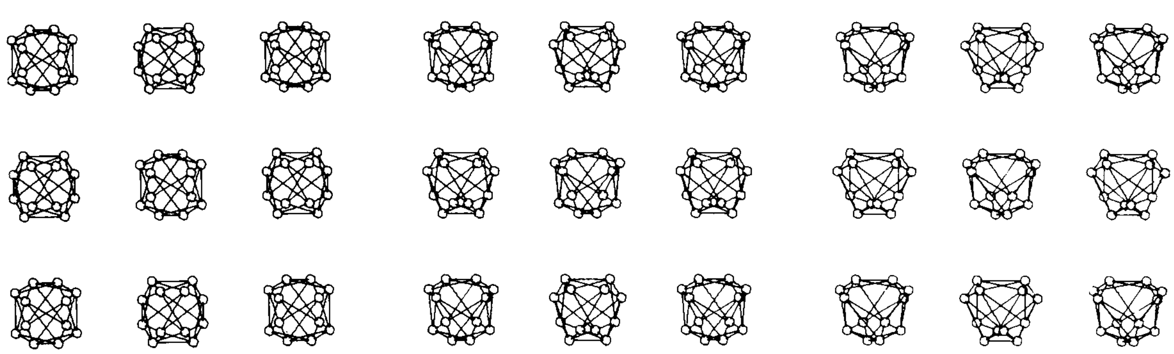
II [2] $I\bar{4}3m$ (217); [4] $F\bar{4}3c$ (219)

International Tables for Crystallography (2006). Vol. A, Space group 219, pp. 666–668.

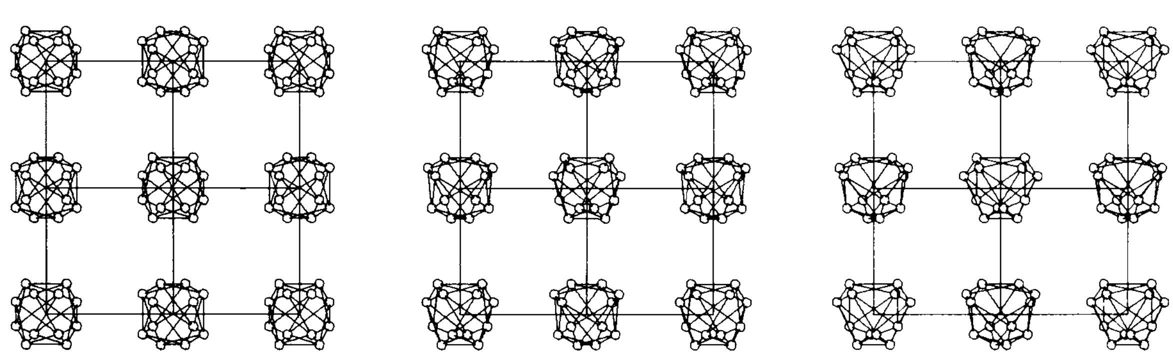
$F\bar{4}3c$	T_d^5	$\bar{4}3m$	Cubic
No. 219	$F\bar{4}3c$		Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Upper half of unit cell



Lower half of unit cell

Origin at 23

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $-\frac{1}{4} \le z \le \frac{1}{4}$; $y \le \min(x, \frac{1}{2} - x)$; $-y \le z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $3^{+}\ x,x,x$	(6) $3^{+}\ \bar{x},x,\bar{x}$	(7) $3^{+}\ x,\bar{x},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x},x$
(9) $3^{-}\ x,x,x$	(10) $3^{-}\ x,\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x},\bar{x},x$	(12) $3^{-}\ \bar{x},x,\bar{x}$
(13) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,z$	(14) $c\quad x+\frac{1}{2},\bar{x},z$	(15) $\bar{4}^{+}\ \frac{1}{2},0,z;\ \frac{1}{2},0,\frac{1}{4}$	(16) $\bar{4}^{-}\ 0,\frac{1}{2},z;\ 0,\frac{1}{2},\frac{1}{4}$
(17) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,y,y$	(18) $\bar{4}^{+}\ x,\frac{1}{2},0;\ \frac{1}{4},\frac{1}{2},0$	(19) $\bar{4}^{-}\ x,0,\frac{1}{2};\ \frac{1}{4},0,\frac{1}{2}$	(20) $a\quad x,y+\frac{1}{2},\bar{y}$
(21) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,y,x$	(22) $\bar{4}^{-}\ \frac{1}{2},y,0;\ \frac{1}{2},\frac{1}{4},0$	(23) $b\quad \bar{x}+\frac{1}{2},y,x$	(24) $\bar{4}^{+}\ 0,y,\frac{1}{2};\ 0,\frac{1}{4},\frac{1}{2}$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2\quad x,\frac{1}{4},\frac{1}{4}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{3},x-\frac{1}{6},x$	(6) $3^{+}\ \bar{x},x+\frac{1}{2},\bar{x}$	(7) $3^{+}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x+\frac{1}{6},x$	(10) $3^{-}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) $3^{-}\ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $g(\frac{1}{4},\frac{1}{4},0)\quad x+\frac{1}{4},x,z$	(14) $g(\frac{1}{4},-\frac{1}{4},0)\quad x+\frac{1}{4},\bar{x},z$	(15) $\bar{4}^{+}\ \frac{1}{4},-\frac{1}{4},z;\ \frac{1}{4},-\frac{1}{4},0$	(16) $\bar{4}^{-}\ \frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},0$
(17) $a\quad x,y,y$	(18) $\bar{4}^{+}\ x,0,0;\ \frac{1}{4},0,0$	(19) $\bar{4}^{-}\ x,0,0;\ \frac{1}{4},0,0$	(20) $a\quad x,y,\bar{y}$
(21) $g(\frac{1}{4},0,\frac{1}{4})\quad x+\frac{1}{4},y,x$	(22) $\bar{4}^{-}\ \frac{1}{4},y,-\frac{1}{4};\ \frac{1}{4},0,-\frac{1}{4}$	(23) $g(\frac{1}{4},0,-\frac{1}{4})\quad \bar{x}+\frac{1}{4},y,x$	(24) $\bar{4}^{+}\ \frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},0,\frac{1}{4}$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,0,\frac{1}{4}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x-\frac{1}{6},x$	(6) $3^{+}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^{+}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x-\frac{1}{3},x$	(10) $3^{-}\ x+\frac{1}{2},\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{1}{2},\bar{x},x$	(12) $3^{-}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $g(\frac{1}{4},\frac{1}{4},0)\quad x-\frac{1}{4},x,z$	(14) $g(-\frac{1}{4},\frac{1}{4},0)\quad x+\frac{1}{4},\bar{x},z$	(15) $\bar{4}^{+}\ \frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},0$	(16) $\bar{4}^{-}\ -\frac{1}{4},\frac{1}{4},z;\ -\frac{1}{4},\frac{1}{4},0$
(17) $g(0,\frac{1}{4},\frac{1}{4})\quad x,y+\frac{1}{4},y$	(18) $\bar{4}^{+}\ x,\frac{1}{4},-\frac{1}{4};\ 0,\frac{1}{4},-\frac{1}{4}$	(19) $\bar{4}^{-}\ x,\frac{1}{4},\frac{1}{4};\ 0,\frac{1}{4},\frac{1}{4}$	(20) $g(0,\frac{1}{4},-\frac{1}{4})\quad x,y+\frac{1}{4},\bar{y}$
(21) $b\quad x,y,x$	(22) $\bar{4}^{-}\ 0,y,0;\ 0,\frac{1}{4},0$	(23) $b\quad \bar{x},y,x$	(24) $\bar{4}^{+}\ 0,y,0;\ 0,\frac{1}{4},0$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x+\frac{1}{3},x$	(6) $3^{+}\ \bar{x}+\frac{1}{2},x,\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x},\bar{x}$	(8) $3^{+}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{3},x+\frac{1}{6},x$	(10) $3^{-}\ x,\bar{x}+\frac{1}{2},\bar{x}$	(11) $3^{-}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^{-}\ \bar{x},x+\frac{1}{2},\bar{x}$
(13) $c\quad x,x,z$	(14) $c\quad x,\bar{x},z$	(15) $\bar{4}^{+}\ 0,0,z;\ 0,0,\frac{1}{4}$	(16) $\bar{4}^{-}\ 0,0,z;\ 0,0,\frac{1}{4}$
(17) $g(0,\frac{1}{4},\frac{1}{4})\quad x,y-\frac{1}{4},y$	(18) $\bar{4}^{+}\ x,\frac{1}{4},\frac{1}{4};\ 0,\frac{1}{4},\frac{1}{4}$	(19) $\bar{4}^{-}\ x,-\frac{1}{4},\frac{1}{4};\ 0,-\frac{1}{4},\frac{1}{4}$	(20) $g(0,-\frac{1}{4},\frac{1}{4})\quad x,y+\frac{1}{4},\bar{y}$
(21) $g(\frac{1}{4},0,\frac{1}{4})\quad x-\frac{1}{4},y,x$	(22) $\bar{4}^{-}\ \frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},0,\frac{1}{4}$	(23) $g(-\frac{1}{4},0,\frac{1}{4})\quad \bar{x}+\frac{1}{4},y,x$	(24) $\bar{4}^{+}\ -\frac{1}{4},y,\frac{1}{4};\ -\frac{1}{4},0,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	Reflection conditions
			$(0,0,0)+\quad (0,\frac{1}{2},\frac{1}{2})+\quad (\frac{1}{2},0,\frac{1}{2})+\quad (\frac{1}{2},\frac{1}{2},0)+$	h,k,l permutable General:
96	*h*	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}$ (4) $x,\bar{y},\bar{z}$ (5) z,x,y (6) $z,\bar{x},\bar{y}$ (7) $\bar{z},\bar{x},y$ (8) $\bar{z},x,\bar{y}$ (9) y,z,x (10) $\bar{y},z,\bar{x}$ (11) $y,\bar{z},\bar{x}$ (12) $\bar{y},\bar{z},x$ (13) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ (14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (17) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$ (18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$ (19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$ (20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$ (21) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$ (22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$ (23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$ (24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	hkl : $h+k=2n$ and $h+l,k+l=2n$ $0kl$: $k,l=2n$ hhl : $h,l=2n$ $h00$: $h=2n$
				Special: as above, plus
48	*g*	2 . .	$x,\frac{1}{4},\frac{1}{4}$ $\bar{x},\frac{3}{4},\frac{1}{4}$ $\frac{1}{4},x,\frac{1}{4}$ $\frac{1}{4},\bar{x},\frac{3}{4}$ $\frac{1}{4},\frac{1}{4},x$ $\frac{3}{4},\frac{1}{4},\bar{x}$ $\frac{3}{4},x+\frac{1}{2},\frac{3}{4}$ $\frac{1}{4},\bar{x}+\frac{1}{2},\frac{3}{4}$ $x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$ $\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},x+\frac{1}{2}$ $\frac{3}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$	hkl : $h=2n$
48	*f*	2 . .	$x,0,0$ $\bar{x},0,0$ $0,x,0$ $0,\bar{x},0$ $0,0,x$ $0,0,\bar{x}$ $\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	hkl : $h=2n$
32	*e*	. 3 .	x,x,x $\bar{x},\bar{x},x$ $\bar{x},x,\bar{x}$ $x,\bar{x},\bar{x}$ $x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	hkl : $h=2n$
24	*d*	$\bar{4}$ . .	$\frac{1}{4},0,0$ $\frac{3}{4},0,0$ $0,\frac{1}{4},0$ $0,\frac{3}{4},0$ $0,0,\frac{1}{4}$ $0,0,\frac{3}{4}$	hkl : $h=2n$
24	*c*	$\bar{4}$ . .	$0,\frac{1}{4},\frac{1}{4}$ $0,\frac{3}{4},\frac{1}{4}$ $\frac{1}{4},0,\frac{1}{4}$ $\frac{1}{4},0,\frac{3}{4}$ $\frac{1}{4},\frac{1}{4},0$ $\frac{3}{4},\frac{1}{4},0$	hkl : $h=2n$
8	*b*	2 3 .	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$	hkl : $h=2n$
8	*a*	2 3 .	$0,0,0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [111] $p31m$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{4}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $F231$ ($F23$, 196) (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+

[3] $F\bar{4}1n$ ($I\bar{4}c2$, 120) (1; 2; 3; 4; 13; 14; 15; 16)+
[3] $F\bar{4}1n$ ($I\bar{4}c2$, 120) (1; 2; 3; 4; 17; 18; 19; 20)+
[3] $F\bar{4}1n$ ($I\bar{4}c2$, 120) (1; 2; 3; 4; 21; 22; 23; 24)+

[4] $F13n$ ($R3c$, 161) (1; 5; 9; 13; 17; 21)+
[4] $F13n$ ($R3c$, 161) (1; 6; 12; 14; 20; 21)+
[4] $F13n$ ($R3c$, 161) (1; 7; 10; 14; 17; 23)+
[4] $F13n$ ($R3c$, 161) (1; 8; 11; 13; 20; 23)+

IIa [4] $P\bar{4}3n$ (218) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24

[4] $P\bar{4}3n$ (218) 1; 2; 3; 4; 13; 14; 15; 16; (9; 10; 11; 12; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (5; 6; 7; 8; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$
[4] $P\bar{4}3n$ (218) 1; 2; 3; 4; 17; 18; 19; 20; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$
[4] $P\bar{4}3n$ (218) 1; 2; 3; 4; 21; 22; 23; 24; (5; 6; 7; 8; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$

[4] $P\bar{4}3n$ (218) 1; 5; 9; 13; 17; 21; (4; 6; 11; 15; 20; 22) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 8; 10; 16; 18; 23) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 7; 12; 14; 19; 24) + $(\frac{1}{2},\frac{1}{2},0)$
[4] $P\bar{4}3n$ (218) 1; 6; 12; 14; 20; 21; (4; 5; 10; 16; 17; 22) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 7; 11; 15; 19; 23) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 8; 9; 13; 18; 24) + $(\frac{1}{2},\frac{1}{2},0)$
[4] $P\bar{4}3n$ (218) 1; 7; 10; 14; 17; 23; (4; 8; 12; 16; 20; 24) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 6; 9; 15; 18; 21) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 5; 11; 13; 19; 22) + $(\frac{1}{2},\frac{1}{2},0)$
[4] $P\bar{4}3n$ (218) 1; 8; 11; 13; 20; 23; (4; 7; 9; 15; 17; 24) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 5; 12; 16; 19; 21) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 6; 10; 14; 18; 22) + $(\frac{1}{2},\frac{1}{2},0)$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $F\bar{4}3c$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (219)

Minimal non-isomorphic supergroups

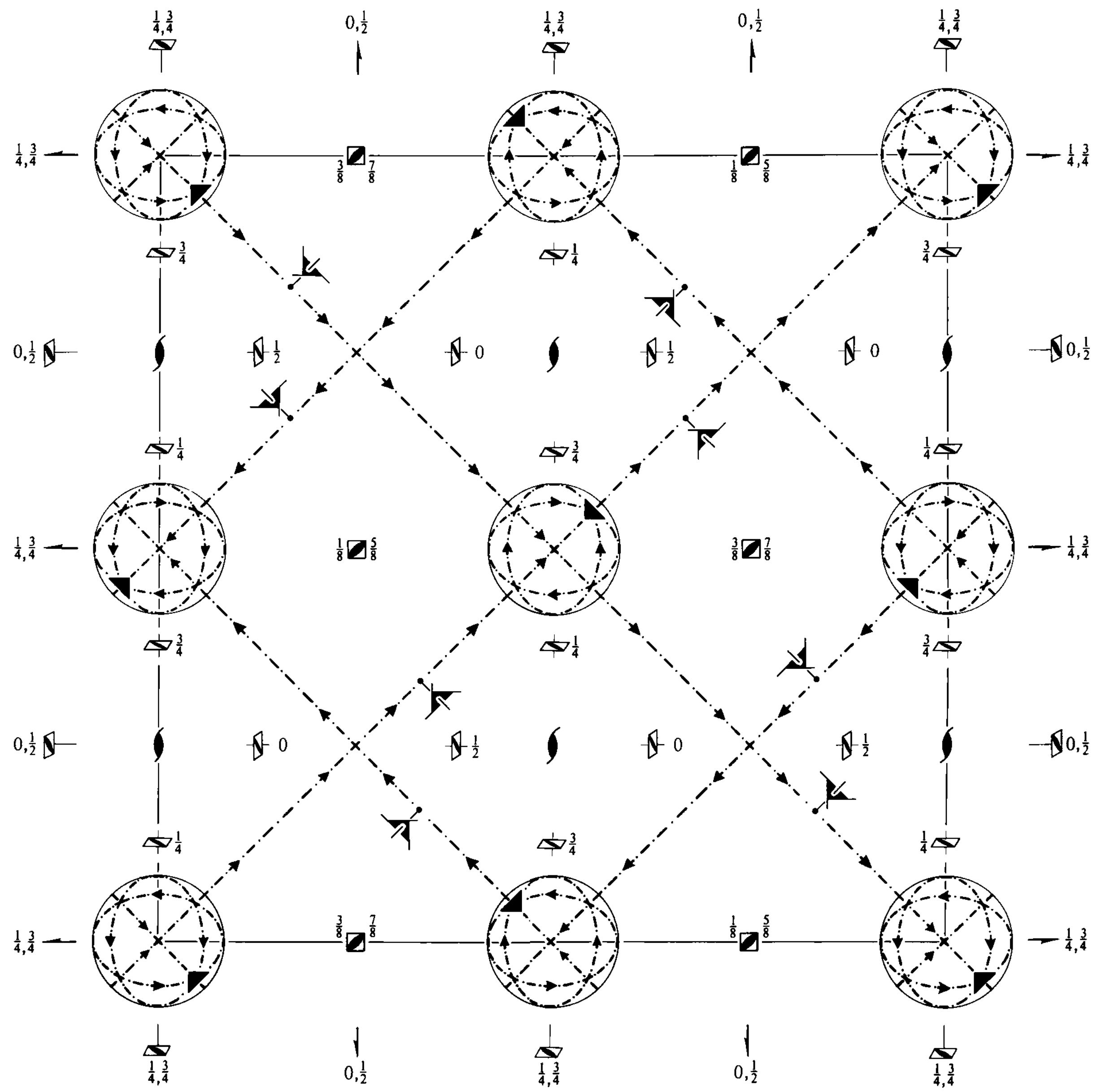
I [2] $Fm\bar{3}c$ (226); [2] $Fd\bar{3}c$ (228)

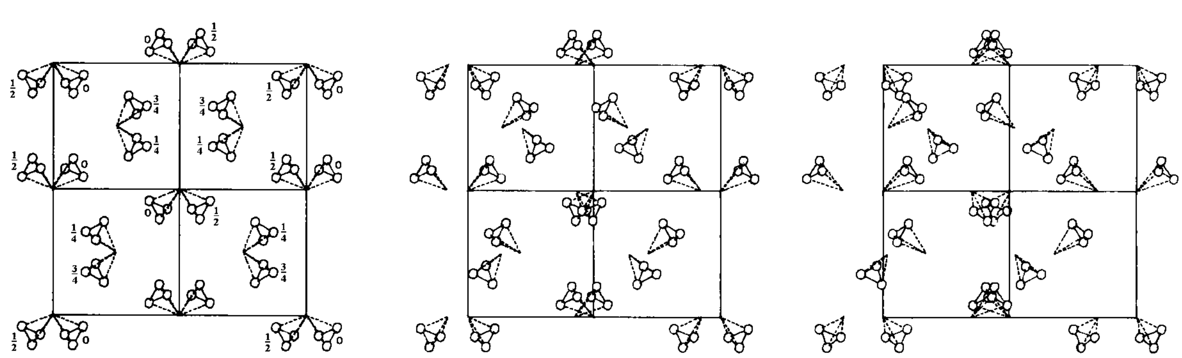
II [2] $P\bar{4}3m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (215)

International Tables for Crystallography (2006). Vol. A, Space group 220, pp. 669–671.

$I\bar{4}3d$ $\quad T_d^6$ $\quad \bar{4}3m$ $\quad$ Cubic

No. 220 $\quad I\bar{4}3d$ $\quad$ Patterson symmetry $Im\bar{3}m$





Origin on 3[111] at midpoint of three non-intersecting pairs of parallel $\bar{4}$ axes and of three non-intersecting pairs of parallel 2_1 axes

Asymmetric unit $\quad \frac{1}{4} \le x \le \frac{1}{2}; \quad \frac{1}{4} \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}; \quad z \le \min(x,y)$

Vertices $\quad \frac{1}{4},\frac{1}{4},0 \quad \frac{1}{2},\frac{1}{4},0 \quad \frac{1}{2},\frac{1}{2},0 \quad \frac{1}{4},\frac{1}{2},0$

$\frac{1}{4},\frac{1}{4},\frac{1}{4} \quad \frac{1}{2},\frac{1}{4},\frac{1}{4} \quad \frac{1}{2},\frac{1}{2},\frac{1}{2} \quad \frac{1}{4},\frac{1}{2},\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},0$
(5) $3^{+}\ x,x,x$	(6) $3^{+}\ \bar{x}+\frac{1}{2},x,\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^{-}\ x,x,x$	(10) $3^{-}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^{-}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\ \ \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^{-}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\ \ \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\ \ x,x,z$	(14) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})\ \ x+\frac{1}{2},\bar{x},z$	(15) $\bar{4}^{+}\ \frac{1}{2},-\frac{1}{4},z;\ \frac{1}{2},-\frac{1}{4},\frac{3}{8}$	(16) $\bar{4}^{-}\ 0,\frac{3}{4},z;\ 0,\frac{3}{4},\frac{1}{8}$
(17) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\ \ x,y,y$	(18) $\bar{4}^{+}\ x,\frac{1}{2},-\frac{1}{4};\ \frac{3}{8},\frac{1}{2},-\frac{1}{4}$	(19) $\bar{4}^{-}\ x,0,\frac{3}{4};\ \frac{1}{8},0,\frac{3}{4}$	(20) $d(\frac{3}{4},-\frac{1}{4},\frac{1}{4})\ \ x,y+\frac{1}{2},\bar{y}$
(21) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\ \ x,y,x$	(22) $\bar{4}^{-}\ \frac{3}{4},y,0;\ \frac{3}{4},\frac{1}{8},0$	(23) $d(\frac{1}{4},\frac{3}{4},-\frac{1}{4})\ \ \bar{x}+\frac{1}{2},y,x$	(24) $\bar{4}^{+}\ -\frac{1}{4},y,\frac{1}{2};\ -\frac{1}{4},\frac{3}{8},\frac{1}{2}$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\ \ 0,\frac{1}{4},z$	(3) $2\ \ \frac{1}{4},y,0$	(4) $2\ \ x,0,\frac{1}{4}$
(5) $3^{+}(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,x,x$	(6) $3^{+}(\frac{1}{6},-\frac{1}{6},\frac{1}{6})\ \ \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$	(7) $3^{+}(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\ \ x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(8) $3^{+}(\frac{1}{6},\frac{1}{6},-\frac{1}{6})\ \ \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(9) $3^{-}(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,x,x$	(10) $3^{-}(\frac{1}{6},-\frac{1}{6},-\frac{1}{6})\ \ x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^{-}(-\frac{1}{6},-\frac{1}{6},\frac{1}{6})\ \ \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^{-}(-\frac{1}{6},\frac{1}{6},-\frac{1}{6})\ \ \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})\ \ x,x,z$	(14) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})\ \ x+\frac{1}{2},\bar{x},z$	(15) $\bar{4}^{+}\ \frac{1}{2},\frac{1}{4},z;\ \frac{1}{2},\frac{1}{4},\frac{1}{8}$	(16) $\bar{4}^{-}\ 0,\frac{1}{4},z;\ 0,\frac{1}{4},\frac{3}{8}$
(17) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})\ \ x,y,y$	(18) $\bar{4}^{+}\ x,\frac{1}{2},\frac{1}{4};\ \frac{1}{8},\frac{1}{2},\frac{1}{4}$	(19) $\bar{4}^{-}\ x,0,\frac{1}{4};\ \frac{3}{8},0,\frac{1}{4}$	(20) $d(\frac{1}{4},\frac{1}{4},-\frac{1}{4})\ \ x,y+\frac{1}{2},\bar{y}$
(21) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})\ \ x,y,x$	(22) $\bar{4}^{-}\ \frac{1}{4},y,0;\ \frac{1}{4},\frac{3}{8},0$	(23) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})\ \ \bar{x}+\frac{1}{2},y,x$	(24) $\bar{4}^{+}\ \frac{1}{4},y,\frac{1}{2};\ \frac{1}{4},\frac{1}{8},\frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
			$(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$						h,k,l permutable General:
48	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$			$hkl:\ h+k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$			$0kl:\ k+l=2n$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$			$hhl:\ 2h+l=4n$
			(13) $y+\frac{1}{4},x+\frac{1}{4},z+\frac{1}{4}$	(14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(15) $y+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$	(16) $\bar{y}+\frac{3}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$			$h00:\ h=4n$
			(17) $x+\frac{1}{4},z+\frac{1}{4},y+\frac{1}{4}$	(18) $\bar{x}+\frac{3}{4},z+\frac{3}{4},\bar{y}+\frac{1}{4}$	(19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$	(20) $x+\frac{3}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$			
			(21) $z+\frac{1}{4},y+\frac{1}{4},x+\frac{1}{4}$	(22) $z+\frac{3}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(23) $\bar{z}+\frac{3}{4},y+\frac{3}{4},\bar{x}+\frac{1}{4}$	(24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$			
									Special: as above, plus
24	d	$2\,.\,.$	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{4},x,0$	$\frac{3}{4},\bar{x}+\frac{1}{2},0$	$0,\frac{1}{4},x$	$0,\frac{3}{4},\bar{x}+\frac{1}{2}$	$hkl:\ h=2n+1$
			$\frac{1}{4},x+\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\bar{x}+\frac{3}{4},0$	$x+\frac{1}{4},\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{3}{4},0,\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},x+\frac{1}{4}$	$0,\frac{1}{4},\bar{x}+\frac{3}{4}$	or $h=4n$
16	c	$.\,3\,.$	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$			$hkl:\ h=2n+1$
			$x+\frac{1}{4},x+\frac{1}{4},x+\frac{1}{4}$	$\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$	$x+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4}$	$\bar{x}+\frac{3}{4},x+\frac{3}{4},\bar{x}+\frac{1}{4}$			or $h+k+l=4n$
12	b	$\bar{4}\,.\,.$	$\frac{7}{8},0,\frac{1}{4}$	$\frac{5}{8},0,\frac{3}{4}$	$\frac{1}{4},\frac{7}{8},0$	$\frac{3}{4},\frac{5}{8},0$	$0,\frac{1}{4},\frac{7}{8}$	$0,\frac{3}{4},\frac{5}{8}$	$hkl:\ h,k=2n,\ h+k+l=4n$ or $h,k=2n+1,\ l=4n+2$
12	a	$\bar{4}\,.\,.$	$\frac{3}{8},0,\frac{1}{4}$	$\frac{1}{8},0,\frac{3}{4}$	$\frac{1}{4},\frac{3}{8},0$	$\frac{3}{4},\frac{1}{8},0$	$0,\frac{1}{4},\frac{3}{8}$	$0,\frac{3}{4},\frac{1}{8}$	or $h=8n,\ k=8n+4$ and $h+k+l=4n+2$ or $h=8n+1$ and $k=8n+3,\ l=4n$ or $h=8n+1$ and $k=8n+5,\ l=4n$ or $h=8n+7$ and $k=8n+3,\ l=4n$ or $h=8n+7$ and $k=8n+5,\ l=4n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})\quad \mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,\frac{1}{4},z$

Along [111] $p31m$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})\quad \mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})\quad \mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x+\frac{1}{4},0$

(*Continued on page 669*)

Maximal non-isomorphic subgroups

I [2] $I2_131$ ($I2_13$, 199) (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+

[3] $I\bar{4}1d$ ($I\bar{4}2d$, 122) (1; 2; 3; 4; 13; 14; 15; 16)+
[3] $I\bar{4}1d$ ($I\bar{4}2d$, 122) (1; 2; 3; 4; 17; 18; 19; 20)+
[3] $I\bar{4}1d$ ($I\bar{4}2d$, 122) (1; 2; 3; 4; 21; 22; 23; 24)+

[4] $I13d$ ($R3c$, 161) (1; 5; 9; 13; 17; 21)+
[4] $I13d$ ($R3c$, 161) (1; 6; 12; 14; 20; 21)+
[4] $I13d$ ($R3c$, 161) (1; 7; 10; 14; 17; 23)+
[4] $I13d$ ($R3c$, 161) (1; 8; 11; 13; 20; 23)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $I\bar{4}3d$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (220)

Minimal non-isomorphic supergroups

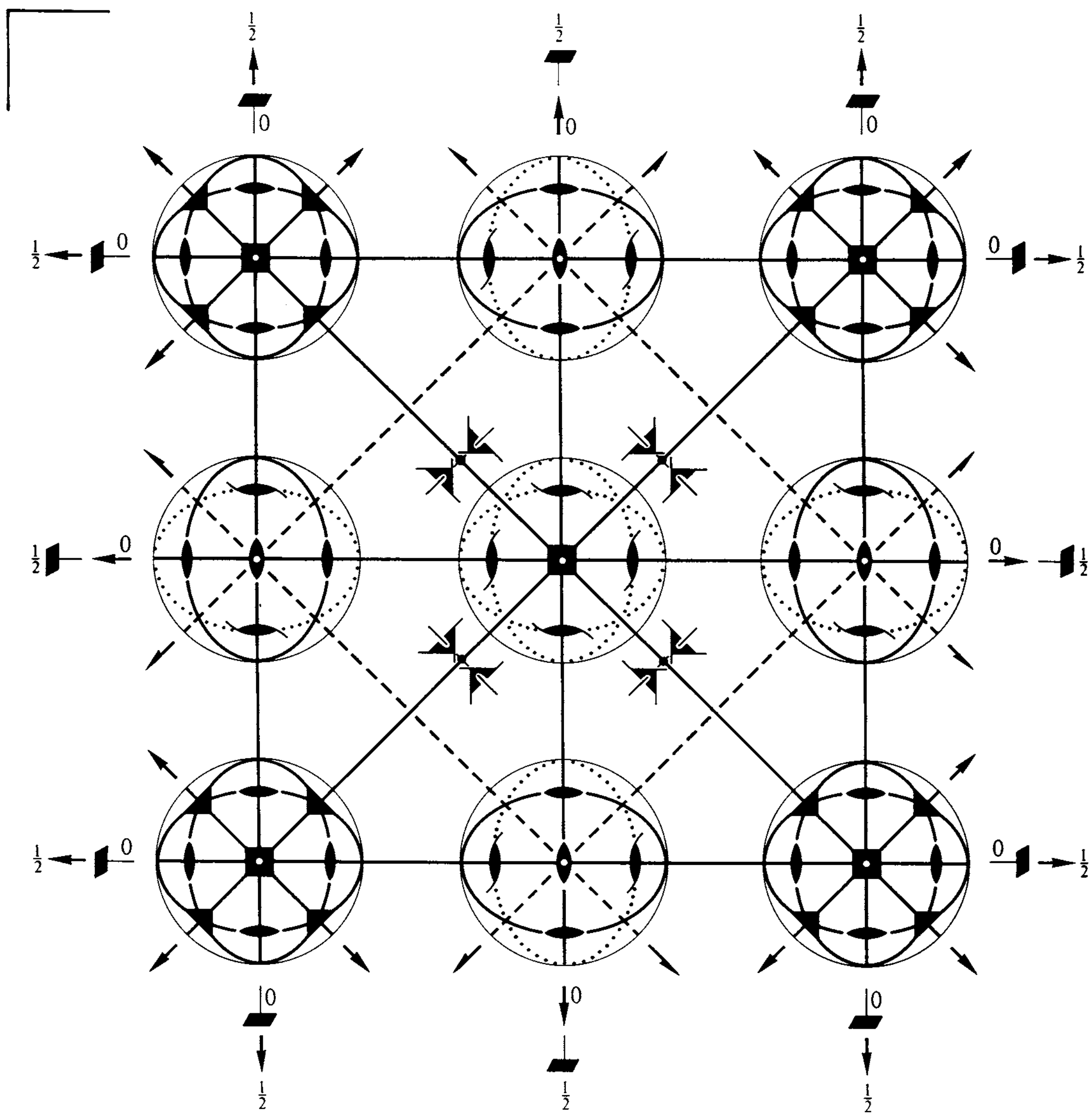
I [2] $Ia\bar{3}d$ (230)

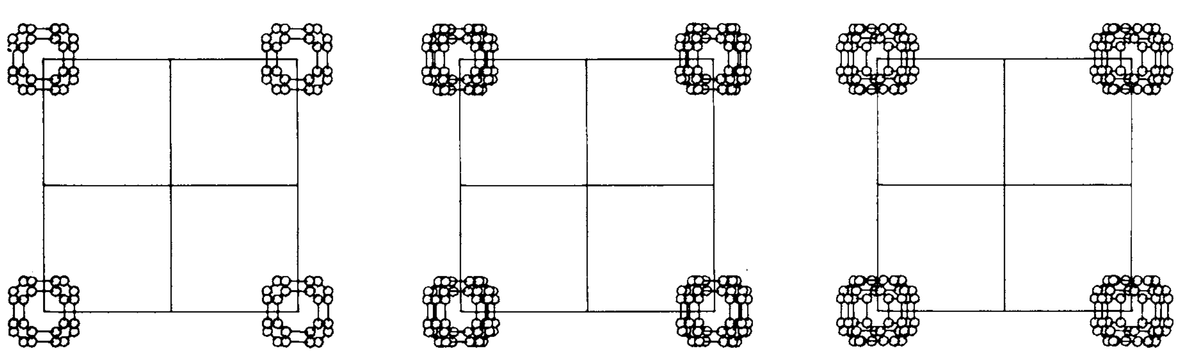
II [4] $P\bar{4}3n$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (218)

International Tables for Crystallography (2006). Vol. A, Space group 221, pp. 672–674.

$Pm\bar{3}m$ O_h^1 $m\bar{3}m$ Cubic

No. 221 $P\ 4/m\ \bar{3}\ 2/m$ Patterson symmetry $Pm\bar{3}m$





Origin at centre ($m\bar{3}m$)

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le x$; $z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(*given on page* 674)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

Reflection conditions: h,k,l permutable

General:

Multiplicity	Wyckoff letter	Site symmetry	Coordinates				Reflection conditions
48	n	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	no conditions
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$	
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$	
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$	
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$	
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$	
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$	
			(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$	
			(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$	
			(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x	

Special: no extra conditions

Multiplicity	Wyckoff letter	Site symmetry	Coordinates					
24	m	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x	$z,\bar{x},\bar{x}$
			$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$
			$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$x,\bar{x},z$	$\bar{x},x,z$	$x,z,\bar{x}$	$\bar{x},z,x$
			$\bar{x},\bar{z},\bar{x}$	$x,\bar{z},x$	$z,x,\bar{x}$	$z,\bar{x},x$	$\bar{z},x,x$	$\bar{z},\bar{x},\bar{x}$
24	l	$m..$	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$	$\frac{1}{2},y,\bar{z}$	$\frac{1}{2},\bar{y},\bar{z}$	$z,\frac{1}{2},y$	$z,\frac{1}{2},\bar{y}$
			$\bar{z},\frac{1}{2},y$	$\bar{z},\frac{1}{2},\bar{y}$	$y,z,\frac{1}{2}$	$\bar{y},z,\frac{1}{2}$	$y,\bar{z},\frac{1}{2}$	$\bar{y},\bar{z},\frac{1}{2}$
			$y,\frac{1}{2},\bar{z}$	$\bar{y},\frac{1}{2},\bar{z}$	$y,\frac{1}{2},z$	$\bar{y},\frac{1}{2},z$	$\frac{1}{2},z,\bar{y}$	$\frac{1}{2},z,y$
			$\frac{1}{2},\bar{z},\bar{y}$	$\frac{1}{2},\bar{z},y$	$z,y,\frac{1}{2}$	$z,\bar{y},\frac{1}{2}$	$\bar{z},y,\frac{1}{2}$	$\bar{z},\bar{y},\frac{1}{2}$
24	k	$m..$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$z,0,y$	$z,0,\bar{y}$
			$\bar{z},0,y$	$\bar{z},0,\bar{y}$	$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$
			$y,0,\bar{z}$	$\bar{y},0,\bar{z}$	$y,0,z$	$\bar{y},0,z$	$0,z,\bar{y}$	$0,z,y$
			$0,\bar{z},\bar{y}$	$0,\bar{z},y$	$z,y,0$	$z,\bar{y},0$	$\bar{z},y,0$	$\bar{z},\bar{y},0$
12	j	$m.m2$	$\frac{1}{2},y,y$	$\frac{1}{2},\bar{y},y$	$\frac{1}{2},y,\bar{y}$	$\frac{1}{2},\bar{y},\bar{y}$	$y,\frac{1}{2},y$	$y,\frac{1}{2},\bar{y}$
			$\bar{y},\frac{1}{2},y$	$\bar{y},\frac{1}{2},\bar{y}$	$y,y,\frac{1}{2}$	$\bar{y},y,\frac{1}{2}$	$y,\bar{y},\frac{1}{2}$	$\bar{y},\bar{y},\frac{1}{2}$
12	i	$m.m2$	$0,y,y$	$0,\bar{y},y$	$0,y,\bar{y}$	$0,\bar{y},\bar{y}$	$y,0,y$	$y,0,\bar{y}$
			$\bar{y},0,y$	$\bar{y},0,\bar{y}$	$y,y,0$	$\bar{y},y,0$	$y,\bar{y},0$	$\bar{y},\bar{y},0$
12	h	$mm2..$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$
			$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\frac{1}{2},\bar{x}$	$0,\frac{1}{2},x$
8	g	$.3m$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$		
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$		
6	f	$4m.m$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$
6	e	$4m.m$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
3	d	$4/mm.m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$			
3	c	$4/mm.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			
1	b	$m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
1	a	$m\bar{3}m$	$0,0,0$					

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\quad \mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad \mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
	[2] $P432$ (207)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[2] $Pm\bar{3}1$ ($Pm\bar{3}$, 200)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36
	[3] $P4/m12/m$ ($P4/mmm$, 123)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40
	[3] $P4/m12/m$ ($P4/mmm$, 123)	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44
	[3] $P4/m12/m$ ($P4/mmm$, 123)	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48
	[4] $P1\bar{3}2/m$ ($R\bar{3}m$, 166)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48
	[4] $P1\bar{3}2/m$ ($R\bar{3}m$, 166)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48
	[4] $P1\bar{3}2/m$ ($R\bar{3}m$, 166)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46
	[4] $P1\bar{3}2/m$ ($R\bar{3}m$, 166)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46

IIa none

IIb [2] $Fm\bar{3}c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (226); [2] $Fm\bar{3}m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (225); [4] $Im\bar{3}m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (229)

Maximal isomorphic subgroups of lowest index

IIc [27] $Pm\bar{3}m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (221)

Minimal non-isomorphic supergroups

I none

II [2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}m$ (225)

Symmetry operations

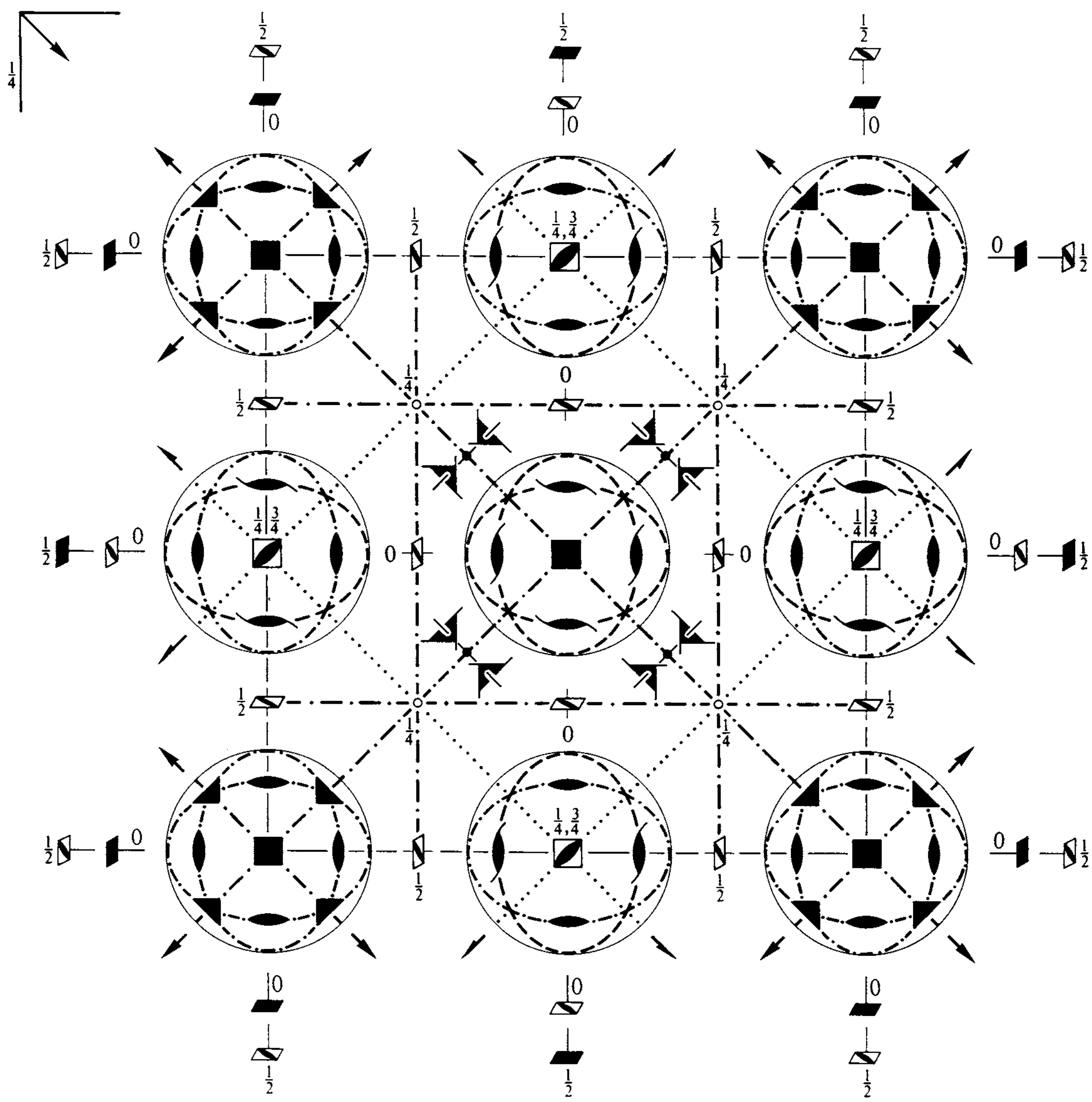
(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) 2 $x,x,0$	(14) 2 $x,\bar{x},0$	(15) 4^- $0,0,z$	(16) 4^+ $0,0,z$
(17) 4^- $x,0,0$	(18) 2 $0,y,y$	(19) 2 $0,y,\bar{y}$	(20) 4^+ $x,0,0$
(21) 4^+ $0,y,0$	(22) 2 $x,0,x$	(23) 4^- $0,y,0$	(24) 2 $\bar{x},0,x$
(25) $\bar{1}$ $0,0,0$	(26) m $x,y,0$	(27) m $x,0,z$	(28) m $0,y,z$
(29) $\bar{3}^+$ x,x,x; $0,0,0$	(30) $\bar{3}^+$ $\bar{x},x,\bar{x}$; $0,0,0$	(31) $\bar{3}^+$ $x,\bar{x},\bar{x}$; $0,0,0$	(32) $\bar{3}^+$ $\bar{x},\bar{x},x$; $0,0,0$
(33) $\bar{3}^-$ x,x,x; $0,0,0$	(34) $\bar{3}^-$ $x,\bar{x},\bar{x}$; $0,0,0$	(35) $\bar{3}^-$ $\bar{x},\bar{x},x$; $0,0,0$	(36) $\bar{3}^-$ $\bar{x},x,\bar{x}$; $0,0,0$
(37) m $x,\bar{x},z$	(38) m x,x,z	(39) $\bar{4}^-$ $0,0,z$; $0,0,0$	(40) $\bar{4}^+$ $0,0,z$; $0,0,0$
(41) $\bar{4}^-$ $x,0,0$; $0,0,0$	(42) m $x,y,\bar{y}$	(43) m x,y,y	(44) $\bar{4}^+$ $x,0,0$; $0,0,0$
(45) $\bar{4}^+$ $0,y,0$; $0,0,0$	(46) m $\bar{x},y,x$	(47) $\bar{4}^-$ $0,y,0$; $0,0,0$	(48) m x,y,x

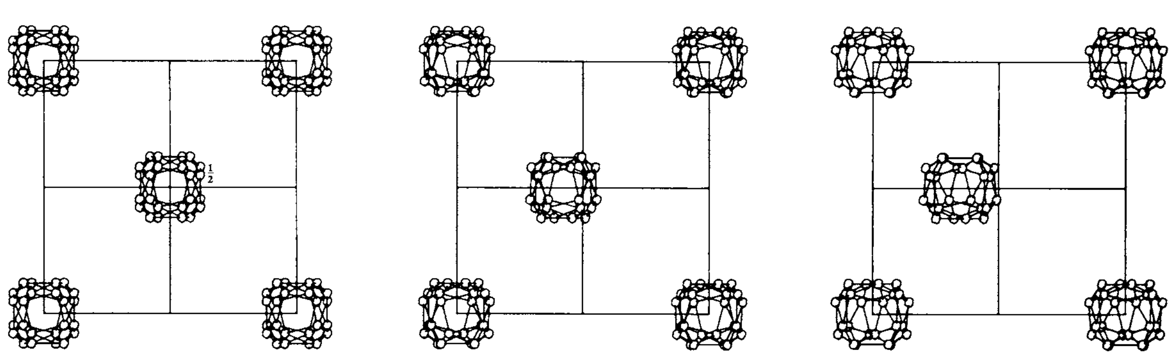
International Tables for Crystallography (2006). Vol. A, Space group 222, pp. 675–679.

$Pn\bar{3}n$ O_h^2 $m\bar{3}m$ Cubic

No. 222 $P\ 4/n\ \bar{3}\ 2/n$ Patterson symmetry $Pm\bar{3}m$

ORIGIN CHOICE 1





Origin at 432, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from centre ($\bar{3}$)

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2};\quad y \le x;\quad z \le y$

Vertices $0,0,0\quad \frac{1}{2},0,0\quad \frac{1}{2},\frac{1}{2},0\quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^{+} x,x,x	(6) 3^{+} $\bar{x},x,\bar{x}$	(7) 3^{+} $x,\bar{x},\bar{x}$	(8) 3^{+} $\bar{x},\bar{x},x$
(9) 3^{-} x,x,x	(10) 3^{-} $x,\bar{x},\bar{x}$	(11) 3^{-} $\bar{x},\bar{x},x$	(12) 3^{-} $\bar{x},x,\bar{x}$
(13) 2 $x,x,0$	(14) 2 $x,\bar{x},0$	(15) 4^{-} $0,0,z$	(16) 4^{+} $0,0,z$
(17) 4^{-} $x,0,0$	(18) 2 $0,y,y$	(19) 2 $0,y,\bar{y}$	(20) 4^{+} $x,0,0$
(21) 4^{+} $0,y,0$	(22) 2 $x,0,x$	(23) 4^{-} $0,y,0$	(24) 2 $\bar{x},0,x$
(25) $\bar{1}$ $\tfrac14,\tfrac14,\tfrac14$	(26) $n(\tfrac12,\tfrac12,0)$ $x,y,\tfrac14$	(27) $n(\tfrac12,0,\tfrac12)$ $x,\tfrac14,z$	(28) $n(0,\tfrac12,\tfrac12)$ $\tfrac14,y,z$
(29) $\bar{3}^{+}$ $x,x,x;$ $\tfrac14,\tfrac14,\tfrac14$	(30) $\bar{3}^{+}$ $\bar{x}-1,x+1,\bar{x};$ $-\tfrac14,\tfrac14,\tfrac34$	(31) $\bar{3}^{+}$ $x,\bar{x}+1,\bar{x};$ $\tfrac14,\tfrac34,-\tfrac14$	(32) $\bar{3}^{+}$ $\bar{x}+1,\bar{x},x;$ $\tfrac34,-\tfrac14,\tfrac14$
(33) $\bar{3}^{-}$ $x,x,x;$ $\tfrac14,\tfrac14,\tfrac14$	(34) $\bar{3}^{-}$ $x+1,\bar{x}-1,\bar{x};$ $\tfrac14,-\tfrac14,\tfrac34$	(35) $\bar{3}^{-}$ $\bar{x},\bar{x}+1,x;$ $-\tfrac14,\tfrac34,\tfrac14$	(36) $\bar{3}^{-}$ $\bar{x}+1,x,\bar{x};$ $\tfrac34,\tfrac14,-\tfrac14$
(37) c $x+\tfrac12,\bar{x},z$	(38) $n(\tfrac12,\tfrac12,\tfrac12)$ x,x,z	(39) $\bar{4}^{-}$ $0,\tfrac12,z;$ $0,\tfrac12,\tfrac14$	(40) $\bar{4}^{+}$ $\tfrac12,0,z;$ $\tfrac12,0,\tfrac14$
(41) $\bar{4}^{-}$ $x,0,\tfrac12;$ $\tfrac14,0,\tfrac12$	(42) a $x,y+\tfrac12,\bar{y}$	(43) $n(\tfrac12,\tfrac12,\tfrac12)$ x,y,y	(44) $\bar{4}^{+}$ $x,\tfrac12,0;$ $\tfrac14,\tfrac12,0$
(45) $\bar{4}^{+}$ $0,y,\tfrac12;$ $0,\tfrac14,\tfrac12$	(46) b $\bar{x}+\tfrac12,y,x$	(47) $\bar{4}^{-}$ $\tfrac12,y,0;$ $\tfrac12,\tfrac14,0$	(48) $n(\tfrac12,\tfrac12,\tfrac12)$ x,y,x

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

h,k,l permutable

General:

48 i 1

(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	$0kl:\ k+l=2n$
(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	$hhl:\ l=2n$
(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	$h00:\ h=2n$
(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$	
(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$	
(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$	
(25) $\bar{x}+\tfrac12,\bar{y}+\tfrac12,\bar{z}+\tfrac12$	(26) $x+\tfrac12,y+\tfrac12,\bar{z}+\tfrac12$	(27) $x+\tfrac12,\bar{y}+\tfrac12,z+\tfrac12$	(28) $\bar{x}+\tfrac12,y+\tfrac12,z+\tfrac12$	
(29) $\bar{z}+\tfrac12,\bar{x}+\tfrac12,\bar{y}+\tfrac12$	(30) $\bar{z}+\tfrac12,x+\tfrac12,y+\tfrac12$	(31) $z+\tfrac12,x+\tfrac12,\bar{y}+\tfrac12$	(32) $z+\tfrac12,\bar{x}+\tfrac12,y+\tfrac12$	
(33) $\bar{y}+\tfrac12,\bar{z}+\tfrac12,\bar{x}+\tfrac12$	(34) $y+\tfrac12,\bar{z}+\tfrac12,x+\tfrac12$	(35) $\bar{y}+\tfrac12,z+\tfrac12,x+\tfrac12$	(36) $y+\tfrac12,z+\tfrac12,\bar{x}+\tfrac12$	
(37) $\bar{y}+\tfrac12,\bar{x}+\tfrac12,z+\tfrac12$	(38) $y+\tfrac12,x+\tfrac12,z+\tfrac12$	(39) $\bar{y}+\tfrac12,x+\tfrac12,\bar{z}+\tfrac12$	(40) $y+\tfrac12,\bar{x}+\tfrac12,\bar{z}+\tfrac12$	
(41) $\bar{x}+\tfrac12,\bar{z}+\tfrac12,y+\tfrac12$	(42) $x+\tfrac12,\bar{z}+\tfrac12,\bar{y}+\tfrac12$	(43) $x+\tfrac12,z+\tfrac12,y+\tfrac12$	(44) $\bar{x}+\tfrac12,z+\tfrac12,\bar{y}+\tfrac12$	
(45) $\bar{z}+\tfrac12,\bar{y}+\tfrac12,x+\tfrac12$	(46) $\bar{z}+\tfrac12,y+\tfrac12,\bar{x}+\tfrac12$	(47) $z+\tfrac12,\bar{y}+\tfrac12,\bar{x}+\tfrac12$	(48) $z+\tfrac12,y+\tfrac12,x+\tfrac12$	

Special: as above, plus

24	h	..2	$0,y,y$	$0,\bar{y},y$	$0,y,\bar{y}$	$0,\bar{y},\bar{y}$					$hkl:\ h+k+l=2n$
			$y,0,y$	$y,0,\bar{y}$	$\bar{y},0,y$	$\bar{y},0,\bar{y}$					
			$y,y,0$	$\bar{y},y,0$	$y,\bar{y},0$	$\bar{y},\bar{y},0$					
			$\tfrac12,\bar{y}+\tfrac12,\bar{y}+\tfrac12$	$\tfrac12,y+\tfrac12,\bar{y}+\tfrac12$	$\tfrac12,\bar{y}+\tfrac12,y+\tfrac12$	$\tfrac12,y+\tfrac12,y+\tfrac12$					
			$\bar{y}+\tfrac12,\tfrac12,\bar{y}+\tfrac12$	$\bar{y}+\tfrac12,\tfrac12,y+\tfrac12$	$y+\tfrac12,\tfrac12,\bar{y}+\tfrac12$	$y+\tfrac12,\tfrac12,y+\tfrac12$					
			$\bar{y}+\tfrac12,\bar{y}+\tfrac12,\tfrac12$	$y+\tfrac12,\bar{y}+\tfrac12,\tfrac12$	$\bar{y}+\tfrac12,y+\tfrac12,\tfrac12$	$y+\tfrac12,y+\tfrac12,\tfrac12$					
24	g	2..	$x,0,\tfrac12$	$\bar{x},0,\tfrac12$	$\tfrac12,x,0$	$\tfrac12,\bar{x},0$	$0,\tfrac12,x$	$0,\tfrac12,\bar{x}$			$hkl:\ h+k+l=2n$
			$0,x,\tfrac12$	$0,\bar{x},\tfrac12$	$x,\tfrac12,0$	$\bar{x},\tfrac12,0$	$\tfrac12,0,\bar{x}$	$\tfrac12,0,x$			
			$\bar{x}+\tfrac12,\tfrac12,0$	$x+\tfrac12,\tfrac12,0$	$0,\bar{x}+\tfrac12,\tfrac12$	$0,x+\tfrac12,\tfrac12$	$\tfrac12,0,\bar{x}+\tfrac12$	$\tfrac12,0,x+\tfrac12$			
			$\tfrac12,\bar{x}+\tfrac12,0$	$\tfrac12,x+\tfrac12,0$	$\bar{x}+\tfrac12,0,\tfrac12$	$x+\tfrac12,0,\tfrac12$	$0,\tfrac12,x+\tfrac12$	$0,\tfrac12,\bar{x}+\tfrac12$			
16	f	.3.	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$					$hkl:\ h+k+l=2n$
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$					
			$\bar{x}+\tfrac12,\bar{x}+\tfrac12,\bar{x}+\tfrac12$	$x+\tfrac12,x+\tfrac12,\bar{x}+\tfrac12$	$x+\tfrac12,\bar{x}+\tfrac12,x+\tfrac12$	$\bar{x}+\tfrac12,x+\tfrac12,x+\tfrac12$					
			$\bar{x}+\tfrac12,\bar{x}+\tfrac12,x+\tfrac12$	$x+\tfrac12,x+\tfrac12,x+\tfrac12$	$\bar{x}+\tfrac12,x+\tfrac12,\bar{x}+\tfrac12$	$x+\tfrac12,\bar{x}+\tfrac12,\bar{x}+\tfrac12$					
12	e	4..	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$			$hkl:\ h+k+l=2n$
			$\bar{x}+\tfrac12,\tfrac12,\tfrac12$	$x+\tfrac12,\tfrac12,\tfrac12$	$\tfrac12,\bar{x}+\tfrac12,\tfrac12$	$\tfrac12,x+\tfrac12,\tfrac12$	$\tfrac12,\tfrac12,\bar{x}+\tfrac12$	$\tfrac12,\tfrac12,x+\tfrac12$			
12	d	$\bar{4}$..	$\tfrac14,0,\tfrac12$	$\tfrac34,0,\tfrac12$	$\tfrac12,\tfrac14,0$	$\tfrac12,\tfrac34,0$	$0,\tfrac12,\tfrac14$	$0,\tfrac12,\tfrac34$			$hkl:\ h+k+l=2n$
			$0,\tfrac14,\tfrac12$	$0,\tfrac34,\tfrac12$	$\tfrac14,\tfrac12,0$	$\tfrac34,\tfrac12,0$	$\tfrac12,0,\tfrac34$	$\tfrac12,0,\tfrac14$			
8	c	.$\bar{3}$.	$\tfrac14,\tfrac14,\tfrac14$	$\tfrac34,\tfrac34,\tfrac14$	$\tfrac34,\tfrac14,\tfrac34$	$\tfrac14,\tfrac34,\tfrac34$	$\tfrac14,\tfrac14,\tfrac34$	$\tfrac34,\tfrac34,\tfrac34$	$\tfrac14,\tfrac34,\tfrac14$	$\tfrac34,\tfrac14,\tfrac14$	$hkl:\ h,k,l=2n$
6	b	42.2	$0,\tfrac12,\tfrac12$	$\tfrac12,0,\tfrac12$	$\tfrac12,\tfrac12,0$	$\tfrac12,0,0$	$0,\tfrac12,0$	$0,0,\tfrac12$			$hkl:\ h+k+l=2n$
2	a	432	$0,0,0$	$\tfrac12,\tfrac12,\tfrac12$							$hkl:\ h+k+l=2n$

(*Continued on page 675*)

ORIGIN CHOICE 1

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

ORIGIN CHOICE 2

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

ORIGIN CHOICES 1 AND 2

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}3n$ (218)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
	[2] $P432$ (207)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[2] $Pn\bar{3}1$ ($Pn\bar{3}$, 201)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36
	{ [3] $P4/n\,1\,2/n$ ($P4/nnc$, 126)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40
	{ [3] $P4/n\,1\,2/n$ ($P4/nnc$, 126)	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44
	{ [3] $P4/n\,1\,2/n$ ($P4/nnc$, 126)	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $Pn\bar{3}n$ ($\mathbf{a}'=3\mathbf{a}, \mathbf{b}'=3\mathbf{b}, \mathbf{c}'=3\mathbf{c}$) (222)

Minimal non-isomorphic supergroups

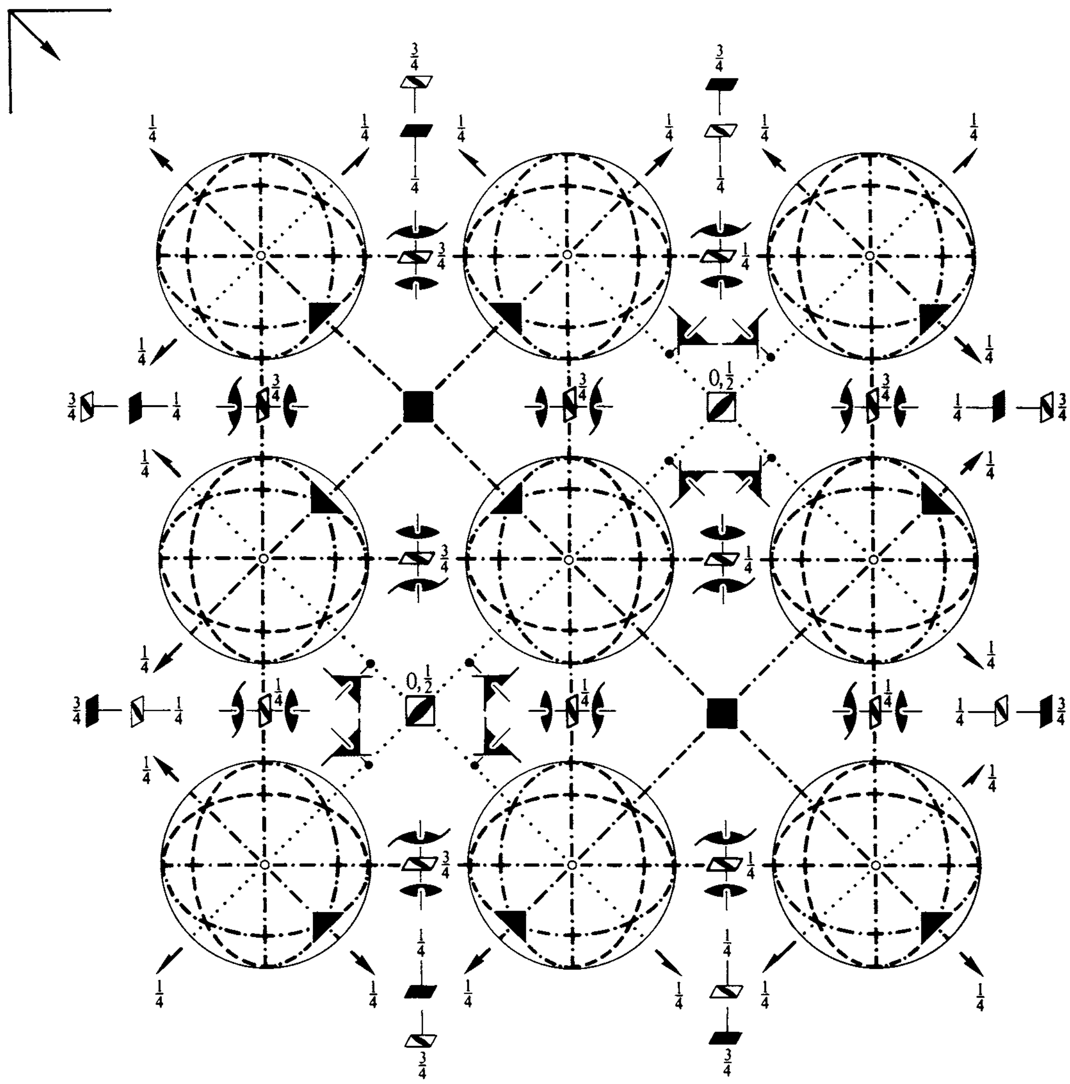
I none

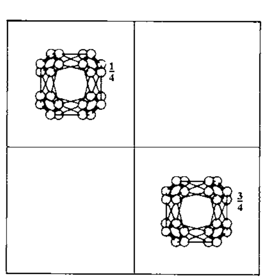
II [2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}c$ (226)

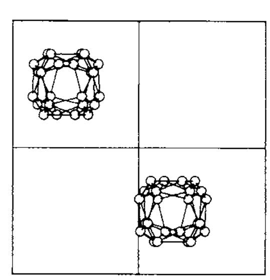
$Pn\bar{3}n$ O_h^2 $m\bar{3}m$ Cubic

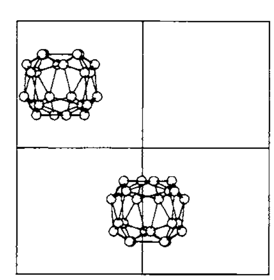
No. 222 $P\ 4/n\ \bar{3}\ 2/n$ Patterson symmetry $Pm\bar{3}m$

ORIGIN CHOICE 2









Origin at centre ($\bar{3}$), at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from 432

Asymmetric unit $\frac{1}{4} \leq x \leq \frac{3}{4}$; $\frac{1}{4} \leq y \leq \frac{3}{4}$; $\frac{1}{4} \leq z \leq \frac{3}{4}$; $y \leq x$; $z \leq y$

Vertices $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$

Symmetry operations

(1) 1	(2) $2\ \ \frac{1}{4},\frac{1}{4},z$	(3) $2\ \ \frac{1}{4},y,\frac{1}{4}$	(4) $2\ \ x,\frac{1}{4},\frac{1}{4}$
(5) $3^{+}\ x,x,x$	(6) $3^{+}\ \bar{x},x+\frac{1}{2},\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x},\bar{x}$	(8) $3^{+}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^{-}\ x,x,x$	(10) $3^{-}\ x+\frac{1}{2},\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) $3^{-}\ \bar{x},x+\frac{1}{2},\bar{x}$
(13) $2\ \ x,x,\frac{1}{4}$	(14) $2\ \ x,\bar{x}+\frac{1}{2},\frac{1}{4}$	(15) $4^{-}\ \frac{1}{4},\frac{1}{4},z$	(16) $4^{+}\ \frac{1}{4},\frac{1}{4},z$
(17) $4^{-}\ x,\frac{1}{4},\frac{1}{4}$	(18) $2\ \ \frac{1}{4},y,y$	(19) $2\ \ \frac{1}{4},y+\frac{1}{2},\bar{y}$	(20) $4^{+}\ x,\frac{1}{4},\frac{1}{4}$
(21) $4^{+}\ \frac{1}{4},y,\frac{1}{4}$	(22) $2\ \ x,\frac{1}{4},x$	(23) $4^{-}\ \frac{1}{4},y,\frac{1}{4}$	(24) $2\ \ \bar{x}+\frac{1}{2},\frac{1}{4},x$
(25) $\bar{1}\ \ 0,0,0$	(26) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$	(27) $n(\frac{1}{2},0,\frac{1}{2})\ \ x,0,z$	(28) $n(0,\frac{1}{2},\frac{1}{2})\ \ 0,y,z$
(29) $\bar{3}^{+}\ x,x,x;\ 0,0,0$	(30) $\bar{3}^{+}\ \bar{x}-1,x+\frac{1}{2},\bar{x};\ -\frac{1}{2},0,\frac{1}{2}$	(31) $\bar{3}^{+}\ x-\frac{1}{2},\bar{x}+1,\bar{x};\ 0,\frac{1}{2},-\frac{1}{2}$	(32) $\bar{3}^{+}\ \bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x;\ \frac{1}{2},-\frac{1}{2},0$
(33) $\bar{3}^{-}\ x,x,x;\ 0,0,0$	(34) $\bar{3}^{-}\ x+\frac{1}{2},\bar{x}-1,\bar{x};\ 0,-\frac{1}{2},\frac{1}{2}$	(35) $\bar{3}^{-}\ \bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x;\ -\frac{1}{2},\frac{1}{2},0$	(36) $\bar{3}^{-}\ \bar{x}+1,x-\frac{1}{2},\bar{x};\ \frac{1}{2},0,-\frac{1}{2}$
(37) $c\ \ x,\bar{x},z$	(38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,x,z$	(39) $\bar{4}^{-}\ -\frac{1}{4},\frac{1}{4},z;\ -\frac{1}{4},\frac{1}{4},0$	(40) $\bar{4}^{+}\ \frac{1}{4},-\frac{1}{4},z;\ \frac{1}{4},-\frac{1}{4},0$
(41) $\bar{4}^{-}\ x,-\frac{1}{4},\frac{1}{4};\ 0,-\frac{1}{4},\frac{1}{4}$	(42) $a\ \ x,y,\bar{y}$	(43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,y,y$	(44) $\bar{4}^{+}\ x,\frac{1}{4},-\frac{1}{4};\ 0,\frac{1}{4},-\frac{1}{4}$
(45) $\bar{4}^{+}\ -\frac{1}{4},y,\frac{1}{4};\ -\frac{1}{4},0,\frac{1}{4}$	(46) $b\ \ \bar{x},y,x$	(47) $\bar{4}^{-}\ \frac{1}{4},y,-\frac{1}{4};\ \frac{1}{4},0,-\frac{1}{4}$	(48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,y,x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

h,k,l permutable

General:

48 i 1

(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$
(5) z,x,y	(6) $z,\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(7) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},y$	(8) $\bar{z}+\frac{1}{2},x,\bar{y}+\frac{1}{2}$
(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	(11) $y,\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},x$
(13) $y,x,\bar{z}+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y,\bar{x}+\frac{1}{2},z$	(16) $\bar{y}+\frac{1}{2},x,z$
(17) $x,z,\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z,y$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x,\bar{z}+\frac{1}{2},y$
(21) $z,y,\bar{x}+\frac{1}{2}$	(22) $z,\bar{y}+\frac{1}{2},x$	(23) $\bar{z}+\frac{1}{2},y,x$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$
(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(27) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(28) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$
(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x+\frac{1}{2},y+\frac{1}{2}$	(31) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}$	(32) $z+\frac{1}{2},\bar{x},y+\frac{1}{2}$
(33) $\bar{y},\bar{z},\bar{x}$	(34) $y+\frac{1}{2},\bar{z},x+\frac{1}{2}$	(35) $\bar{y},z+\frac{1}{2},x+\frac{1}{2}$	(36) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}$
(37) $\bar{y},\bar{x},z+\frac{1}{2}$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y},x+\frac{1}{2},\bar{z}$	(40) $y+\frac{1}{2},\bar{x},\bar{z}$
(41) $\bar{x},\bar{z},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z},\bar{y}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x},z+\frac{1}{2},\bar{y}$
(45) $\bar{z},\bar{y},x+\frac{1}{2}$	(46) $\bar{z},y+\frac{1}{2},\bar{x}$	(47) $z+\frac{1}{2},\bar{y},\bar{x}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$

$0kl:\ k+l=2n$
$hhl:\ l=2n$
$h00:\ h=2n$

Special: as above, plus

24 h $..2$

$\frac{1}{4},y,y$	$\frac{1}{4},\bar{y}+\frac{1}{2},y$	$\frac{1}{4},y,\bar{y}+\frac{1}{2}$	$\frac{1}{4},\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{2}$
$y,\frac{1}{4},y$	$y,\frac{1}{4},\bar{y}+\frac{1}{2}$	$\bar{y}+\frac{1}{2},\frac{1}{4},y$	$\bar{y}+\frac{1}{2},\frac{1}{4},\bar{y}+\frac{1}{2}$
$y,y,\frac{1}{4}$	$\bar{y}+\frac{1}{2},y,\frac{1}{4}$	$y,\bar{y}+\frac{1}{2},\frac{1}{4}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{4}$
$\frac{3}{4},\bar{y},\bar{y}$	$\frac{3}{4},y+\frac{1}{2},\bar{y}$	$\frac{3}{4},\bar{y},y+\frac{1}{2}$	$\frac{3}{4},y+\frac{1}{2},y+\frac{1}{2}$
$\bar{y},\frac{3}{4},\bar{y}$	$\bar{y},\frac{3}{4},y+\frac{1}{2}$	$y+\frac{1}{2},\frac{3}{4},\bar{y}$	$y+\frac{1}{2},\frac{3}{4},y+\frac{1}{2}$
$\bar{y},\bar{y},\frac{3}{4}$	$y+\frac{1}{2},\bar{y},\frac{3}{4}$	$\bar{y},y+\frac{1}{2},\frac{3}{4}$	$y+\frac{1}{2},y+\frac{1}{2},\frac{3}{4}$

$hkl:\ h+k+l=2n$

24 g $2..$

$x,\frac{3}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{3}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$
$\frac{3}{4},x,\frac{1}{4}$	$\frac{3}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$	$x,\frac{1}{4},\frac{3}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\bar{x}+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},x$
$\bar{x},\frac{1}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{1}{4}$	$\frac{3}{4},x+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\bar{x}$	$\frac{1}{4},\frac{3}{4},x+\frac{1}{2}$
$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},x+\frac{1}{2},\frac{3}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},x+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\bar{x}$

$hkl:\ h+k+l=2n$

16 f $.3.$

x,x,x	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	$\bar{x}+\frac{1}{2},x,\bar{x}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$
$x,x,\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},x$	$\bar{x}+\frac{1}{2},x,x$
$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{x}$	$x+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},x+\frac{1}{2}$
$\bar{x},\bar{x},x+\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}$	$x+\frac{1}{2},\bar{x},\bar{x}$

$hkl:\ h+k+l=2n$

12 e $4..$

$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{1}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$
$\bar{x},\frac{3}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{3}{4}$	$\frac{3}{4},x+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\bar{x}$	$\frac{3}{4},\frac{3}{4},x+\frac{1}{2}$

$hkl:\ h+k+l=2n$

12 d $\bar{4}..$

$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$
$\frac{3}{4},0,\frac{1}{4}$	$\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{4},\frac{3}{4}$	$\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$

$hkl:\ h+k+l=2n$

8 c $.\bar{3}.$ $0,0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},0,\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$ $0,0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $0,\frac{1}{2},0$ $\frac{1}{2},0,0$ $hkl:\ h,k,l=2n$

6 b 42.2 $\frac{3}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{3}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},\frac{3}{4}$ $\frac{1}{4},\frac{3}{4},\frac{3}{4}$ $\frac{3}{4},\frac{1}{4},\frac{3}{4}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$ $hkl:\ h+k+l=2n$

2 a 432 $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$ $hkl:\ h+k+l=2n$

(*Continued on page 675*)

ORIGIN CHOICE 1

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

ORIGIN CHOICE 2

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

ORIGIN CHOICES 1 AND 2

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}3n$ (218)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
	[2] $P432$ (207)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[2] $Pn\bar{3}1$ ($Pn\bar{3}$, 201)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36
	{ [3] $P4/n12/n$ ($P4/nnc$, 126)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40
	{ [3] $P4/n12/n$ ($P4/nnc$, 126)	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44
	{ [3] $P4/n12/n$ ($P4/nnc$, 126)	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46
	{ [4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46
IIa	none	
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $Pn\bar{3}n$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (222)

Minimal non-isomorphic supergroups

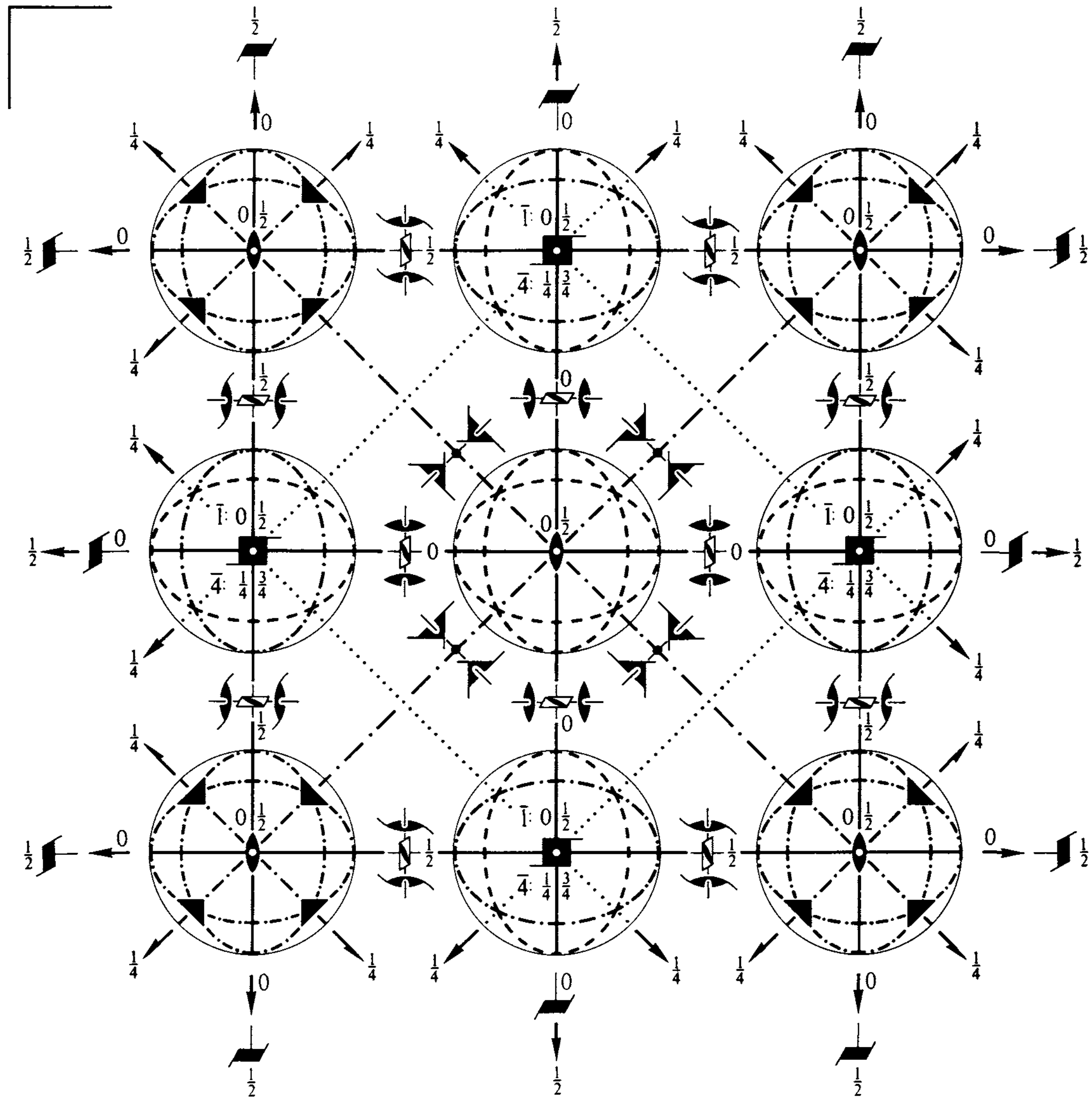
I none

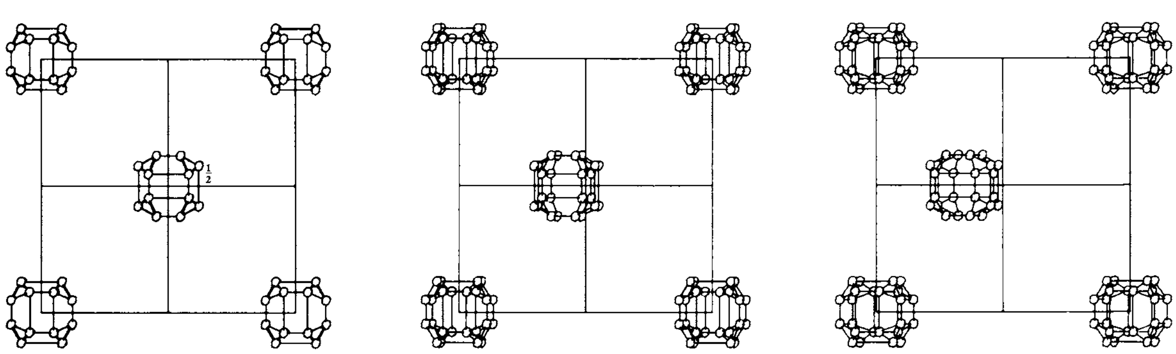
II [2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}c$ (226)

International Tables for Crystallography (2006). Vol. A, Space group 223, pp. 680–682.

$Pm\bar{3}n$ O_h^3 $m\bar{3}m$ Cubic

No. 223 $P\ 4_2/m\ \bar{3}\ 2/n$ Patterson symmetry $Pm\bar{3}m$





Origin at centre ($m\bar{3}$)

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$; $z \le \min(x, \frac{1}{2}-x, y, \frac{1}{2}-y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

Symmetry operations

(*given on page* 682)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									h,k,l permutable
									General:
48	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			hhl : $l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			$h00$: $h=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			
			(13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$			
			(17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$			
			(21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$			
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$			
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$			
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$			
			(37) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$			
			(41) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$			
			(45) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(46) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$			
									Special: as above, plus
24	k	$m\,.\,.$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$			no extra conditions
			$z,0,y$	$z,0,\bar{y}$	$\bar{z},0,y$	$\bar{z},0,\bar{y}$			
			$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$			
			$y+\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\bar{y}+\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$y+\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\bar{y}+\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			
			$\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	$\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	$\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	$\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$			
			$z+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$z+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\bar{z}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$			
24	j	$.\,.\,2$	$\frac{1}{4},y,y+\frac{1}{2}$	$\frac{3}{4},\bar{y},y+\frac{1}{2}$	$\frac{3}{4},y,\bar{y}+\frac{1}{2}$	$\frac{1}{4},\bar{y},\bar{y}+\frac{1}{2}$			hkl : $h=2n$
			$y+\frac{1}{2},\frac{1}{4},y$	$y+\frac{1}{2},\frac{3}{4},\bar{y}$	$\bar{y}+\frac{1}{2},\frac{3}{4},y$	$\bar{y}+\frac{1}{2},\frac{1}{4},\bar{y}$			
			$y,y+\frac{1}{2},\frac{1}{4}$	$\bar{y},y+\frac{1}{2},\frac{3}{4}$	$y,\bar{y}+\frac{1}{2},\frac{3}{4}$	$\bar{y},\bar{y}+\frac{1}{2},\frac{1}{4}$			
			$\frac{3}{4},\bar{y},\bar{y}+\frac{1}{2}$	$\frac{1}{4},y,\bar{y}+\frac{1}{2}$	$\frac{1}{4},\bar{y},y+\frac{1}{2}$	$\frac{3}{4},y,y+\frac{1}{2}$			
			$\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}$	$\bar{y}+\frac{1}{2},\frac{1}{4},y$	$y+\frac{1}{2},\frac{1}{4},\bar{y}$	$y+\frac{1}{2},\frac{3}{4},y$			
			$\bar{y},\bar{y}+\frac{1}{2},\frac{3}{4}$	$y,\bar{y}+\frac{1}{2},\frac{1}{4}$	$\bar{y},y+\frac{1}{2},\frac{1}{4}$	$y,y+\frac{1}{2},\frac{3}{4}$			
16	i	$.\,3\,.$	x,x,x	$\bar{x},\bar{x},x$					hkl : $h+k+l=2n$
			$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$					
			$x+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$					
			$x+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$					
			$\bar{x},\bar{x},\bar{x}$	$x,x,\bar{x}$					
			$x,\bar{x},x$	$\bar{x},x,x$					
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$					
			$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$					
12	h	$m\,m\,2\,.\,.$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$			hkl : $h=2n$
			$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$	$0,x+\frac{1}{2},\frac{1}{2}$	$0,\bar{x}+\frac{1}{2},\frac{1}{2}$			
			$x+\frac{1}{2},\frac{1}{2},0$	$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\bar{x}+\frac{1}{2}$	$\frac{1}{2},0,x+\frac{1}{2}$			
12	g	$m\,m\,2\,.\,.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$			hkl : $h=2n$
			$0,\frac{1}{2},x$	$0,\frac{1}{2},\bar{x}$	$\frac{1}{2},x+\frac{1}{2},0$	$\frac{1}{2},\bar{x}+\frac{1}{2},0$			
			$x+\frac{1}{2},0,\frac{1}{2}$	$\bar{x}+\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\bar{x}+\frac{1}{2}$	$0,\frac{1}{2},x+\frac{1}{2}$			
12	f	$m\,m\,2\,.\,.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$			hkl : $h+k+l=2n$
			$0,0,x$	$0,0,\bar{x}$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$			
			$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$			
8	e	$.\,3\,2$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$			hkl : $h,k,l=2n$
			$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$			
6	d	$\bar{4}\,m\,.\,2$	$\frac{1}{4},\frac{1}{2},0$	$\frac{3}{4},\frac{1}{2},0$	$0,\frac{1}{4},\frac{1}{2}$	$0,\frac{3}{4},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	hkl : $h+k+l=2n$ or $h=2n+1$, $k=4n$ and $l=4n+2$ (for d and c)
6	c	$\bar{4}\,m\,.\,2$	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},0$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	
6	b	$m\,m\,m\,.\,.$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	hkl : $h+k+l=2n$
2	a	$m\,\bar{3}\,.$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, \frac{1}{2}, z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
Origin at x, x, x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}3n$ (218)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
	[2] $P4_232$ (208)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[2] $Pm\bar{3}1$ ($Pm\bar{3}$, 200)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36
	[3] $P4_2/m12/n$ ($P4_2/mmc$, 131)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40
	[3] $P4_2/m12/n$ ($P4_2/mmc$, 131)	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44
	[3] $P4_2/m12/n$ ($P4_2/mmc$, 131)	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48
	[4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48
	[4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48
	[4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46
	[4] $P1\bar{3}2/n$ ($R\bar{3}c$, 167)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46

IIa none

IIb [4] $Ia\bar{3}d$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (230)

Maximal isomorphic subgroups of lowest index

IIc [27] $Pm\bar{3}n$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (223)

Minimal non-isomorphic supergroups

I none

II [2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}c$ (226)

Symmetry operations

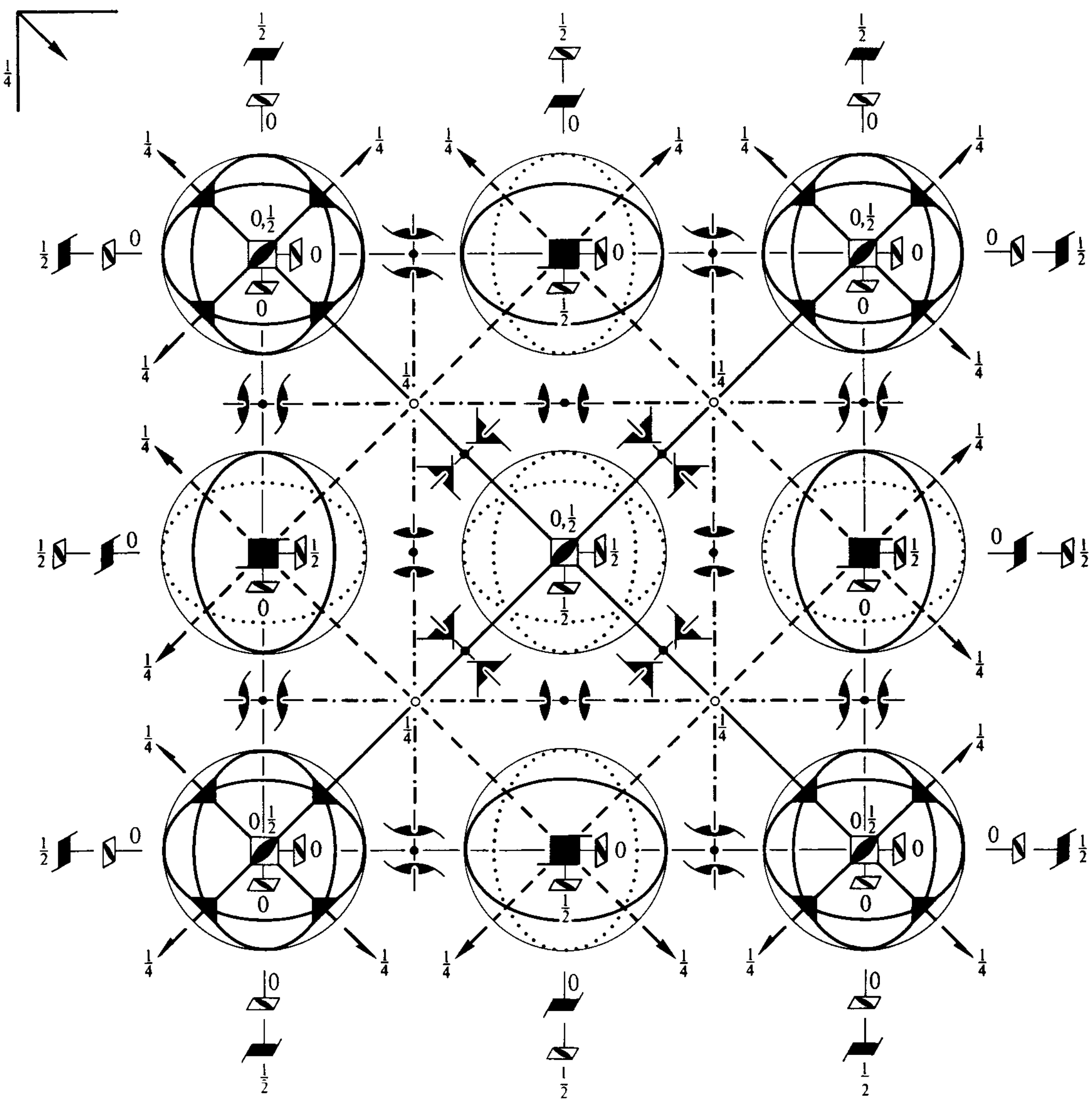
(1) 1	(2) $2\ \ 0,0,z$	(3) $2\ \ 0,y,0$	(4) $2\ \ x,0,0$
(5) $3^+\ x,x,x$	(6) $3^+\ \bar{x},x,\bar{x}$	(7) $3^+\ x,\bar{x},\bar{x}$	(8) $3^+\ \bar{x},\bar{x},x$
(9) $3^-\ x,x,x$	(10) $3^-\ x,\bar{x},\bar{x}$	(11) $3^-\ \bar{x},\bar{x},x$	(12) $3^-\ \bar{x},x,\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x,\frac{1}{4}$	(14) $2\ \ x,\bar{x}+\frac{1}{2},\frac{1}{4}$	(15) $4^-(0,0,\frac{1}{2})\ \ \frac{1}{2},0,z$	(16) $4^+(0,0,\frac{1}{2})\ \ 0,\frac{1}{2},z$
(17) $4^-(\frac{1}{2},0,0)\ \ x,\frac{1}{2},0$	(18) $2(0,\frac{1}{2},\frac{1}{2})\ \ \frac{1}{4},y,y$	(19) $2\ \ \frac{1}{4},y+\frac{1}{2},\bar{y}$	(20) $4^+(\frac{1}{2},0,0)\ \ x,0,\frac{1}{2}$
(21) $4^+(0,\frac{1}{2},0)\ \ \frac{1}{2},y,0$	(22) $2(\frac{1}{2},0,\frac{1}{2})\ \ x,\frac{1}{4},x$	(23) $4^-(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{2}$	(24) $2\ \ \bar{x}+\frac{1}{2},\frac{1}{4},x$
(25) $\bar{1}\ \ 0,0,0$	(26) $m\ \ x,y,0$	(27) $m\ \ x,0,z$	(28) $m\ \ 0,y,z$
(29) $\bar{3}^+\ x,x,x;\ \ 0,0,0$	(30) $\bar{3}^+\ \bar{x},x,\bar{x};\ \ 0,0,0$	(31) $\bar{3}^+\ x,\bar{x},\bar{x};\ \ 0,0,0$	(32) $\bar{3}^+\ \bar{x},\bar{x},x;\ \ 0,0,0$
(33) $\bar{3}^-\ x,x,x;\ \ 0,0,0$	(34) $\bar{3}^-\ x,\bar{x},\bar{x};\ \ 0,0,0$	(35) $\bar{3}^-\ \bar{x},\bar{x},x;\ \ 0,0,0$	(36) $\bar{3}^-\ \bar{x},x,\bar{x};\ \ 0,0,0$
(37) $c\ \ x+\frac{1}{2},\bar{x},z$	(38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,x,z$	(39) $\bar{4}^-\ 0,\frac{1}{2},z;\ \ 0,\frac{1}{2},\frac{1}{4}$	(40) $\bar{4}^+\ \frac{1}{2},0,z;\ \ \frac{1}{2},0,\frac{1}{4}$
(41) $\bar{4}^-\ x,0,\frac{1}{2};\ \ \frac{1}{4},0,\frac{1}{2}$	(42) $a\ \ x,y+\frac{1}{2},\bar{y}$	(43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,y,y$	(44) $\bar{4}^+\ x,\frac{1}{2},0;\ \ \frac{1}{4},\frac{1}{2},0$
(45) $\bar{4}^+\ 0,y,\frac{1}{2};\ \ 0,\frac{1}{4},\frac{1}{2}$	(46) $b\ \ \bar{x}+\frac{1}{2},y,x$	(47) $\bar{4}^-\ \frac{1}{2},y,0;\ \ \frac{1}{2},\frac{1}{4},0$	(48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,y,x$

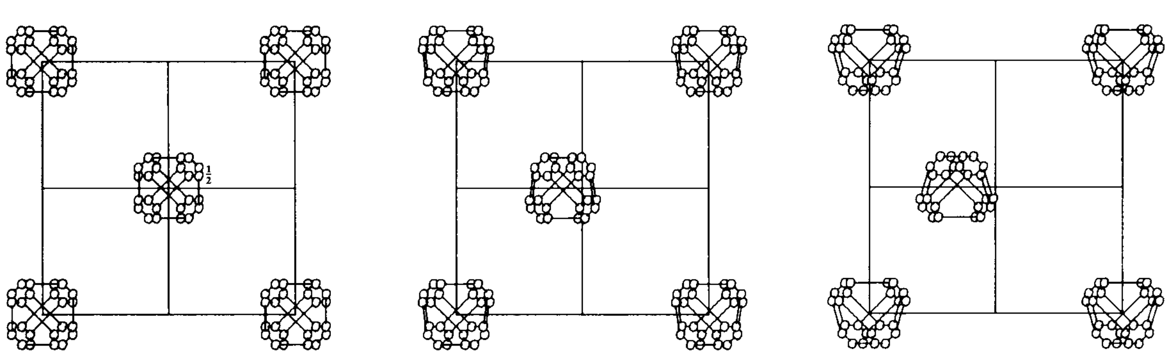
International Tables for Crystallography (2006). Vol. A, Space group 224, pp. 683–687.

$Pn\bar{3}m$ O_h^4 $m\bar{3}m$ Cubic

No. 224 $P\ 4_2/n\ \bar{3}\ 2/m$ Patterson symmetry $Pm\bar{3}m$

ORIGIN CHOICE 1





Origin at $\bar{4}3m$, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from centre ($\bar{3}m$)

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $-\frac{1}{4} \le z \le \frac{1}{4}$; $y \le x$; $\max(x-\frac{1}{2},-y) \le z \le \min(\frac{1}{2}-x,y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$

Symmetry operations

(*given on page* 683)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

h,k,l permutable

General:

Mult.	Letter	Site symm.	Coordinates				Reflection conditions
48	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	$0kl$: $k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	$h00$: $h=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	
			(13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	
			(17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	
			(21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	
			(25) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(26) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(27) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	
			(29) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y+\frac{1}{2}$	(31) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	(32) $z+\frac{1}{2},\bar{x}+\frac{1}{2},y+\frac{1}{2}$	
			(33) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(34) $y+\frac{1}{2},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x+\frac{1}{2}$	(36) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	
			(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$	
			(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$	
			(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x	

Special: as above, plus

Mult.	Letter	Site symm.	Coordinates						Reflection conditions
24	k	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$			no extra conditions
			z,x,x	$z,\bar{x},\bar{x}$	$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$			
			x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$			
			$x+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$			
			$x+\frac{1}{2},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},z+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{z}+\frac{1}{2},x+\frac{1}{2}$			
			$z+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$z+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{z}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$			
24	j	$..2$	$\frac{1}{4},y,y+\frac{1}{2}$	$\frac{3}{4},\bar{y},y+\frac{1}{2}$	$\frac{3}{4},y,\bar{y}+\frac{1}{2}$	$\frac{1}{4},\bar{y},\bar{y}+\frac{1}{2}$	$y+\frac{1}{2},\frac{1}{4},y$	$y+\frac{1}{2},\frac{3}{4},\bar{y}$	no extra conditions
			$\bar{y}+\frac{1}{2},\frac{3}{4},y$	$\bar{y}+\frac{1}{2},\frac{1}{4},\bar{y}$	$y,y+\frac{1}{2},\frac{1}{4}$	$\bar{y},y+\frac{1}{2},\frac{3}{4}$	$y,\bar{y}+\frac{1}{2},\frac{3}{4}$	$\bar{y},\bar{y}+\frac{1}{2},\frac{1}{4}$	
			$\frac{1}{4},\bar{y}+\frac{1}{2},\bar{y}$	$\frac{3}{4},y+\frac{1}{2},\bar{y}$	$\frac{3}{4},\bar{y}+\frac{1}{2},y$	$\frac{1}{4},y+\frac{1}{2},y$	$\bar{y},\frac{1}{4},\bar{y}+\frac{1}{2}$	$\bar{y},\frac{3}{4},y+\frac{1}{2}$	
			$y,\frac{3}{4},\bar{y}+\frac{1}{2}$	$y,\frac{1}{4},y+\frac{1}{2}$	$\bar{y}+\frac{1}{2},\bar{y},\frac{1}{4}$	$y+\frac{1}{2},\bar{y},\frac{3}{4}$	$\bar{y}+\frac{1}{2},y,\frac{3}{4}$	$y+\frac{1}{2},y,\frac{1}{4}$	
24	i	$..2$	$\frac{1}{4},y,\bar{y}+\frac{1}{2}$	$\frac{3}{4},\bar{y},\bar{y}+\frac{1}{2}$	$\frac{3}{4},y,y+\frac{1}{2}$	$\frac{1}{4},\bar{y},y+\frac{1}{2}$	$\bar{y}+\frac{1}{2},\frac{1}{4},y$	$\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}$	no extra conditions
			$y+\frac{1}{2},\frac{3}{4},y$	$y+\frac{1}{2},\frac{1}{4},\bar{y}$	$y,\bar{y}+\frac{1}{2},\frac{1}{4}$	$\bar{y},\bar{y}+\frac{1}{2},\frac{3}{4}$	$y,y+\frac{1}{2},\frac{3}{4}$	$\bar{y},y+\frac{1}{2},\frac{1}{4}$	
			$\frac{1}{4},\bar{y}+\frac{1}{2},y$	$\frac{3}{4},y+\frac{1}{2},y$	$\frac{3}{4},\bar{y}+\frac{1}{2},\bar{y}$	$\frac{1}{4},y+\frac{1}{2},\bar{y}$	$y,\frac{1}{4},\bar{y}+\frac{1}{2}$	$y,\frac{3}{4},y+\frac{1}{2}$	
			$\bar{y},\frac{3}{4},\bar{y}+\frac{1}{2}$	$\bar{y},\frac{1}{4},y+\frac{1}{2}$	$\bar{y}+\frac{1}{2},y,\frac{1}{4}$	$y+\frac{1}{2},y,\frac{3}{4}$	$\bar{y}+\frac{1}{2},\bar{y},\frac{3}{4}$	$y+\frac{1}{2},\bar{y},\frac{1}{4}$	
24	h	$2..$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$0,\frac{1}{2},x$	$0,\frac{1}{2},\bar{x}$	hkl : $h+k+l=2n$
			$\frac{1}{2},x+\frac{1}{2},0$	$\frac{1}{2},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},0,\frac{1}{2}$	$\bar{x}+\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\bar{x}+\frac{1}{2}$	$0,\frac{1}{2},x+\frac{1}{2}$	
			$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},0$	$0,\bar{x}+\frac{1}{2},\frac{1}{2}$	$0,x+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\bar{x}+\frac{1}{2}$	$\frac{1}{2},0,x+\frac{1}{2}$	
			$0,\bar{x},\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\frac{1}{2},0$	$x,\frac{1}{2},0$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$	
12	g	$2.mm$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	hkl : $h+k+l=2n$
			$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$	
12	f	2.22	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},0$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	hkl : $h+k+l=2n$
			$\frac{1}{4},\frac{1}{2},0$	$\frac{3}{4},\frac{1}{2},0$	$0,\frac{1}{4},\frac{1}{2}$	$0,\frac{3}{4},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	
8	e	$.3m$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			no extra conditions
			$x+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$			
6	d	$\bar{4}2.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	hkl : $h+k+l=2n$
4	c	$.\bar{3}m$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$			hkl : $h+k,h+l,k+l=2n$
4	b	$.\bar{3}m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$			hkl : $h+k,h+l,k+l=2n$
2	a	$\bar{4}3m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					hkl : $h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{1}{4}$

(*Continued on page 683*)

ORIGIN CHOICES 1 AND 2

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
	[2] $P4_232$ (208)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[2] $Pn\bar{3}1$ ($Pn\bar{3}$, 201)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36
	[3] $P4_2/n12/m$ ($P4_2/nnm$, 134)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40
	[3] $P4_2/n12/m$ ($P4_2/nnm$, 134)	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44
	[3] $P4_2/n12/m$ ($P4_2/nnm$, 134)	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48
	[4] $P1\bar{3}2/m$ ($R\bar{3}m$, 166)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48
	[4] $P1\bar{3}2/m$ ($R\bar{3}m$, 166)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48
	[4] $P1\bar{3}2/m$ ($R\bar{3}m$, 166)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46
	[4] $P1\bar{3}2/m$ ($R\bar{3}m$, 166)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46
IIa	none	
IIb	[2] $Fd\bar{3}c$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (228); [2] $Fd\bar{3}m$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (227)	

Maximal isomorphic subgroups of lowest index

IIc [27] $Pn\bar{3}m$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (224)

Minimal non-isomorphic supergroups

I none

II [2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}m$ (225)

ORIGIN CHOICE 1

Symmetry operations

(1) 1	(2) $2\ \ 0,0,z$	(3) $2\ \ 0,y,0$	(4) $2\ \ x,0,0$
(5) $3^+\ x,x,x$	(6) $3^+\ \bar{x},x,\bar{x}$	(7) $3^+\ x,\bar{x},\bar{x}$	(8) $3^+\ \bar{x},\bar{x},x$
(9) $3^-\ x,x,x$	(10) $3^-\ x,\bar{x},\bar{x}$	(11) $3^-\ \bar{x},\bar{x},x$	(12) $3^-\ \bar{x},x,\bar{x}$
(13) $2(\tfrac{1}{2},\tfrac{1}{2},0)\ \ x,x,\tfrac{1}{4}$	(14) $2\ \ x,\bar{x}+\tfrac{1}{2},\tfrac{1}{4}$	(15) $4^-(0,0,\tfrac{1}{2})\ \ \tfrac{1}{2},0,z$	(16) $4^+(0,0,\tfrac{1}{2})\ \ 0,\tfrac{1}{2},z$
(17) $4^-(\tfrac{1}{2},0,0)\ \ x,\tfrac{1}{2},0$	(18) $2(0,\tfrac{1}{2},\tfrac{1}{2})\ \ \tfrac{1}{4},y,y$	(19) $2\ \ \tfrac{1}{4},y+\tfrac{1}{2},\bar{y}$	(20) $4^+(\tfrac{1}{2},0,0)\ \ x,0,\tfrac{1}{2}$
(21) $4^+(0,\tfrac{1}{2},0)\ \ \tfrac{1}{2},y,0$	(22) $2(\tfrac{1}{2},0,\tfrac{1}{2})\ \ x,\tfrac{1}{4},x$	(23) $4^-(0,\tfrac{1}{2},0)\ \ 0,y,\tfrac{1}{2}$	(24) $2\ \ \bar{x}+\tfrac{1}{2},\tfrac{1}{4},x$
(25) $\bar{1}\ \ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$	(26) $n(\tfrac{1}{2},\tfrac{1}{2},0)\ \ x,y,\tfrac{1}{4}$	(27) $n(\tfrac{1}{2},0,\tfrac{1}{2})\ \ x,\tfrac{1}{4},z$	(28) $n(0,\tfrac{1}{2},\tfrac{1}{2})\ \ \tfrac{1}{4},y,z$
(29) $\bar{3}^+\ x,x,x;\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$	(30) $\bar{3}^+\ \bar{x}-1,x+1,\bar{x};\ -\tfrac{1}{4},\tfrac{1}{4},\tfrac{3}{4}$	(31) $\bar{3}^+\ x,\bar{x}+1,\bar{x};\ \tfrac{1}{4},\tfrac{3}{4},-\tfrac{1}{4}$	(32) $\bar{3}^+\ \bar{x}+1,\bar{x},x;\ \tfrac{3}{4},-\tfrac{1}{4},\tfrac{1}{4}$
(33) $\bar{3}^-\ x,x,x;\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$	(34) $\bar{3}^-\ x+1,\bar{x}-1,\bar{x};\ \tfrac{1}{4},-\tfrac{1}{4},\tfrac{3}{4}$	(35) $\bar{3}^-\ \bar{x},\bar{x}+1,x;\ -\tfrac{1}{4},\tfrac{3}{4},\tfrac{1}{4}$	(36) $\bar{3}^-\ \bar{x}+1,x,\bar{x};\ \tfrac{3}{4},\tfrac{1}{4},-\tfrac{1}{4}$
(37) $m\ \ x,\bar{x},z$	(38) $m\ \ x,x,z$	(39) $\bar{4}^-\ 0,0,z;\ 0,0,0$	(40) $\bar{4}^+\ 0,0,z;\ 0,0,0$
(41) $\bar{4}^-\ x,0,0;\ 0,0,0$	(42) $m\ \ x,y,\bar{y}$	(43) $m\ \ x,y,y$	(44) $\bar{4}^+\ x,0,0;\ 0,0,0$
(45) $\bar{4}^+\ 0,y,0;\ 0,0,0$	(46) $m\ \ \bar{x},y,x$	(47) $\bar{4}^-\ 0,y,0;\ 0,0,0$	(48) $m\ \ x,y,x$

ORIGIN CHOICE 2

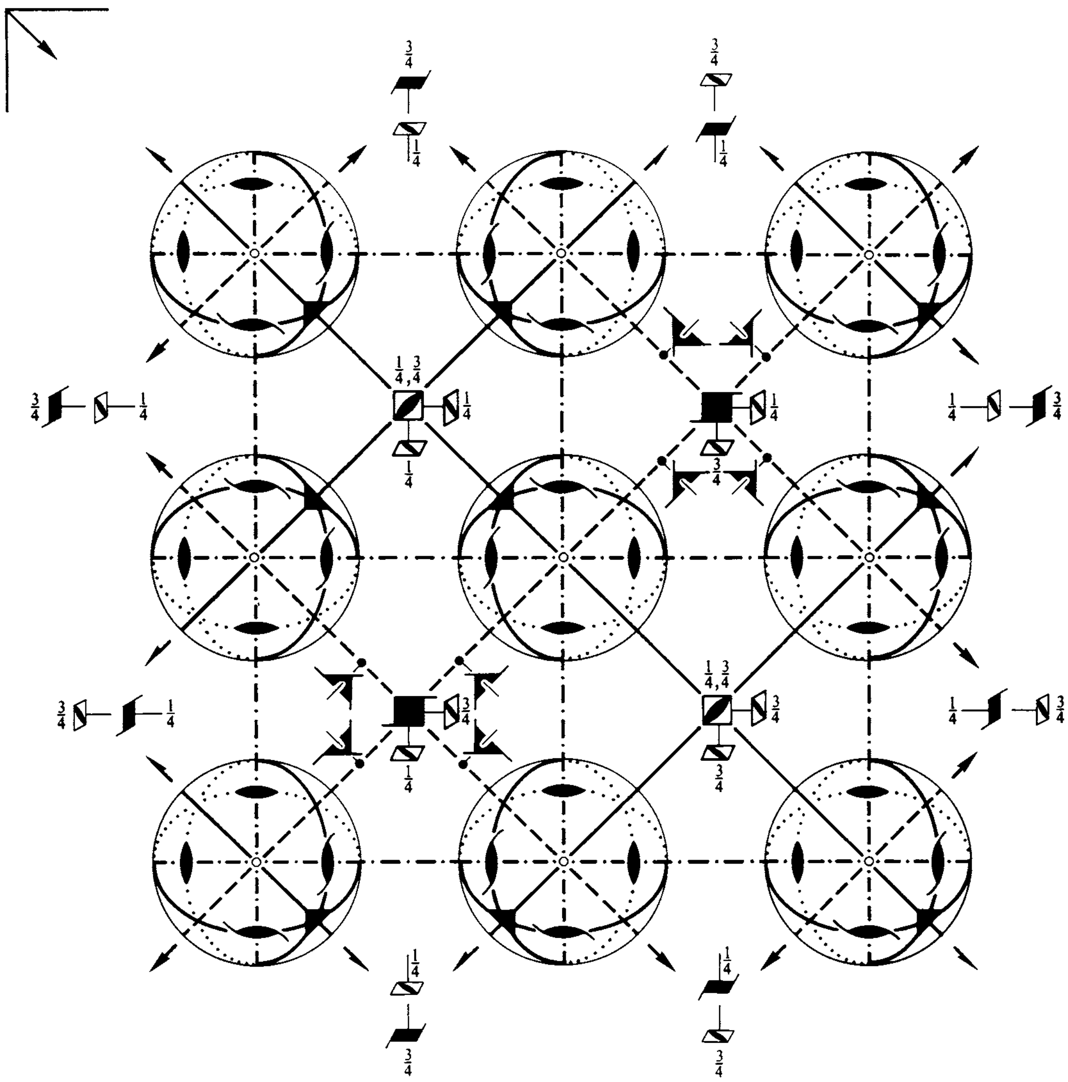
Symmetry operations

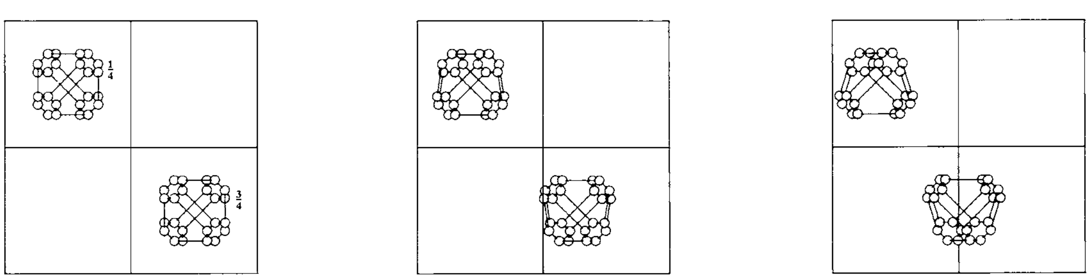
(1) 1	(2) $2\ \ \tfrac{1}{4},\tfrac{1}{4},z$	(3) $2\ \ \tfrac{1}{4},y,\tfrac{1}{4}$	(4) $2\ \ x,\tfrac{1}{4},\tfrac{1}{4}$
(5) $3^+\ x,x,x$	(6) $3^+\ \bar{x},x+\tfrac{1}{2},\bar{x}$	(7) $3^+\ x+\tfrac{1}{2},\bar{x},\bar{x}$	(8) $3^+\ \bar{x}+\tfrac{1}{2},\bar{x}+\tfrac{1}{2},x$
(9) $3^-\ x,x,x$	(10) $3^-\ x+\tfrac{1}{2},\bar{x},\bar{x}$	(11) $3^-\ \bar{x}+\tfrac{1}{2},\bar{x}+\tfrac{1}{2},x$	(12) $3^-\ \bar{x},x+\tfrac{1}{2},\bar{x}$
(13) $2(\tfrac{1}{2},\tfrac{1}{2},0)\ \ x,x,0$	(14) $2\ \ x,\bar{x},0$	(15) $4^-(0,0,\tfrac{1}{2})\ \ \tfrac{1}{4},-\tfrac{1}{4},z$	(16) $4^+(0,0,\tfrac{1}{2})\ \ -\tfrac{1}{4},\tfrac{1}{4},z$
(17) $4^-(\tfrac{1}{2},0,0)\ \ x,\tfrac{1}{4},-\tfrac{1}{4}$	(18) $2(0,\tfrac{1}{2},\tfrac{1}{2})\ \ 0,y,y$	(19) $2\ \ 0,y,\bar{y}$	(20) $4^+(\tfrac{1}{2},0,0)\ \ x,-\tfrac{1}{4},\tfrac{1}{4}$
(21) $4^+(0,\tfrac{1}{2},0)\ \ \tfrac{1}{4},y,-\tfrac{1}{4}$	(22) $2(\tfrac{1}{2},0,\tfrac{1}{2})\ \ x,0,x$	(23) $4^-(0,\tfrac{1}{2},0)\ \ -\tfrac{1}{4},y,\tfrac{1}{4}$	(24) $2\ \ \bar{x},0,x$
(25) $\bar{1}\ \ 0,0,0$	(26) $n(\tfrac{1}{2},\tfrac{1}{2},0)\ \ x,y,0$	(27) $n(\tfrac{1}{2},0,\tfrac{1}{2})\ \ x,0,z$	(28) $n(0,\tfrac{1}{2},\tfrac{1}{2})\ \ 0,y,z$
(29) $\bar{3}^+\ x,x,x;\ 0,0,0$	(30) $\bar{3}^+\ \bar{x}-1,x+\tfrac{1}{2},\bar{x};\ -\tfrac{1}{2},0,\tfrac{1}{2}$	(31) $\bar{3}^+\ x-\tfrac{1}{2},\bar{x}+1,\bar{x};\ 0,\tfrac{1}{2},-\tfrac{1}{2}$	(32) $\bar{3}^+\ \bar{x}+\tfrac{1}{2},\bar{x}-\tfrac{1}{2},x;\ \tfrac{1}{2},-\tfrac{1}{2},0$
(33) $\bar{3}^-\ x,x,x;\ 0,0,0$	(34) $\bar{3}^-\ x+\tfrac{1}{2},\bar{x}-1,\bar{x};\ 0,-\tfrac{1}{2},\tfrac{1}{2}$	(35) $\bar{3}^-\ \bar{x}-\tfrac{1}{2},\bar{x}+\tfrac{1}{2},x;\ -\tfrac{1}{2},\tfrac{1}{2},0$	(36) $\bar{3}^-\ \bar{x}+1,x-\tfrac{1}{2},\bar{x};\ \tfrac{1}{2},0,-\tfrac{1}{2}$
(37) $m\ \ x+\tfrac{1}{2},\bar{x},z$	(38) $m\ \ x,x,z$	(39) $\bar{4}^-\ \tfrac{1}{4},\tfrac{1}{4},z;\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$	(40) $\bar{4}^+\ \tfrac{1}{4},\tfrac{1}{4},z;\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$
(41) $\bar{4}^-\ x,\tfrac{1}{4},\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$	(42) $m\ \ x,y+\tfrac{1}{2},\bar{y}$	(43) $m\ \ x,y,y$	(44) $\bar{4}^+\ x,\tfrac{1}{4},\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$
(45) $\bar{4}^+\ \tfrac{1}{4},y,\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$	(46) $m\ \ \bar{x}+\tfrac{1}{2},y,x$	(47) $\bar{4}^-\ \tfrac{1}{4},y,\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$	(48) $m\ \ x,y,x$

$Pn\bar{3}m$ O_h^4 $m\bar{3}m$ Cubic

No. 224 $P\ 4_2/n\ \bar{3}\ 2/m$ Patterson symmetry $Pm\bar{3}m$

ORIGIN CHOICE 2





Origin at centre ($\bar{3}m$), at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{4}3m$

Asymmetric unit $\frac{1}{4} \le x \le \frac{3}{4}$; $\frac{1}{4} \le y \le \frac{3}{4}$; $0 \le z \le \frac{1}{2}$; $y \le x$; $\max(x-\frac{1}{2},\frac{1}{2}-y) \le z \le \min(y,1-x)$

Vertices $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},0$

Symmetry operations

(*given on page* 683)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

h,k,l permutable

General:

48 l 1

(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$
(5) z,x,y	(6) $z,\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(7) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},y$	(8) $\bar{z}+\frac{1}{2},x,\bar{y}+\frac{1}{2}$
(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	(11) $y,\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},x$
(13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y+\frac{1}{2},\bar{x},z+\frac{1}{2}$	(16) $\bar{y},x+\frac{1}{2},z+\frac{1}{2}$
(17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}$	(18) $\bar{x},z+\frac{1}{2},y+\frac{1}{2}$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x+\frac{1}{2},\bar{z},y+\frac{1}{2}$
(21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}$	(22) $z+\frac{1}{2},\bar{y},x+\frac{1}{2}$	(23) $\bar{z},y+\frac{1}{2},x+\frac{1}{2}$	(24) $\bar{z},\bar{y},\bar{x}$
(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(27) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(28) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$
(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x+\frac{1}{2},y+\frac{1}{2}$	(31) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}$	(32) $z+\frac{1}{2},\bar{x},y+\frac{1}{2}$
(33) $\bar{y},\bar{z},\bar{x}$	(34) $y+\frac{1}{2},\bar{z},x+\frac{1}{2}$	(35) $\bar{y},z+\frac{1}{2},x+\frac{1}{2}$	(36) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}$
(37) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(38) y,x,z	(39) $\bar{y}+\frac{1}{2},x,\bar{z}+\frac{1}{2}$	(40) $y,\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$
(41) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y$	(42) $x,\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(43) x,z,y	(44) $\bar{x}+\frac{1}{2},z,\bar{y}+\frac{1}{2}$
(45) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x$	(46) $\bar{z}+\frac{1}{2},y,\bar{x}+\frac{1}{2}$	(47) $z,\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(48) z,y,x

Reflection conditions: $0kl: k+l=2n$; $h00: h=2n$

Special: as above, plus

24 k $..m$ — no extra conditions

x,x,z	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,\bar{z}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$
z,x,x	$z,\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	$\bar{z}+\frac{1}{2},x,\bar{x}+\frac{1}{2}$
x,z,x	$\bar{x}+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	$x,\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},x$
$x+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$x+\frac{1}{2},\bar{x},z+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},z+\frac{1}{2}$
$x+\frac{1}{2},z+\frac{1}{2},\bar{x}$	$\bar{x},z+\frac{1}{2},x+\frac{1}{2}$	$\bar{x},\bar{z},\bar{x}$	$x+\frac{1}{2},\bar{z},x+\frac{1}{2}$
$z+\frac{1}{2},x+\frac{1}{2},\bar{x}$	$z+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{z},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{z},\bar{x},\bar{x}$

24 j $..2$ — no extra conditions

$\frac{1}{2},y,\bar{y}$	$0,\bar{y}+\frac{1}{2},\bar{y}$	$0,y,y+\frac{1}{2}$	$\frac{1}{2},\bar{y}+\frac{1}{2},y+\frac{1}{2}$
$\bar{y},\frac{1}{2},y$	$\bar{y},0,\bar{y}+\frac{1}{2}$	$y+\frac{1}{2},0,y$	$y+\frac{1}{2},\frac{1}{2},\bar{y}+\frac{1}{2}$
$y,\bar{y},\frac{1}{2}$	$\bar{y}+\frac{1}{2},\bar{y},0$	$y,y+\frac{1}{2},0$	$\bar{y}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$
$\frac{1}{2},\bar{y},y$	$0,y+\frac{1}{2},y$	$0,\bar{y},\bar{y}+\frac{1}{2}$	$\frac{1}{2},y+\frac{1}{2},\bar{y}+\frac{1}{2}$
$y,\frac{1}{2},\bar{y}$	$y,0,y+\frac{1}{2}$	$\bar{y}+\frac{1}{2},0,\bar{y}$	$\bar{y}+\frac{1}{2},\frac{1}{2},y+\frac{1}{2}$
$\bar{y},y,\frac{1}{2}$	$y+\frac{1}{2},y,0$	$\bar{y},\bar{y}+\frac{1}{2},0$	$y+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$

24 i $..2$ — no extra conditions

$\frac{1}{2},y,y+\frac{1}{2}$	$0,\bar{y}+\frac{1}{2},y+\frac{1}{2}$	$0,y,\bar{y}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\bar{y}$
$y+\frac{1}{2},\frac{1}{2},y$	$y+\frac{1}{2},0,\bar{y}+\frac{1}{2}$	$\bar{y},0,y$	$\bar{y},\frac{1}{2},\bar{y}+\frac{1}{2}$
$y,y+\frac{1}{2},\frac{1}{2}$	$\bar{y}+\frac{1}{2},y+\frac{1}{2},0$	$y,\bar{y},0$	$\bar{y}+\frac{1}{2},\bar{y},\frac{1}{2}$
$\frac{1}{2},\bar{y},\bar{y}+\frac{1}{2}$	$0,y+\frac{1}{2},\bar{y}+\frac{1}{2}$	$0,\bar{y},y$	$\frac{1}{2},y+\frac{1}{2},y$
$\bar{y}+\frac{1}{2},\frac{1}{2},\bar{y}$	$\bar{y}+\frac{1}{2},0,y+\frac{1}{2}$	$y,0,\bar{y}$	$y,\frac{1}{2},y+\frac{1}{2}$
$\bar{y},\bar{y}+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},\bar{y}+\frac{1}{2},0$	$\bar{y},y,0$	$y+\frac{1}{2},y,\frac{1}{2}$

24 h $2..$ — $hkl: h+k+l=2n$

$x,\frac{1}{4},\frac{3}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},x,\frac{1}{4}$	$\frac{3}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},x$	$\frac{1}{4},\frac{3}{4},\bar{x}+\frac{1}{2}$
$\frac{3}{4},x+\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},\bar{x},\frac{1}{4}$	$x+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\bar{x},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\bar{x}$	$\frac{1}{4},\frac{3}{4},x+\frac{1}{2}$
$\bar{x},\frac{3}{4},\frac{1}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},x+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\bar{x}$	$\frac{3}{4},\frac{1}{4},x+\frac{1}{2}$
$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\frac{1}{4},x,\frac{3}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$x,\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$

12 g $2.mm$ — $hkl: h+k+l=2n$

$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{1}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$
$\frac{3}{4},x+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{3}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\bar{x}$	$\frac{3}{4},\frac{3}{4},x+\frac{1}{2}$

12 f 2.22 — $hkl: h+k+l=2n$

$\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$0,\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},0,\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$
$\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{2},\frac{3}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},0$

8 e $.3m$ — no extra conditions

x,x,x	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	$\bar{x}+\frac{1}{2},x,\bar{x}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$
$x+\frac{1}{2},x+\frac{1}{2},\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},x+\frac{1}{2}$

6 d $\bar{4}2.m$ — $\frac{1}{4},\frac{3}{4},\frac{3}{4}$ — $\frac{3}{4},\frac{1}{4},\frac{3}{4}$ — $\frac{3}{4},\frac{3}{4},\frac{1}{4}$ — $\frac{1}{4},\frac{3}{4},\frac{1}{4}$ — $\frac{3}{4},\frac{1}{4},\frac{1}{4}$ — $\frac{1}{4},\frac{1}{4},\frac{3}{4}$ — $hkl: h+k+l=2n$

4 c $.\bar{3}m$ — $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ — $0,0,\frac{1}{2}$ — $0,\frac{1}{2},0$ — $\frac{1}{2},0,0$ — $hkl: h+k,h+l,k+l=2n$

4 b $.\bar{3}m$ — $0,0,0$ — $\frac{1}{2},\frac{1}{2},0$ — $\frac{1}{2},0,\frac{1}{2}$ — $0,\frac{1}{2},\frac{1}{2}$ — $hkl: h+k,h+l,k+l=2n$

2 a $\bar{4}3m$ — $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ — $\frac{3}{4},\frac{3}{4},\frac{3}{4}$ — $hkl: h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [111] $p6mm$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

(*Continued on page 683*)

ORIGIN CHOICES 1 AND 2

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
	[2] $P4_232$ (208)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
	[2] $Pn\bar{3}1$ ($Pn\bar{3}$, 201)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36
	[3] $P4_2/n12/m$ ($P4_2/nnm$, 134)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40
	[3] $P4_2/n12/m$ ($P4_2/nnm$, 134)	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44
	[3] $P4_2/n12/m$ ($P4_2/nnm$, 134)	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48
	[4] $P1\bar{3}2/m$ ($R\bar{3}m$, 166)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48
	[4] $P1\bar{3}2/m$ ($R\bar{3}m$, 166)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48
	[4] $P1\bar{3}2/m$ ($R\bar{3}m$, 166)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46
	[4] $P1\bar{3}2/m$ ($R\bar{3}m$, 166)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46

IIa none

IIb [2] $Fd\bar{3}c$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (228); [2] $Fd\bar{3}m$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (227)

Maximal isomorphic subgroups of lowest index

IIc [27] $Pn\bar{3}m$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b},\mathbf{c}'=3\mathbf{c}$) (224)

Minimal non-isomorphic supergroups

I none

II [2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}m$ (225)

ORIGIN CHOICE 1

Symmetry operations

(1) 1	(2) $2\ \ 0,0,z$	(3) $2\ \ 0,y,0$	(4) $2\ \ x,0,0$
(5) $3^+\ x,x,x$	(6) $3^+\ \bar{x},x,\bar{x}$	(7) $3^+\ x,\bar{x},\bar{x}$	(8) $3^+\ \bar{x},\bar{x},x$
(9) $3^-\ x,x,x$	(10) $3^-\ x,\bar{x},\bar{x}$	(11) $3^-\ \bar{x},\bar{x},x$	(12) $3^-\ \bar{x},x,\bar{x}$
(13) $2(\tfrac{1}{2},\tfrac{1}{2},0)\ \ x,x,\tfrac{1}{4}$	(14) $2\ \ x,\bar{x}+\tfrac{1}{2},\tfrac{1}{4}$	(15) $4^-(0,0,\tfrac{1}{2})\ \ \tfrac{1}{2},0,z$	(16) $4^+(0,0,\tfrac{1}{2})\ \ 0,\tfrac{1}{2},z$
(17) $4^-(\tfrac{1}{2},0,0)\ \ x,\tfrac{1}{2},0$	(18) $2(0,\tfrac{1}{2},\tfrac{1}{2})\ \ \tfrac{1}{4},y,y$	(19) $2\ \ \tfrac{1}{4},y+\tfrac{1}{2},\bar{y}$	(20) $4^+(\tfrac{1}{2},0,0)\ \ x,0,\tfrac{1}{2}$
(21) $4^+(0,\tfrac{1}{2},0)\ \ \tfrac{1}{2},y,0$	(22) $2(\tfrac{1}{2},0,\tfrac{1}{2})\ \ x,\tfrac{1}{4},x$	(23) $4^-(0,\tfrac{1}{2},0)\ \ 0,y,\tfrac{1}{2}$	(24) $2\ \ \bar{x}+\tfrac{1}{2},\tfrac{1}{4},x$
(25) $\bar{1}\ \ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$	(26) $n(\tfrac{1}{2},\tfrac{1}{2},0)\ \ x,y,\tfrac{1}{4}$	(27) $n(\tfrac{1}{2},0,\tfrac{1}{2})\ \ x,\tfrac{1}{4},z$	(28) $n(0,\tfrac{1}{2},\tfrac{1}{2})\ \ \tfrac{1}{4},y,z$
(29) $\bar{3}^+\ x,x,x;\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$	(30) $\bar{3}^+\ \bar{x}-1,x+1,\bar{x};\ -\tfrac{1}{4},\tfrac{1}{4},\tfrac{3}{4}$	(31) $\bar{3}^+\ x,\bar{x}+1,\bar{x};\ \tfrac{1}{4},\tfrac{3}{4},-\tfrac{1}{4}$	(32) $\bar{3}^+\ \bar{x}+1,\bar{x},x;\ \tfrac{3}{4},-\tfrac{1}{4},\tfrac{1}{4}$
(33) $\bar{3}^-\ x,x,x;\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$	(34) $\bar{3}^-\ x+1,\bar{x}-1,\bar{x};\ \tfrac{1}{4},-\tfrac{1}{4},\tfrac{3}{4}$	(35) $\bar{3}^-\ \bar{x},\bar{x}+1,x;\ -\tfrac{1}{4},\tfrac{3}{4},\tfrac{1}{4}$	(36) $\bar{3}^-\ \bar{x}+1,x,\bar{x};\ \tfrac{3}{4},\tfrac{1}{4},-\tfrac{1}{4}$
(37) $m\ \ x,\bar{x},z$	(38) $m\ \ x,x,z$	(39) $\bar{4}^-\ 0,0,z;\ 0,0,0$	(40) $\bar{4}^+\ 0,0,z;\ 0,0,0$
(41) $\bar{4}^-\ x,0,0;\ 0,0,0$	(42) $m\ \ x,y,\bar{y}$	(43) $m\ \ x,y,y$	(44) $\bar{4}^+\ x,0,0;\ 0,0,0$
(45) $\bar{4}^+\ 0,y,0;\ 0,0,0$	(46) $m\ \ \bar{x},y,x$	(47) $\bar{4}^-\ 0,y,0;\ 0,0,0$	(48) $m\ \ x,y,x$

ORIGIN CHOICE 2

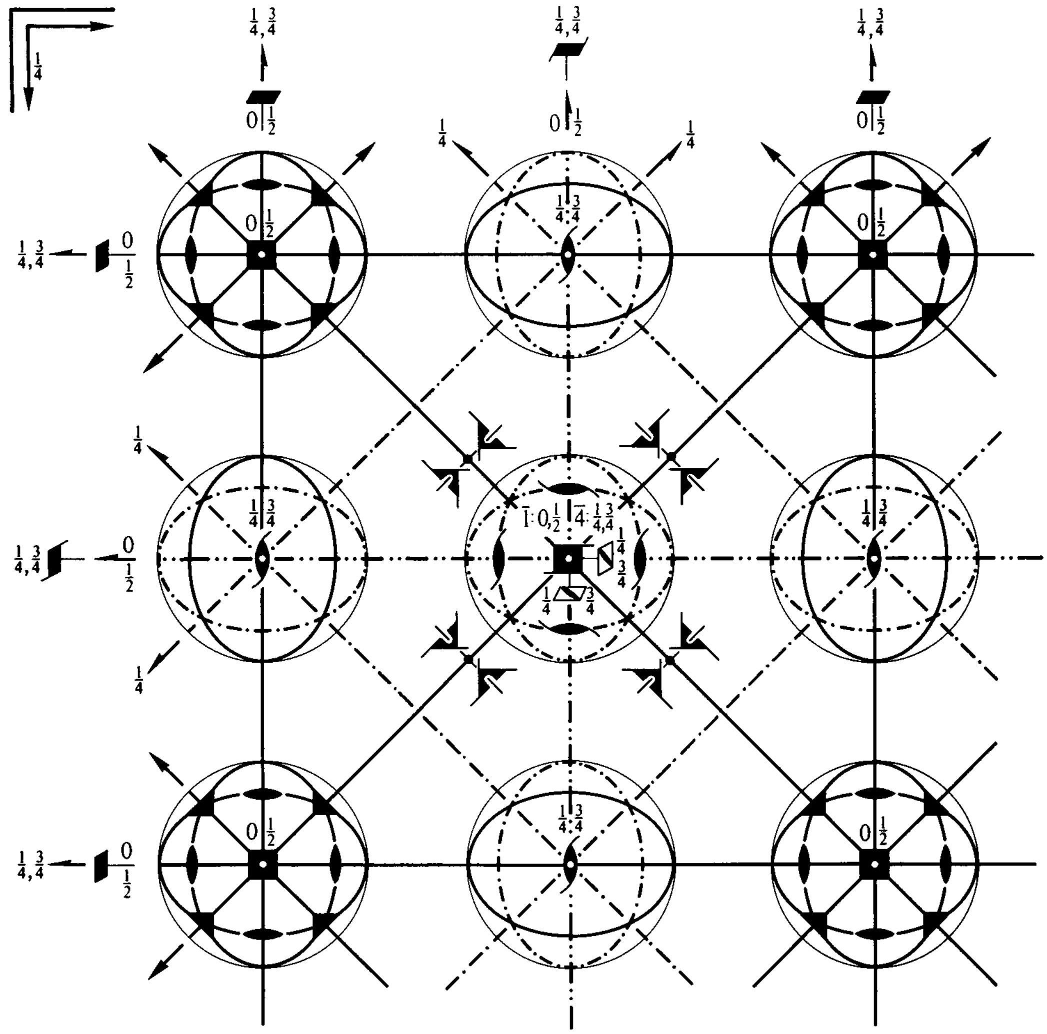
Symmetry operations

(1) 1	(2) $2\ \ \tfrac{1}{4},\tfrac{1}{4},z$	(3) $2\ \ \tfrac{1}{4},y,\tfrac{1}{4}$	(4) $2\ \ x,\tfrac{1}{4},\tfrac{1}{4}$
(5) $3^+\ x,x,x$	(6) $3^+\ \bar{x},x+\tfrac{1}{2},\bar{x}$	(7) $3^+\ x+\tfrac{1}{2},\bar{x},\bar{x}$	(8) $3^+\ \bar{x}+\tfrac{1}{2},\bar{x}+\tfrac{1}{2},x$
(9) $3^-\ x,x,x$	(10) $3^-\ x+\tfrac{1}{2},\bar{x},\bar{x}$	(11) $3^-\ \bar{x}+\tfrac{1}{2},\bar{x}+\tfrac{1}{2},x$	(12) $3^-\ \bar{x},x+\tfrac{1}{2},\bar{x}$
(13) $2(\tfrac{1}{2},\tfrac{1}{2},0)\ \ x,x,0$	(14) $2\ \ x,\bar{x},0$	(15) $4^-(0,0,\tfrac{1}{2})\ \ \tfrac{1}{4},-\tfrac{1}{4},z$	(16) $4^+(0,0,\tfrac{1}{2})\ \ -\tfrac{1}{4},\tfrac{1}{4},z$
(17) $4^-(\tfrac{1}{2},0,0)\ \ x,\tfrac{1}{4},-\tfrac{1}{4}$	(18) $2(0,\tfrac{1}{2},\tfrac{1}{2})\ \ 0,y,y$	(19) $2\ \ 0,y,\bar{y}$	(20) $4^+(\tfrac{1}{2},0,0)\ \ x,-\tfrac{1}{4},\tfrac{1}{4}$
(21) $4^+(0,\tfrac{1}{2},0)\ \ \tfrac{1}{4},y,-\tfrac{1}{4}$	(22) $2(\tfrac{1}{2},0,\tfrac{1}{2})\ \ x,0,x$	(23) $4^-(0,\tfrac{1}{2},0)\ \ -\tfrac{1}{4},y,\tfrac{1}{4}$	(24) $2\ \ \bar{x},0,x$
(25) $\bar{1}\ \ 0,0,0$	(26) $n(\tfrac{1}{2},\tfrac{1}{2},0)\ \ x,y,0$	(27) $n(\tfrac{1}{2},0,\tfrac{1}{2})\ \ x,0,z$	(28) $n(0,\tfrac{1}{2},\tfrac{1}{2})\ \ 0,y,z$
(29) $\bar{3}^+\ x,x,x;\ 0,0,0$	(30) $\bar{3}^+\ \bar{x}-1,x+\tfrac{1}{2},\bar{x};\ -\tfrac{1}{2},0,\tfrac{1}{2}$	(31) $\bar{3}^+\ x-\tfrac{1}{2},\bar{x}+1,\bar{x};\ 0,\tfrac{1}{2},-\tfrac{1}{2}$	(32) $\bar{3}^+\ \bar{x}+\tfrac{1}{2},\bar{x}-\tfrac{1}{2},x;\ \tfrac{1}{2},-\tfrac{1}{2},0$
(33) $\bar{3}^-\ x,x,x;\ 0,0,0$	(34) $\bar{3}^-\ x+\tfrac{1}{2},\bar{x}-1,\bar{x};\ 0,-\tfrac{1}{2},\tfrac{1}{2}$	(35) $\bar{3}^-\ \bar{x}-\tfrac{1}{2},\bar{x}+\tfrac{1}{2},x;\ -\tfrac{1}{2},\tfrac{1}{2},0$	(36) $\bar{3}^-\ \bar{x}+1,x-\tfrac{1}{2},\bar{x};\ \tfrac{1}{2},0,-\tfrac{1}{2}$
(37) $m\ \ x+\tfrac{1}{2},\bar{x},z$	(38) $m\ \ x,x,z$	(39) $\bar{4}^-\ \tfrac{1}{4},\tfrac{1}{4},z;\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$	(40) $\bar{4}^+\ \tfrac{1}{4},\tfrac{1}{4},z;\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$
(41) $\bar{4}^-\ x,\tfrac{1}{4},\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$	(42) $m\ \ x,y+\tfrac{1}{2},\bar{y}$	(43) $m\ \ x,y,y$	(44) $\bar{4}^+\ x,\tfrac{1}{4},\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$
(45) $\bar{4}^+\ \tfrac{1}{4},y,\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$	(46) $m\ \ \bar{x}+\tfrac{1}{2},y,x$	(47) $\bar{4}^-\ \tfrac{1}{4},y,\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}$	(48) $m\ \ x,y,x$

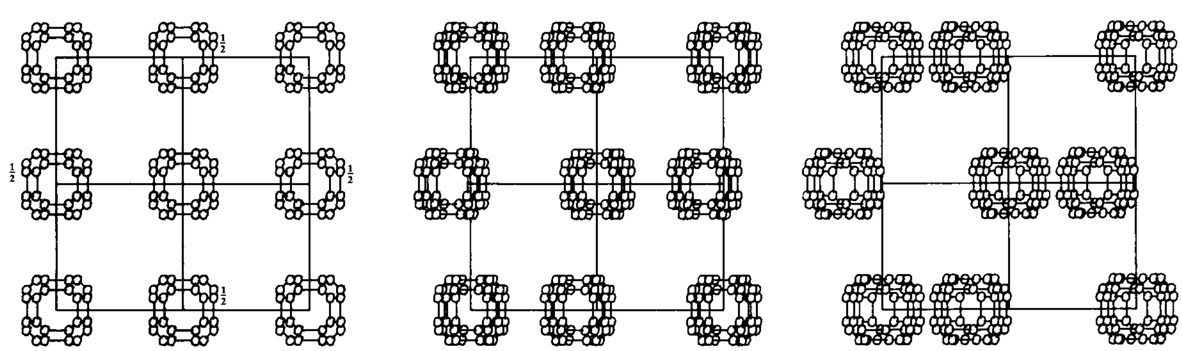
International Tables for Crystallography (2006). Vol. A, Space group 225, pp. 688–691.

$Fm\bar{3}m$ $\quad O_h^5$ $\quad m\bar{3}m$ $\quad$ Cubic

No. 225 $\quad F\ 4/m\ \bar{3}\ 2/m$ $\quad$ Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Origin at centre ($m\bar{3}m$)

Asymmetric unit $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le \frac{1}{4};\quad y \le \min(x, \frac{1}{2} - x);\quad z \le y$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{4},\frac{1}{4},0 \quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$

Symmetry operations

(*given on page* 691)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates: $(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$ — Reflection conditions: h,k,l permutable

General:

							Reflection conditions
192	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hkl : $h+k,h+l,k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	hhl : $h+l=2n$
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$	$h00$: $h=2n$
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$	
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$	
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$	
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$	
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$	
			(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$	
			(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$	
			(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x	

Special: as above, plus

									Reflection conditions
96	k	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x	$z,\bar{x},\bar{x}$	no extra conditions
			$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$	
			$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$x,\bar{x},z$	$\bar{x},x,z$	$x,z,\bar{x}$	$\bar{x},z,x$	
			$\bar{x},\bar{z},\bar{x}$	$x,\bar{z},x$	$z,x,\bar{x}$	$z,\bar{x},x$	$\bar{z},x,x$	$\bar{z},\bar{x},\bar{x}$	
96	j	$m..$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$z,0,y$	$z,0,\bar{y}$	no extra conditions
			$\bar{z},0,y$	$\bar{z},0,\bar{y}$	$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$	
			$y,0,\bar{z}$	$\bar{y},0,\bar{z}$	$y,0,z$	$\bar{y},0,z$	$0,z,\bar{y}$	$0,z,y$	
			$0,\bar{z},\bar{y}$	$0,\bar{z},y$	$z,y,0$	$z,\bar{y},0$	$\bar{z},y,0$	$\bar{z},\bar{y},0$	
48	i	$m.m2$	$\frac{1}{2},y,y$	$\frac{1}{2},\bar{y},y$	$\frac{1}{2},y,\bar{y}$	$\frac{1}{2},\bar{y},\bar{y}$	$y,\frac{1}{2},y$	$y,\frac{1}{2},\bar{y}$	no extra conditions
			$\bar{y},\frac{1}{2},y$	$\bar{y},\frac{1}{2},\bar{y}$	$y,y,\frac{1}{2}$	$\bar{y},y,\frac{1}{2}$	$y,\bar{y},\frac{1}{2}$	$\bar{y},\bar{y},\frac{1}{2}$	
48	h	$m.m2$	$0,y,y$	$0,\bar{y},y$	$0,y,\bar{y}$	$0,\bar{y},\bar{y}$	$y,0,y$	$y,0,\bar{y}$	no extra conditions
			$\bar{y},0,y$	$\bar{y},0,\bar{y}$	$y,y,0$	$\bar{y},y,0$	$y,\bar{y},0$	$\bar{y},\bar{y},0$	
48	g	$2.mm$	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}$	hkl : $h=2n$
			$\frac{1}{4},x,\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{3}{4}$	$x,\frac{1}{4},\frac{3}{4}$	$\bar{x},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\bar{x}$	$\frac{1}{4},\frac{3}{4},x$	
32	f	$.3m$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			no extra conditions
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$			
24	e	$4m.m$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	no extra conditions
24	d	$m.mm$	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl : $h=2n$
8	c	$\bar{4}3m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$					hkl : $h=2n$
4	b	$m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						no extra conditions
4	a	$m\bar{3}m$	$0,0,0$						no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}'=\frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $F\bar{4}3m$ (216)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+
	[2] $F432$ (209)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+
	[2] $Fm\bar{3}1$ ($Fm\bar{3}$, 202)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+
	[3] $F4/m12/m$ ($I4/mmm$, 139)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
	[3] $F4/m12/m$ ($I4/mmm$, 139)	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
	[3] $F4/m12/m$ ($I4/mmm$, 139)	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
	[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
	[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
	[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
	[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+
IIa	[4] $Pn\bar{3}m$ (224)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48; (4; 6; 11; 16; 18; 23; 28; 30; 35; 40; 42; 47) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 8; 10; 15; 20; 22; 27; 32; 34; 39; 44; 46) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 7; 12; 13; 17; 21; 26; 31; 36; 37; 41; 45) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pn\bar{3}m$ (224)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48; (4; 5; 10; 15; 19; 23; 28; 29; 34; 39; 43; 47) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 7; 11; 16; 17; 22; 27; 31; 35; 40; 41; 46) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 8; 9; 14; 20; 21; 26; 32; 33; 38; 44; 45) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pn\bar{3}m$ (224)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46; (4; 8; 12; 15; 18; 21; 28; 32; 36; 39; 42; 45) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 6; 9; 16; 20; 24; 27; 30; 33; 40; 44; 48) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 5; 11; 14; 17; 23; 26; 29; 35; 38; 41; 47) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pn\bar{3}m$ (224)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46; (4; 7; 9; 16; 19; 21; 28; 31; 33; 40; 43; 45) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 5; 12; 15; 17; 24; 27; 29; 36; 39; 41; 48) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 6; 10; 13; 20; 23; 26; 30; 34; 37; 44; 47) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
	[4] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40; (9; 10; 11; 12; 17; 18; 19; 20; 33; 34; 35; 36; 41; 42; 43; 44) + $(0,\frac{1}{2},\frac{1}{2})$; (5; 6; 7; 8; 21; 22; 23; 24; 29; 30; 31; 32; 45; 46; 47; 48) + $(\frac{1}{2},0,\frac{1}{2})$
	[4] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44; (9; 10; 11; 12; 21; 22; 23; 24; 33; 34; 35; 36; 45; 46; 47; 48) + $(\frac{1}{2},0,\frac{1}{2})$; (5; 6; 7; 8; 13; 14; 15; 16; 29; 30; 31; 32; 37; 38; 39; 40) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48; (5; 6; 7; 8; 17; 18; 19; 20; 29; 30; 31; 32; 41; 42; 43; 44) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16; 33; 34; 35; 36; 37; 38; 39; 40) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $Fm\bar{3}m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (225)

Minimal non-isomorphic supergroups

I none

II [2] $Pm\bar{3}m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (221)

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\ \ 0,0,z$	(3) $2\ \ 0,y,0$	(4) $2\ \ x,0,0$
(5) $3^{+}\ x,x,x$	(6) $3^{+}\ \bar{x},x,\bar{x}$	(7) $3^{+}\ x,\bar{x},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x},x$
(9) $3^{-}\ x,x,x$	(10) $3^{-}\ x,\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x},\bar{x},x$	(12) $3^{-}\ \bar{x},x,\bar{x}$
(13) $2\ \ x,x,0$	(14) $2\ \ x,\bar{x},0$	(15) $4^{-}\ 0,0,z$	(16) $4^{+}\ 0,0,z$
(17) $4^{-}\ x,0,0$	(18) $2\ \ 0,y,y$	(19) $2\ \ 0,y,\bar{y}$	(20) $4^{+}\ x,0,0$
(21) $4^{+}\ 0,y,0$	(22) $2\ \ x,0,x$	(23) $4^{-}\ 0,y,0$	(24) $2\ \ \bar{x},0,x$
(25) $\bar{1}\ \ 0,0,0$	(26) $m\ \ x,y,0$	(27) $m\ \ x,0,z$	(28) $m\ \ 0,y,z$
(29) $\bar{3}^{+}\ x,x,x;\ 0,0,0$	(30) $\bar{3}^{+}\ \bar{x},x,\bar{x};\ 0,0,0$	(31) $\bar{3}^{+}\ x,\bar{x},\bar{x};\ 0,0,0$	(32) $\bar{3}^{+}\ \bar{x},\bar{x},x;\ 0,0,0$
(33) $\bar{3}^{-}\ x,x,x;\ 0,0,0$	(34) $\bar{3}^{-}\ x,\bar{x},\bar{x};\ 0,0,0$	(35) $\bar{3}^{-}\ \bar{x},\bar{x},x;\ 0,0,0$	(36) $\bar{3}^{-}\ \bar{x},x,\bar{x};\ 0,0,0$
(37) $m\ \ x,\bar{x},z$	(38) $m\ \ x,x,z$	(39) $\bar{4}^{-}\ 0,0,z;\ 0,0,0$	(40) $\bar{4}^{+}\ 0,0,z;\ 0,0,0$
(41) $\bar{4}^{-}\ x,0,0;\ 0,0,0$	(42) $m\ \ x,y,\bar{y}$	(43) $m\ \ x,y,y$	(44) $\bar{4}^{+}\ x,0,0;\ 0,0,0$
(45) $\bar{4}^{+}\ 0,y,0;\ 0,0,0$	(46) $m\ \ \bar{x},y,x$	(47) $\bar{4}^{-}\ 0,y,0;\ 0,0,0$	(48) $m\ \ x,y,x$

For $(0,\frac12,\frac12)+$ set

(1) $t(0,\frac12,\frac12)$	(2) $2(0,0,\frac12)\ \ 0,\frac14,z$	(3) $2(0,\frac12,0)\ \ 0,y,\frac14$	(4) $2\ \ x,\frac14,\frac14$
(5) $3^{+}(\frac13,\frac13,\frac13)\ \ x-\frac13,x-\frac16,x$	(6) $3^{+}\ \bar{x},x+\frac12,\bar{x}$	(7) $3^{+}(-\frac13,\frac13,\frac13)\ \ x+\frac13,\bar{x}-\frac16,\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x}+\frac12,x$
(9) $3^{-}(\frac13,\frac13,\frac13)\ \ x-\frac16,x+\frac16,x$	(10) $3^{-}(-\frac13,\frac13,\frac13)\ \ x+\frac16,\bar{x}+\frac16,\bar{x}$	(11) $3^{-}\ \bar{x}+\frac12,\bar{x}+\frac12,x$	(12) $3^{-}\ \bar{x}-\frac12,x+\frac12,\bar{x}$
(13) $2(\frac14,\frac14,0)\ \ x,x+\frac14,\frac14$	(14) $2(-\frac14,\frac14,0)\ \ x,\bar{x}+\frac14,\frac14$	(15) $4^{-}(0,0,\frac12)\ \ \frac14,\frac14,z$	(16) $4^{+}(0,0,\frac12)\ \ -\frac14,\frac14,z$
(17) $4^{-}\ x,\frac12,0$	(18) $2(0,\frac12,\frac12)\ \ 0,y,y$	(19) $2\ \ 0,y+\frac12,\bar{y}$	(20) $4^{+}\ x,0,\frac12$
(21) $4^{+}(0,\frac12,0)\ \ \frac14,y,\frac14$	(22) $2(\frac14,0,\frac14)\ \ x-\frac14,\frac14,x$	(23) $4^{-}(0,\frac12,0)\ \ -\frac14,y,\frac14$	(24) $2(-\frac14,0,\frac14)\ \ \bar{x}+\frac14,\frac14,x$
(25) $\bar{1}\ \ 0,\frac14,\frac14$	(26) $b\ \ x,y,\frac14$	(27) $c\ \ x,\frac14,z$	(28) $n(0,\frac12,\frac12)\ \ 0,y,z$
(29) $\bar{3}^{+}\ x,x+\frac12,x;\ 0,\frac12,0$	(30) $\bar{3}^{+}\ \bar{x}-1,x+\frac12,\bar{x};\ -\frac12,0,\frac12$	(31) $\bar{3}^{+}\ x,\bar{x}+\frac12,\bar{x};\ 0,\frac12,0$	(32) $\bar{3}^{+}\ \bar{x}+1,\bar{x}+\frac12,x;\ \frac12,0,\frac12$
(33) $\bar{3}^{-}\ x-\frac12,x-\frac12,x;\ 0,0,\frac12$	(34) $\bar{3}^{-}\ x+\frac12,\bar{x}-\frac12,\bar{x};\ 0,0,\frac12$	(35) $\bar{3}^{-}\ \bar{x}-\frac12,\bar{x}+\frac12,x;\ -\frac12,\frac12,0$	(36) $\bar{3}^{-}\ \bar{x}+\frac12,x+\frac12,\bar{x};\ \frac12,\frac12,0$
(37) $g(-\frac14,\frac14,\frac12)\ \ x+\frac14,\bar{x},z$	(38) $g(\frac14,\frac14,\frac12)\ \ x-\frac14,x,z$	(39) $\bar{4}^{-}\ -\frac14,\frac14,z;\ -\frac14,\frac14,\frac14$	(40) $\bar{4}^{+}\ \frac14,\frac14,z;\ \frac14,\frac14,\frac14$
(41) $\bar{4}^{-}\ x,0,\frac12;\ 0,0,\frac12$	(42) $m\ \ x,y+\frac12,\bar{y}$	(43) $g(0,\frac12,\frac12)\ \ x,y,y$	(44) $\bar{4}^{+}\ x,\frac12,0;\ 0,\frac12,0$
(45) $\bar{4}^{+}\ -\frac14,y,\frac14;\ -\frac14,\frac14,\frac14$	(46) $g(-\frac14,\frac12,\frac14)\ \ \bar{x}+\frac14,y,x$	(47) $\bar{4}^{-}\ \frac14,y,\frac14;\ \frac14,\frac14,\frac14$	(48) $g(\frac14,\frac12,\frac14)\ \ x-\frac14,y,x$

For $(\frac12,0,\frac12)+$ set

(1) $t(\frac12,0,\frac12)$	(2) $2(0,0,\frac12)\ \ \frac14,0,z$	(3) $2\ \ \frac14,y,\frac14$	(4) $2(\frac12,0,0)\ \ x,0,\frac14$
(5) $3^{+}(\frac13,\frac13,\frac13)\ \ x+\frac16,x-\frac16,x$	(6) $3^{+}(\frac13,-\frac13,\frac13)\ \ \bar{x}+\frac16,x+\frac16,\bar{x}$	(7) $3^{+}\ x+\frac12,\bar{x}-\frac12,\bar{x}$	(8) $3^{+}\ \bar{x}+\frac12,\bar{x}+\frac12,x$
(9) $3^{-}(\frac13,\frac13,\frac13)\ \ x-\frac16,x-\frac13,x$	(10) $3^{-}\ x+\frac12,\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac12,\bar{x},x$	(12) $3^{-}(\frac13,-\frac13,\frac13)\ \ \bar{x}-\frac16,x+\frac13,\bar{x}$
(13) $2(\frac14,\frac14,0)\ \ x,x-\frac14,\frac14$	(14) $2(\frac14,-\frac14,0)\ \ x,\bar{x}+\frac14,\frac14$	(15) $4^{-}(0,0,\frac12)\ \ \frac14,-\frac14,z$	(16) $4^{+}(0,0,\frac12)\ \ \frac14,\frac14,z$
(17) $4^{-}(\frac12,0,0)\ \ x,\frac14,\frac14$	(18) $2(0,\frac14,\frac14)\ \ \frac14,y-\frac14,y$	(19) $2(0,-\frac14,\frac14)\ \ \frac14,y+\frac14,\bar{y}$	(20) $4^{+}(\frac12,0,0)\ \ x,-\frac14,\frac14$
(21) $4^{+}\ \frac12,y,0$	(22) $2(\frac12,0,\frac12)\ \ x,0,x$	(23) $4^{-}\ 0,y,\frac12$	(24) $2\ \ \bar{x}+\frac12,0,x$
(25) $\bar{1}\ \ \frac14,0,\frac14$	(26) $a\ \ x,y,\frac14$	(27) $n(\frac12,0,\frac12)\ \ x,0,z$	(28) $c\ \ \frac14,y,z$
(29) $\bar{3}^{+}\ x-\frac12,x-\frac12,x;\ 0,0,\frac12$	(30) $\bar{3}^{+}\ \bar{x}-\frac12,x+\frac12,\bar{x};\ 0,0,\frac12$	(31) $\bar{3}^{+}\ x+\frac12,\bar{x}+\frac12,\bar{x};\ \frac12,\frac12,0$	(32) $\bar{3}^{+}\ \bar{x}+\frac12,\bar{x}-\frac12,x;\ \frac12,-\frac12,0$
(33) $\bar{3}^{-}\ x+\frac12,x,x;\ \frac12,0,0$	(34) $\bar{3}^{-}\ x+\frac12,\bar{x}-1,\bar{x};\ 0,-\frac12,\frac12$	(35) $\bar{3}^{-}\ \bar{x}+\frac12,\bar{x}+1,x;\ 0,\frac12,\frac12$	(36) $\bar{3}^{-}\ \bar{x}+\frac12,x,\bar{x};\ \frac12,0,0$
(37) $g(\frac14,-\frac14,\frac12)\ \ x+\frac14,\bar{x},z$	(38) $g(\frac14,\frac14,\frac12)\ \ x+\frac14,x,z$	(39) $\bar{4}^{-}\ \frac14,\frac14,z;\ \frac14,\frac14,\frac14$	(40) $\bar{4}^{+}\ \frac14,-\frac14,z;\ \frac14,-\frac14,\frac14$
(41) $\bar{4}^{-}\ x,-\frac14,\frac14;\ \frac14,-\frac14,\frac14$	(42) $g(\frac12,-\frac14,\frac14)\ \ x,y+\frac14,\bar{y}$	(43) $g(\frac12,\frac14,\frac14)\ \ x,y-\frac14,y$	(44) $\bar{4}^{+}\ x,\frac14,\frac14;\ \frac14,\frac14,\frac14$
(45) $\bar{4}^{+}\ 0,y,\frac12;\ 0,0,\frac12$	(46) $m\ \ \bar{x}+\frac12,y,x$	(47) $\bar{4}^{-}\ \frac12,y,0;\ \frac12,0,0$	(48) $g(\frac12,0,\frac12)\ \ x,y,x$

For $(\frac12,\frac12,0)+$ set

(1) $t(\frac12,\frac12,0)$	(2) $2\ \ \frac14,\frac14,z$	(3) $2(0,\frac12,0)\ \ \frac14,y,0$	(4) $2(\frac12,0,0)\ \ x,\frac14,0$
(5) $3^{+}(\frac13,\frac13,\frac13)\ \ x+\frac16,x+\frac13,x$	(6) $3^{+}\ \bar{x}+\frac12,x,\bar{x}$	(7) $3^{+}\ x+\frac12,\bar{x},\bar{x}$	(8) $3^{+}(\frac13,\frac13,-\frac13)\ \ \bar{x}+\frac16,\bar{x}+\frac13,x$
(9) $3^{-}(\frac13,\frac13,\frac13)\ \ x+\frac13,x+\frac16,x$	(10) $3^{-}\ x,\bar{x}+\frac12,\bar{x}$	(11) $3^{-}(\frac13,\frac13,-\frac13)\ \ \bar{x}+\frac13,\bar{x}+\frac16,x$	(12) $3^{-}\ \bar{x},x+\frac12,\bar{x}$
(13) $2(\frac12,\frac12,0)\ \ x,x,0$	(14) $2\ \ x,\bar{x}+\frac12,0$	(15) $4^{-}\ \frac12,0,z$	(16) $4^{+}\ 0,\frac12,z$
(17) $4^{-}(\frac12,0,0)\ \ x,\frac14,-\frac14$	(18) $2(0,\frac14,\frac14)\ \ \frac14,y+\frac14,y$	(19) $2(0,\frac14,-\frac14)\ \ \frac14,y+\frac14,\bar{y}$	(20) $4^{+}(\frac12,0,0)\ \ x,\frac14,\frac14$
(21) $4^{+}(0,\frac12,0)\ \ \frac14,y,-\frac14$	(22) $2(\frac14,0,\frac14)\ \ x+\frac14,\frac14,x$	(23) $4^{-}(0,\frac12,0)\ \ \frac14,y,\frac14$	(24) $2(\frac14,0,-\frac14)\ \ \bar{x}+\frac14,\frac14,x$
(25) $\bar{1}\ \ \frac14,\frac14,0$	(26) $n(\frac12,\frac12,0)\ \ x,y,0$	(27) $a\ \ x,\frac14,z$	(28) $b\ \ \frac14,y,z$
(29) $\bar{3}^{+}\ x+\frac12,x,x;\ \frac12,0,0$	(30) $\bar{3}^{+}\ \bar{x}-\frac12,x+1,\bar{x};\ 0,\frac12,\frac12$	(31) $\bar{3}^{+}\ x-\frac12,\bar{x}+1,\bar{x};\ 0,\frac12,-\frac12$	(32) $\bar{3}^{+}\ \bar{x}+\frac12,\bar{x},x;\ \frac12,0,0$
(33) $\bar{3}^{-}\ x,x+\frac12,x;\ 0,\frac12,0$	(34) $\bar{3}^{-}\ x+1,\bar{x}-\frac12,\bar{x};\ \frac12,0,\frac12$	(35) $\bar{3}^{-}\ \bar{x},\bar{x}+\frac12,x;\ 0,\frac12,0$	(36) $\bar{3}^{-}\ \bar{x}+1,x-\frac12,\bar{x};\ \frac12,0,-\frac12$
(37) $m\ \ x+\frac12,\bar{x},z$	(38) $g(\frac12,\frac12,0)\ \ x,x,z$	(39) $\bar{4}^{-}\ 0,\frac12,z;\ 0,\frac12,0$	(40) $\bar{4}^{+}\ \frac12,0,z;\ \frac12,0,0$
(41) $\bar{4}^{-}\ x,\frac14,\frac14;\ \frac14,\frac14,\frac14$	(42) $g(\frac12,\frac14,-\frac14)\ \ x,y+\frac14,\bar{y}$	(43) $g(\frac12,\frac14,\frac14)\ \ x,y+\frac14,y$	(44) $\bar{4}^{+}\ x,\frac14,-\frac14;\ \frac14,\frac14,-\frac14$
(45) $\bar{4}^{+}\ \frac14,y,\frac14;\ \frac14,\frac14,\frac14$	(46) $g(\frac14,\frac12,-\frac14)\ \ \bar{x}+\frac14,y,x$	(47) $\bar{4}^{-}\ \frac14,y,-\frac14;\ \frac14,\frac14,-\frac14$	(48) $g(\frac14,\frac12,\frac14)\ \ x+\frac14,y,x$

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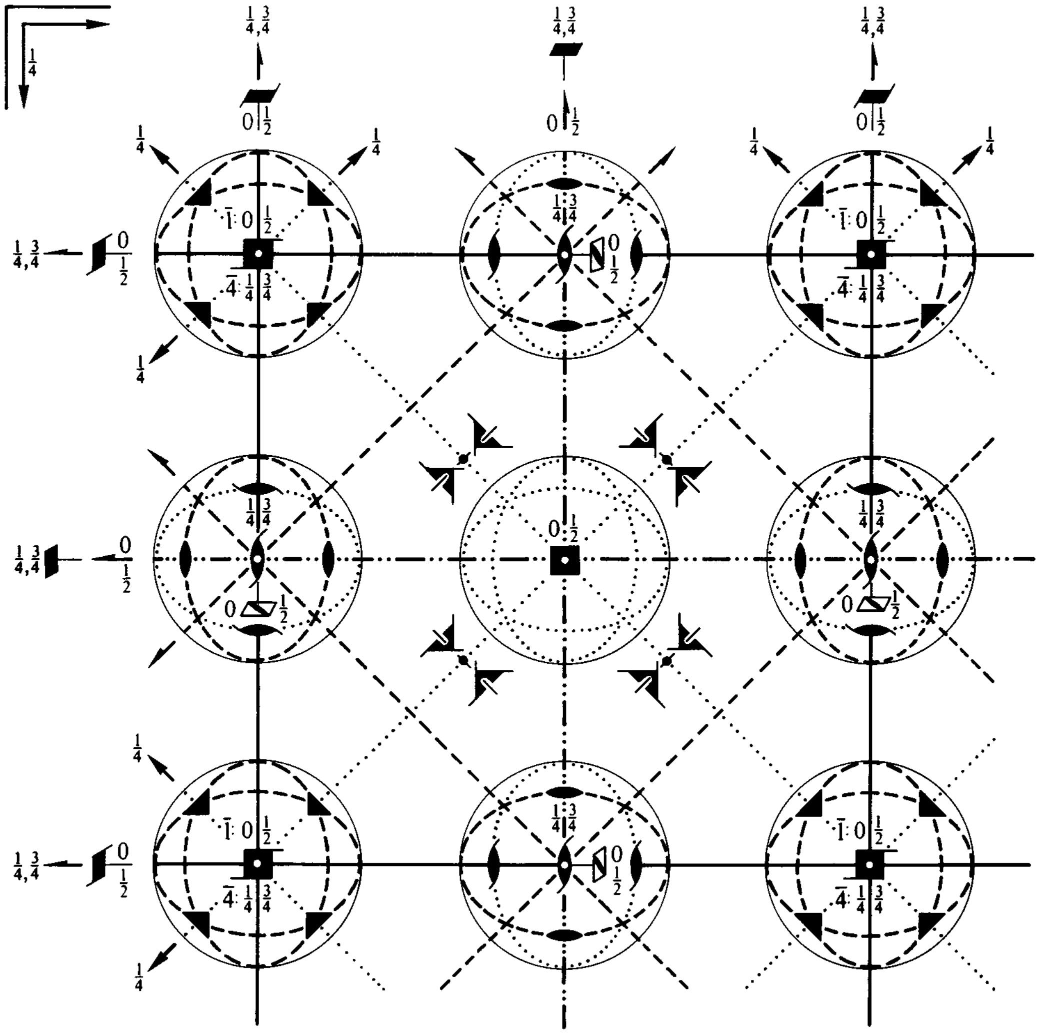
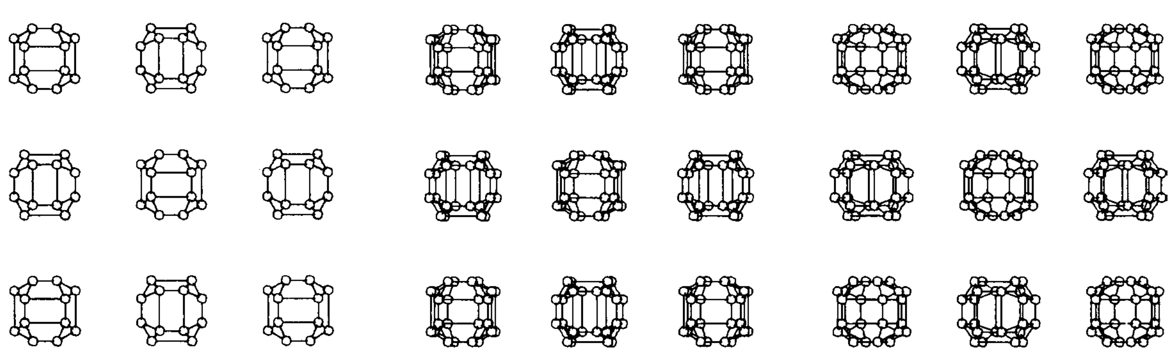
$Fm\bar{3}c$ O_h^6 $m\bar{3}m$ Cubic

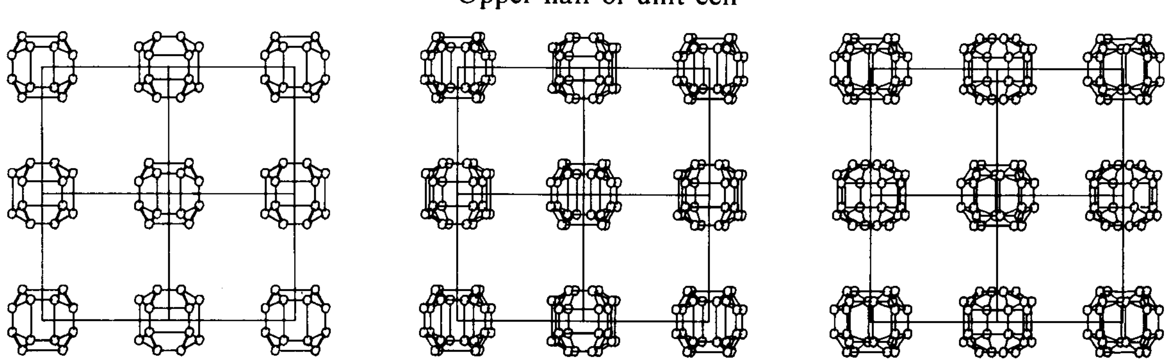
No. 226 $F\ 4/m\ \bar{3}\ 2/c$ Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Upper half of unit cell



Lower half of unit cell

Origin at centre ($m\bar{3}$)

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le \frac{1}{4};\quad y \le \min(x, \frac{1}{2}-x);\quad z \le y$

Vertices $0,0,0\quad \frac{1}{2},0,0\quad \frac{1}{4},\frac{1}{4},0\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$

Symmetry operations

(*given on page* 695)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

$(0,0,0)+\quad (0,\frac{1}{2},\frac{1}{2})+\quad (\frac{1}{2},0,\frac{1}{2})+\quad (\frac{1}{2},\frac{1}{2},0)+$

h,k,l permutable

General:

192	*j*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hkl : $h+k=2n$ and $h+l,k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	hhl : $h,l=2n$
			(13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$h00$: $h=2n$
			(17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	
			(21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$	
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$	
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$	
			(37) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	
			(41) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	
			(45) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(46) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	

Special: as above, plus

96	*i*	$m\,.\,.$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$			no extra conditions
			$z,0,y$	$z,0,\bar{y}$	$\bar{z},0,y$	$\bar{z},0,\bar{y}$			
			$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$			
			$y+\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\bar{y}+\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$y+\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\bar{y}+\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			
			$\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	$\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	$\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	$\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$			
			$z+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$z+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\bar{z}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$			
96	*h*	$.\,.\,2$	$\frac{1}{4},y,y$	$\frac{3}{4},\bar{y},y$	$\frac{3}{4},y,\bar{y}$	$\frac{1}{4},\bar{y},\bar{y}$	$y,\frac{1}{4},y$	$y,\frac{3}{4},\bar{y}$	hkl : $h=2n$
			$\bar{y},\frac{3}{4},y$	$\bar{y},\frac{1}{4},\bar{y}$	$y,y,\frac{1}{4}$	$\bar{y},y,\frac{3}{4}$	$y,\bar{y},\frac{3}{4}$	$\bar{y},\bar{y},\frac{1}{4}$	
			$\frac{3}{4},\bar{y},\bar{y}$	$\frac{1}{4},y,\bar{y}$	$\frac{1}{4},\bar{y},y$	$\frac{3}{4},y,y$	$\bar{y},\frac{3}{4},\bar{y}$	$\bar{y},\frac{1}{4},y$	
			$y,\frac{1}{4},\bar{y}$	$y,\frac{3}{4},y$	$\bar{y},\bar{y},\frac{3}{4}$	$y,\bar{y},\frac{1}{4}$	$\bar{y},y,\frac{1}{4}$	$y,y,\frac{3}{4}$	
64	*g*	$.\,3\,.$	x,x,x	$\bar{x},\bar{x},x$					hkl : $h=2n$
			$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$					
			$x+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$					
			$x+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$					
			$\bar{x},\bar{x},\bar{x}$	$x,x,\bar{x}$					
			$x,\bar{x},x$	$\bar{x},x,x$					
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$					
			$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$					
48	*f*	$4\,.\,.$	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}$	hkl : $h=2n$
			$\bar{x},\frac{3}{4},\frac{3}{4}$	$x,\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{3}{4}$	$\frac{3}{4},x,\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\bar{x}$	$\frac{1}{4},\frac{3}{4},x$	
48	*e*	$m\,m\,2\,.\,.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$			hkl : $h=2n$
			$0,0,x$	$0,0,\bar{x}$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$			
			$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$			
24	*d*	$4/m\,.\,.$	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl : $h=2n$
24	*c*	$\bar{4}\,m\,.\,2$	$\frac{1}{4},0,0$	$\frac{3}{4},0,0$	$0,\frac{1}{4},0$	$0,\frac{3}{4},0$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$	hkl : $h=2n$
8	*b*	$m\,\bar{3}\,.$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					hkl : $h=2n$
8	*a*	$4\,3\,2$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$					hkl : $h=2n$

Symmetry of special projections

Along [001] $p4mm$	Along [111] $p6mm$	Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\quad \mathbf{b}' = \frac{1}{2}\mathbf{b}$	$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\quad \mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$	$\mathbf{a}' = \frac{1}{4}(-\mathbf{a}+\mathbf{b})$ $\quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $0,0,z$	Origin at x,x,x	Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $F\bar{4}3c$ (219)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+
	[2] $F432$ (209)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+
	[2] $Fm\bar{3}1$ ($Fm\bar{3}$, 202)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+
	[3] $F4_2/m12/n$ ($I4/mcm$, 140)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
	[3] $F4_2/m12/n$ ($I4/mcm$, 140)	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
	[3] $F4_2/m12/n$ ($I4/mcm$, 140)	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
	[4] $F1\bar{3}2/n$ ($R\bar{3}c$, 167)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
	[4] $F1\bar{3}2/n$ ($R\bar{3}c$, 167)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
	[4] $F1\bar{3}2/n$ ($R\bar{3}c$, 167)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
	[4] $F1\bar{3}2/n$ ($R\bar{3}c$, 167)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+
IIa	[4] $Pm\bar{3}n$ (223)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
	[4] $Pm\bar{3}n$ (223)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40; (9; 10; 11; 12; 17; 18; 19; 20; 33; 34; 35; 36; 41; 42; 43; 44) + $(0,\frac{1}{2},\frac{1}{2})$; (5; 6; 7; 8; 21; 22; 23; 24; 29; 30; 31; 32; 45; 46; 47; 48) + $(\frac{1}{2},0,\frac{1}{2})$
	[4] $Pm\bar{3}n$ (223)	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44; (9; 10; 11; 12; 21; 22; 23; 24; 33; 34; 35; 36; 45; 46; 47; 48) + $(\frac{1}{2},0,\frac{1}{2})$; (5; 6; 7; 8; 13; 14; 15; 16; 29; 30; 31; 32; 37; 38; 39; 40) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pm\bar{3}n$ (223)	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48; (5; 6; 7; 8; 17; 18; 19; 20; 29; 30; 31; 32; 41; 42; 43; 44) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16; 33; 34; 35; 36; 37; 38; 39; 40) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pn\bar{3}n$ (222)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48; (4; 6; 11; 16; 18; 23; 28; 30; 35; 40; 42; 47) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 8; 10; 15; 20; 22; 27; 32; 34; 39; 44; 46) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 7; 12; 13; 17; 21; 26; 31; 36; 37; 41; 45) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pn\bar{3}n$ (222)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48; (4; 5; 10; 15; 19; 23; 28; 29; 34; 39; 43; 47) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 7; 11; 16; 17; 22; 27; 31; 35; 40; 41; 46) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 8; 9; 14; 20; 21; 26; 32; 33; 38; 44; 45) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pn\bar{3}n$ (222)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46; (4; 8; 12; 15; 18; 21; 28; 32; 36; 39; 42; 45) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 6; 9; 16; 20; 24; 27; 30; 33; 40; 44; 48) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 5; 11; 14; 17; 23; 26; 29; 35; 38; 41; 47) + $(\frac{1}{2},\frac{1}{2},0)$
	[4] $Pn\bar{3}n$ (222)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46; (4; 7; 9; 16; 19; 21; 28; 31; 33; 40; 43; 45) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 5; 12; 15; 17; 24; 27; 29; 36; 39; 41; 48) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 6; 10; 13; 20; 23; 26; 30; 34; 37; 44; 47) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $Fm\bar{3}c$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (226)

Minimal non-isomorphic supergroups

I none

II [2] $Pm\bar{3}m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (221)

(*from page* 693)

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\ \ 0,0,z$	(3) $2\ \ 0,y,0$	(4) $2\ \ x,0,0$
(5) $3^{+}\ x,x,x$	(6) $3^{+}\ \bar{x},x,\bar{x}$	(7) $3^{+}\ x,\bar{x},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x},x$
(9) $3^{-}\ x,x,x$	(10) $3^{-}\ x,\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x},\bar{x},x$	(12) $3^{-}\ \bar{x},x,\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x,\frac{1}{4}$	(14) $2\ \ x,\bar{x}+\frac{1}{2},\frac{1}{4}$	(15) $4^{-}(0,0,\frac{1}{2})\ \ \frac{1}{2},0,z$	(16) $4^{+}(0,0,\frac{1}{2})\ \ 0,\frac{1}{2},z$
(17) $4^{-}(\frac{1}{2},0,0)\ \ x,\frac{1}{2},0$	(18) $2(0,\frac{1}{2},\frac{1}{2})\ \ \frac{1}{4},y,y$	(19) $2\ \ \frac{1}{4},y+\frac{1}{2},\bar{y}$	(20) $4^{+}(\frac{1}{2},0,0)\ \ x,0,\frac{1}{2}$
(21) $4^{+}(0,\frac{1}{2},0)\ \ \frac{1}{2},y,0$	(22) $2(\frac{1}{2},0,\frac{1}{2})\ \ x,\frac{1}{4},x$	(23) $4^{-}(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{2}$	(24) $2\ \ \bar{x}+\frac{1}{2},\frac{1}{4},x$
(25) $\bar{1}\ \ 0,0,0$	(26) $m\ \ x,y,0$	(27) $m\ \ x,0,z$	(28) $m\ \ 0,y,z$
(29) $\bar{3}^{+}\ x,x,x;\ 0,0,0$	(30) $\bar{3}^{+}\ \bar{x},x,\bar{x};\ 0,0,0$	(31) $\bar{3}^{+}\ x,\bar{x},\bar{x};\ 0,0,0$	(32) $\bar{3}^{+}\ \bar{x},\bar{x},x;\ 0,0,0$
(33) $\bar{3}^{-}\ x,x,x;\ 0,0,0$	(34) $\bar{3}^{-}\ x,\bar{x},\bar{x};\ 0,0,0$	(35) $\bar{3}^{-}\ \bar{x},\bar{x},x;\ 0,0,0$	(36) $\bar{3}^{-}\ \bar{x},x,\bar{x};\ 0,0,0$
(37) $c\ \ x+\frac{1}{2},\bar{x},z$	(38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,x,z$	(39) $\bar{4}^{-}\ 0,\frac{1}{2},z;\ 0,\frac{1}{2},\frac{1}{4}$	(40) $\bar{4}^{+}\ \frac{1}{2},0,z;\ \frac{1}{2},0,\frac{1}{4}$
(41) $\bar{4}^{-}\ x,0,\frac{1}{2};\ \frac{1}{4},0,\frac{1}{2}$	(42) $a\ \ x,y+\frac{1}{2},\bar{y}$	(43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,y,y$	(44) $\bar{4}^{+}\ x,\frac{1}{2},0;\ \frac{1}{4},\frac{1}{2},0$
(45) $\bar{4}^{+}\ 0,y,\frac{1}{2};\ 0,\frac{1}{4},\frac{1}{2}$	(46) $b\ \ \bar{x}+\frac{1}{2},y,x$	(47) $\bar{4}^{-}\ \frac{1}{2},y,0;\ \frac{1}{2},\frac{1}{4},0$	(48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,y,x$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\ \ 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{4}$	(4) $2\ \ x,\frac{1}{4},\frac{1}{4}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x-\frac{1}{3},x-\frac{1}{6},x$	(6) $3^{+}\ \bar{x},x+\frac{1}{2},\bar{x}$	(7) $3^{+}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x-\frac{1}{6},x+\frac{1}{6},x$	(10) $3^{-}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) $3^{-}\ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)\ \ x,x-\frac{1}{4},0$	(14) $2(\frac{1}{4},-\frac{1}{4},0)\ \ x,\bar{x}+\frac{1}{4},0$	(15) $4^{-}\ \frac{1}{4},-\frac{1}{4},z$	(16) $4^{+}\ \frac{1}{4},\frac{1}{4},z$
(17) $4^{-}(\frac{1}{2},0,0)\ \ x,0,0$	(18) $2\ \ \frac{1}{4},y,y$	(19) $2\ \ \frac{1}{4},y,\bar{y}$	(20) $4^{+}(\frac{1}{2},0,0)\ \ x,0,0$
(21) $4^{+}\ \frac{1}{4},y,-\frac{1}{4}$	(22) $2(\frac{1}{4},0,\frac{1}{4})\ \ x+\frac{1}{4},0,x$	(23) $4^{-}\ \frac{1}{4},y,\frac{1}{4}$	(24) $2(\frac{1}{4},0,-\frac{1}{4})\ \ \bar{x}+\frac{1}{4},0,x$
(25) $\bar{1}\ \ 0,\frac{1}{4},\frac{1}{4}$	(26) $b\ \ x,y,\frac{1}{4}$	(27) $c\ \ x,\frac{1}{4},z$	(28) $n(0,\frac{1}{2},\frac{1}{2})\ \ 0,y,z$
(29) $\bar{3}^{+}\ x,x+\frac{1}{2},x;\ 0,\frac{1}{2},0$	(30) $\bar{3}^{+}\ \bar{x}-1,x+\frac{1}{2},\bar{x};\ -\frac{1}{2},0,\frac{1}{2}$	(31) $\bar{3}^{+}\ x,\bar{x}+\frac{1}{2},\bar{x};\ 0,\frac{1}{2},0$	(32) $\bar{3}^{+}\ \bar{x}+1,\bar{x}+\frac{1}{2},x;\ \frac{1}{2},0,\frac{1}{2}$
(33) $\bar{3}^{-}\ x-\frac{1}{2},x-\frac{1}{2},x;\ 0,0,\frac{1}{2}$	(34) $\bar{3}^{-}\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};\ 0,0,\frac{1}{2}$	(35) $\bar{3}^{-}\ \bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x;\ -\frac{1}{2},\frac{1}{2},0$	(36) $\bar{3}^{-}\ \bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x};\ \frac{1}{2},\frac{1}{2},0$
(37) $g(\frac{1}{4},-\frac{1}{4},0)\ \ x+\frac{1}{4},\bar{x},z$	(38) $g(\frac{1}{4},\frac{1}{4},0)\ \ x+\frac{1}{4},x,z$	(39) $\bar{4}^{-}\ \frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},0$	(40) $\bar{4}^{+}\ \frac{1}{4},-\frac{1}{4},z;\ \frac{1}{4},-\frac{1}{4},0$
(41) $\bar{4}^{-}\ x,0,0;\ \frac{1}{4},0,0$	(42) $a\ \ x,y,\bar{y}$	(43) $a\ \ x,y,y$	(44) $\bar{4}^{+}\ x,0,0;\ \frac{1}{4},0,0$
(45) $\bar{4}^{+}\ \frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},0,\frac{1}{4}$	(46) $g(\frac{1}{4},0,-\frac{1}{4})\ \ \bar{x}+\frac{1}{4},y,x$	(47) $\bar{4}^{-}\ \frac{1}{4},y,-\frac{1}{4};\ \frac{1}{4},0,-\frac{1}{4}$	(48) $g(\frac{1}{4},0,\frac{1}{4})\ \ x+\frac{1}{4},y,x$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},0,z$	(3) $2\ \ \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\ \ x,0,\frac{1}{4}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{6},x-\frac{1}{6},x$	(6) $3^{+}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\ \ \bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^{+}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x-\frac{1}{6},x-\frac{1}{3},x$	(10) $3^{-}\ x+\frac{1}{2},\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{1}{2},\bar{x},x$	(12) $3^{-}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\ \ \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)\ \ x,x+\frac{1}{4},0$	(14) $2(-\frac{1}{4},\frac{1}{4},0)\ \ x,\bar{x}+\frac{1}{4},0$	(15) $4^{-}\ \frac{1}{4},\frac{1}{4},z$	(16) $4^{+}\ -\frac{1}{4},\frac{1}{4},z$
(17) $4^{-}\ x,\frac{1}{4},-\frac{1}{4}$	(18) $2(0,\frac{1}{4},\frac{1}{4})\ \ 0,y+\frac{1}{4},y$	(19) $2(0,\frac{1}{4},-\frac{1}{4})\ \ 0,y+\frac{1}{4},\bar{y}$	(20) $4^{+}\ x,\frac{1}{4},\frac{1}{4}$
(21) $4^{+}(0,\frac{1}{2},0)\ \ 0,y,0$	(22) $2\ \ x,\frac{1}{4},x$	(23) $4^{-}(0,\frac{1}{2},0)\ \ 0,y,0$	(24) $2\ \ \bar{x},\frac{1}{4},x$
(25) $\bar{1}\ \ \frac{1}{4},0,\frac{1}{4}$	(26) $a\ \ x,y,\frac{1}{4}$	(27) $n(\frac{1}{2},0,\frac{1}{2})\ \ x,0,z$	(28) $c\ \ \frac{1}{4},y,z$
(29) $\bar{3}^{+}\ x-\frac{1}{2},x-\frac{1}{2},x;\ 0,0,\frac{1}{2}$	(30) $\bar{3}^{+}\ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x};\ 0,0,\frac{1}{2}$	(31) $\bar{3}^{+}\ x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x};\ \frac{1}{2},\frac{1}{2},0$	(32) $\bar{3}^{+}\ \bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x;\ \frac{1}{2},-\frac{1}{2},0$
(33) $\bar{3}^{-}\ x+\frac{1}{2},x,x;\ \frac{1}{2},0,0$	(34) $\bar{3}^{-}\ x+\frac{1}{2},\bar{x}-1,\bar{x};\ 0,-\frac{1}{2},\frac{1}{2}$	(35) $\bar{3}^{-}\ \bar{x}+\frac{1}{2},\bar{x}+1,x;\ 0,\frac{1}{2},\frac{1}{2}$	(36) $\bar{3}^{-}\ \bar{x}+\frac{1}{2},x,\bar{x};\ \frac{1}{2},0,0$
(37) $g(-\frac{1}{4},\frac{1}{4},0)\ \ x+\frac{1}{4},\bar{x},z$	(38) $g(\frac{1}{4},\frac{1}{4},0)\ \ x-\frac{1}{4},x,z$	(39) $\bar{4}^{-}\ -\frac{1}{4},\frac{1}{4},z;\ -\frac{1}{4},\frac{1}{4},0$	(40) $\bar{4}^{+}\ \frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},0$
(41) $\bar{4}^{-}\ x,\frac{1}{4},\frac{1}{4};\ 0,\frac{1}{4},\frac{1}{4}$	(42) $g(0,\frac{1}{4},-\frac{1}{4})\ \ x,y+\frac{1}{4},\bar{y}$	(43) $g(0,\frac{1}{4},\frac{1}{4})\ \ x,y+\frac{1}{4},y$	(44) $\bar{4}^{+}\ x,\frac{1}{4},-\frac{1}{4};\ 0,\frac{1}{4},-\frac{1}{4}$
(45) $\bar{4}^{+}\ 0,y,0;\ 0,\frac{1}{4},0$	(46) $b\ \ \bar{x},y,x$	(47) $\bar{4}^{-}\ 0,y,0;\ 0,\frac{1}{4},0$	(48) $b\ \ x,y,x$

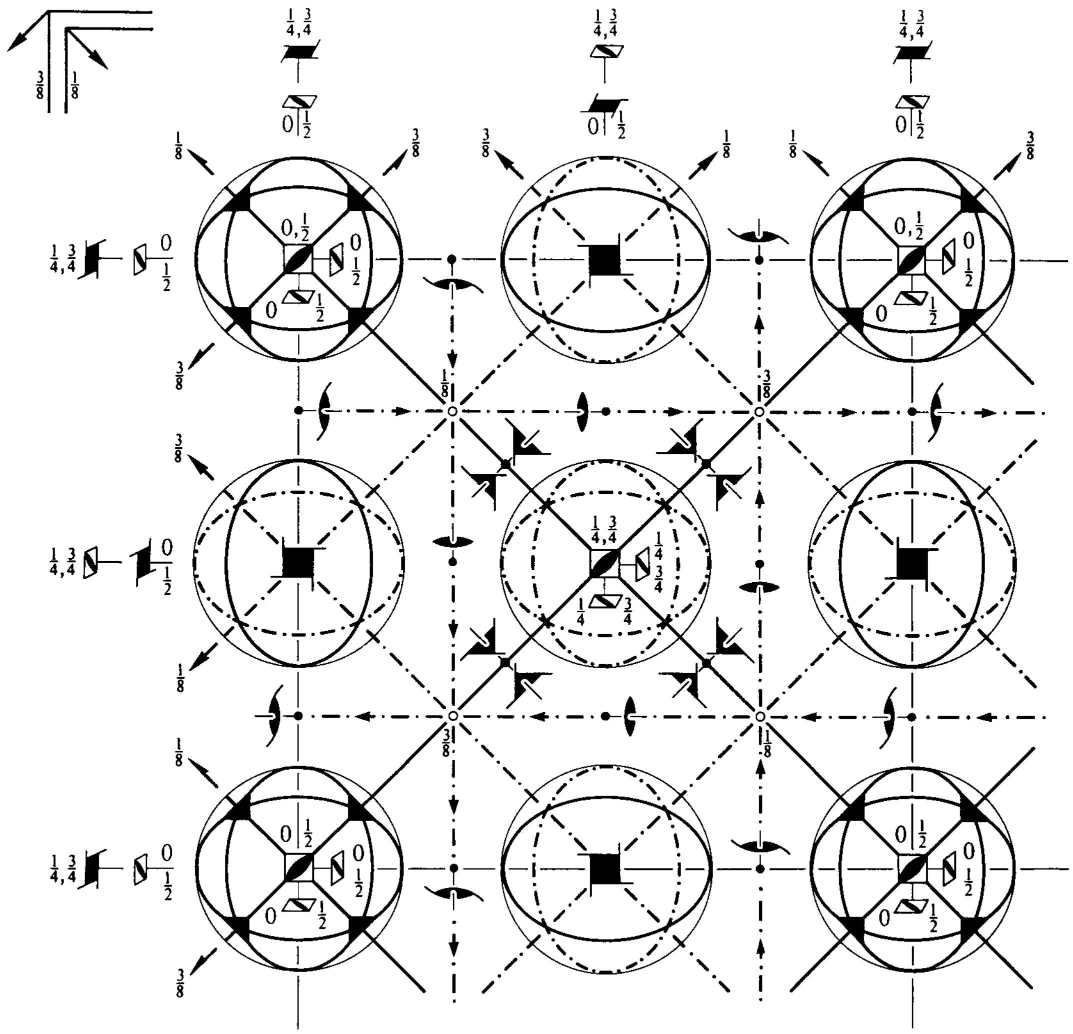
For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\ \ \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\ \ \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},0$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{6},x+\frac{1}{3},x$	(6) $3^{+}\ \bar{x}+\frac{1}{2},x,\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x},\bar{x}$	(8) $3^{+}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\ \ \bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{3},x+\frac{1}{6},x$	(10) $3^{-}\ x,\bar{x}+\frac{1}{2},\bar{x}$	(11) $3^{-}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\ \ \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^{-}\ \bar{x},x+\frac{1}{2},\bar{x}$
(13) $2\ \ x,x,\frac{1}{4}$	(14) $2\ \ x,\bar{x},\frac{1}{4}$	(15) $4^{-}(0,0,\frac{1}{2})\ \ 0,0,z$	(16) $4^{+}(0,0,\frac{1}{2})\ \ 0,0,z$
(17) $4^{-}\ x,\frac{1}{4},\frac{1}{4}$	(18) $2(0,\frac{1}{4},\frac{1}{4})\ \ 0,y-\frac{1}{4},y$	(19) $2(0,-\frac{1}{4},\frac{1}{4})\ \ 0,y+\frac{1}{4},\bar{y}$	(20) $4^{+}\ x,-\frac{1}{4},\frac{1}{4}$
(21) $4^{+}\ \frac{1}{4},y,\frac{1}{4}$	(22) $2(\frac{1}{4},0,\frac{1}{4})\ \ x-\frac{1}{4},0,x$	(23) $4^{-}\ -\frac{1}{4},y,\frac{1}{4}$	(24) $2(-\frac{1}{4},0,\frac{1}{4})\ \ \bar{x}+\frac{1}{4},0,x$
(25) $\bar{1}\ \ \frac{1}{4},\frac{1}{4},0$	(26) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$	(27) $a\ \ x,\frac{1}{4},z$	(28) $b\ \ \frac{1}{4},y,z$
(29) $\bar{3}^{+}\ x+\frac{1}{2},x,x;\ \frac{1}{2},0,0$	(30) $\bar{3}^{+}\ \bar{x}-\frac{1}{2},x+1,\bar{x};\ 0,\frac{1}{2},\frac{1}{2}$	(31) $\bar{3}^{+}\ x-\frac{1}{2},\bar{x}+1,\bar{x};\ 0,\frac{1}{2},-\frac{1}{2}$	(32) $\bar{3}^{+}\ \bar{x}+\frac{1}{2},\bar{x},x;\ \frac{1}{2},0,0$
(33) $\bar{3}^{-}\ x,x+\frac{1}{2},x;\ 0,\frac{1}{2},0$	(34) $\bar{3}^{-}\ x+1,\bar{x}-\frac{1}{2},\bar{x};\ \frac{1}{2},0,\frac{1}{2}$	(35) $\bar{3}^{-}\ \bar{x},\bar{x}+\frac{1}{2},x;\ 0,\frac{1}{2},0$	(36) $\bar{3}^{-}\ \bar{x}+1,x-\frac{1}{2},\bar{x};\ \frac{1}{2},0,-\frac{1}{2}$
(37) $c\ \ x,\bar{x},z$	(38) $c\ \ x,x,z$	(39) $\bar{4}^{-}\ 0,0,z;\ 0,0,\frac{1}{4}$	(40) $\bar{4}^{+}\ 0,0,z;\ 0,0,\frac{1}{4}$
(41) $\bar{4}^{-}\ x,-\frac{1}{4},\frac{1}{4};\ 0,-\frac{1}{4},\frac{1}{4}$	(42) $g(0,-\frac{1}{4},\frac{1}{4})\ \ x,y+\frac{1}{4},\bar{y}$	(43) $g(0,\frac{1}{4},\frac{1}{4})\ \ x,y-\frac{1}{4},y$	(44) $\bar{4}^{+}\ x,\frac{1}{4},\frac{1}{4};\ 0,\frac{1}{4},\frac{1}{4}$
(45) $\bar{4}^{+}\ -\frac{1}{4},y,\frac{1}{4};\ -\frac{1}{4},0,\frac{1}{4}$	(46) $g(-\frac{1}{4},0,\frac{1}{4})\ \ \bar{x}+\frac{1}{4},y,x$	(47) $\bar{4}^{-}\ \frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},0,\frac{1}{4}$	(48) $g(\frac{1}{4},0,\frac{1}{4})\ \ x-\frac{1}{4},y,x$

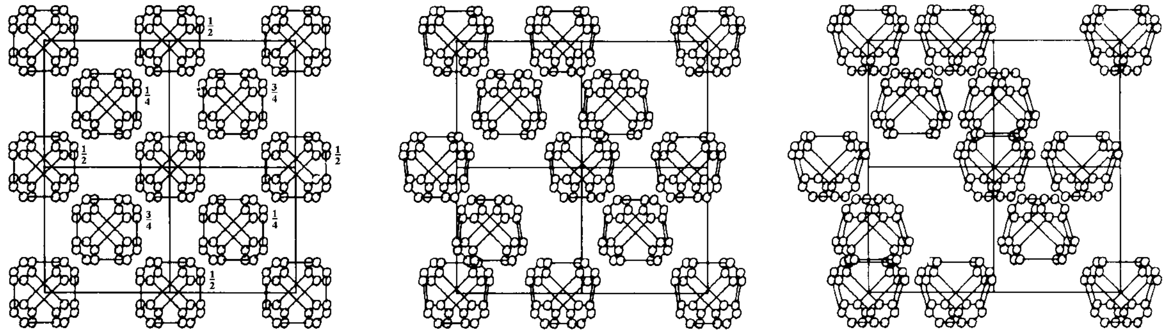
$Fd\bar{3}m$ O_h^7 $m\bar{3}m$ Cubic

No. 227 $F\ 4_1/d\ \bar{3}\ 2/m$ Patterson symmetry $Fm\bar{3}m$

ORIGIN CHOICE 1



Upper left quadrant only



Origin at $\bar{4}3m$, at $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ from centre ($\bar{3}m$)

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{8};\quad -\frac{1}{8} \le z \le \frac{1}{8};\quad y \le \min(\frac{1}{2}-x, x);\quad -y \le z \le y$

Vertices $0,0,0\quad \frac{1}{2},0,0\quad \frac{3}{8},\frac{1}{8},\frac{1}{8}\quad \frac{1}{8},\frac{1}{8},\frac{1}{8}\quad \frac{3}{8},\frac{1}{8},-\frac{1}{8}\quad \frac{1}{8},\frac{1}{8},-\frac{1}{8}$

Symmetry operations

(*given on page* 699)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\tfrac12,\tfrac12)$; $t(\tfrac12,0,\tfrac12)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

$(0,0,0)+\quad (0,\tfrac12,\tfrac12)+\quad (\tfrac12,0,\tfrac12)+\quad (\tfrac12,\tfrac12,0)+$

h,k,l permutable

General:

192 i 1

(1) x,y,z	(2) $\bar{x},\bar{y}+\tfrac12,z+\tfrac12$	(3) $\bar{x}+\tfrac12,y+\tfrac12,\bar{z}$	(4) $x+\tfrac12,\bar{y},\bar{z}+\tfrac12$
(5) z,x,y	(6) $z+\tfrac12,\bar{x},\bar{y}+\tfrac12$	(7) $\bar{z},\bar{x}+\tfrac12,y+\tfrac12$	(8) $\bar{z}+\tfrac12,x+\tfrac12,\bar{y}$
(9) y,z,x	(10) $\bar{y}+\tfrac12,z+\tfrac12,\bar{x}$	(11) $y+\tfrac12,\bar{z},\bar{x}+\tfrac12$	(12) $\bar{y},\bar{z}+\tfrac12,x+\tfrac12$
(13) $y+\tfrac34,x+\tfrac14,\bar{z}+\tfrac34$	(14) $\bar{y}+\tfrac14,\bar{x}+\tfrac14,\bar{z}+\tfrac14$	(15) $y+\tfrac14,\bar{x}+\tfrac34,z+\tfrac34$	(16) $\bar{y}+\tfrac34,x+\tfrac34,z+\tfrac14$
(17) $x+\tfrac34,z+\tfrac14,\bar{y}+\tfrac34$	(18) $\bar{x}+\tfrac34,z+\tfrac34,y+\tfrac14$	(19) $\bar{x}+\tfrac14,\bar{z}+\tfrac14,\bar{y}+\tfrac14$	(20) $x+\tfrac14,\bar{z}+\tfrac34,y+\tfrac34$
(21) $z+\tfrac34,y+\tfrac14,\bar{x}+\tfrac34$	(22) $z+\tfrac14,\bar{y}+\tfrac34,x+\tfrac34$	(23) $\bar{z}+\tfrac34,y+\tfrac34,x+\tfrac14$	(24) $\bar{z}+\tfrac14,\bar{y}+\tfrac14,\bar{x}+\tfrac14$
(25) $\bar{x}+\tfrac14,\bar{y}+\tfrac14,\bar{z}+\tfrac14$	(26) $x+\tfrac14,y+\tfrac34,\bar{z}+\tfrac34$	(27) $x+\tfrac34,\bar{y}+\tfrac34,z+\tfrac14$	(28) $\bar{x}+\tfrac34,y+\tfrac14,z+\tfrac34$
(29) $\bar{z}+\tfrac14,\bar{x}+\tfrac14,\bar{y}+\tfrac14$	(30) $\bar{z}+\tfrac34,x+\tfrac14,y+\tfrac34$	(31) $z+\tfrac14,x+\tfrac34,\bar{y}+\tfrac34$	(32) $z+\tfrac34,\bar{x}+\tfrac34,y+\tfrac14$
(33) $\bar{y}+\tfrac14,\bar{z}+\tfrac14,\bar{x}+\tfrac14$	(34) $y+\tfrac34,\bar{z}+\tfrac34,x+\tfrac14$	(35) $\bar{y}+\tfrac34,z+\tfrac14,x+\tfrac34$	(36) $y+\tfrac14,z+\tfrac34,\bar{x}+\tfrac34$
(37) $\bar{y}+\tfrac12,\bar{x},z+\tfrac12$	(38) y,x,z	(39) $\bar{y},x+\tfrac12,\bar{z}+\tfrac12$	(40) $y+\tfrac12,\bar{x}+\tfrac12,\bar{z}$
(41) $\bar{x}+\tfrac12,\bar{z},y+\tfrac12$	(42) $x+\tfrac12,\bar{z}+\tfrac12,\bar{y}$	(43) x,z,y	(44) $\bar{x},z+\tfrac12,\bar{y}+\tfrac12$
(45) $\bar{z}+\tfrac12,\bar{y},x+\tfrac12$	(46) $\bar{z},y+\tfrac12,\bar{x}+\tfrac12$	(47) $z+\tfrac12,\bar{y}+\tfrac12,\bar{x}$	(48) z,y,x

Reflection conditions (general):
hkl : $h+k=2n$ and $h+l,k+l=2n$
$0kl$: $k+l=4n$ and $k,l=2n$
hhl : $h+l=2n$
$h00$: $h=4n$

Special: as above, plus

96 h ..2 — no extra conditions

$\tfrac18,y,\bar{y}+\tfrac14$	$\tfrac78,\bar{y}+\tfrac12,\bar{y}+\tfrac34$	$\tfrac38,y+\tfrac12,y+\tfrac34$	$\tfrac58,\bar{y},y+\tfrac14$
$\bar{y}+\tfrac14,\tfrac18,y$	$\bar{y}+\tfrac34,\tfrac78,\bar{y}+\tfrac12$	$y+\tfrac34,\tfrac38,y+\tfrac12$	$y+\tfrac14,\tfrac58,\bar{y}$
$y,\bar{y}+\tfrac14,\tfrac18$	$\bar{y}+\tfrac12,\bar{y}+\tfrac34,\tfrac78$	$y+\tfrac12,y+\tfrac34,\tfrac38$	$\bar{y},y+\tfrac14,\tfrac58$
$\tfrac18,\bar{y}+\tfrac14,y$	$\tfrac38,y+\tfrac34,y+\tfrac12$	$\tfrac78,\bar{y}+\tfrac34,\bar{y}+\tfrac12$	$\tfrac58,y+\tfrac14,\bar{y}$
$y,\tfrac18,\bar{y}+\tfrac14$	$y+\tfrac12,\tfrac38,y+\tfrac34$	$\bar{y}+\tfrac12,\tfrac78,\bar{y}+\tfrac34$	$\bar{y},\tfrac58,y+\tfrac14$
$\bar{y}+\tfrac14,y,\tfrac18$	$y+\tfrac34,y+\tfrac12,\tfrac38$	$\bar{y}+\tfrac34,\bar{y}+\tfrac12,\tfrac78$	$y+\tfrac14,\bar{y},\tfrac58$

96 g ..m — no extra conditions

x,x,z	$\bar{x},\bar{x}+\tfrac12,z+\tfrac12$	$\bar{x}+\tfrac12,x+\tfrac12,\bar{z}$	$x+\tfrac12,\bar{x},\bar{z}+\tfrac12$
z,x,x	$z+\tfrac12,\bar{x},\bar{x}+\tfrac12$	$\bar{z},\bar{x}+\tfrac12,x+\tfrac12$	$\bar{z}+\tfrac12,x+\tfrac12,\bar{x}$
x,z,x	$\bar{x}+\tfrac12,z+\tfrac12,\bar{x}$	$x+\tfrac12,\bar{z},\bar{x}+\tfrac12$	$\bar{x},\bar{z}+\tfrac12,x+\tfrac12$
$x+\tfrac34,x+\tfrac14,\bar{z}+\tfrac34$	$\bar{x}+\tfrac14,\bar{x}+\tfrac14,\bar{z}+\tfrac14$	$x+\tfrac14,\bar{x}+\tfrac34,z+\tfrac34$	$\bar{x}+\tfrac34,x+\tfrac34,z+\tfrac14$
$x+\tfrac34,z+\tfrac14,\bar{x}+\tfrac34$	$\bar{x}+\tfrac34,z+\tfrac34,x+\tfrac14$	$\bar{x}+\tfrac14,\bar{z}+\tfrac14,\bar{x}+\tfrac14$	$x+\tfrac14,\bar{z}+\tfrac34,x+\tfrac34$
$z+\tfrac34,x+\tfrac14,\bar{x}+\tfrac34$	$z+\tfrac14,\bar{x}+\tfrac34,x+\tfrac34$	$\bar{z}+\tfrac34,x+\tfrac34,x+\tfrac14$	$\bar{z}+\tfrac14,\bar{x}+\tfrac14,\bar{x}+\tfrac14$

48 f 2.mm — hkl : $h=2n+1$ or $h+k+l=4n$

$x,0,0$	$\bar{x},\tfrac12,\tfrac12$	$0,x,0$	$\tfrac12,\bar{x},\tfrac12$	$0,0,x$	$\tfrac12,\tfrac12,\bar{x}$
$\tfrac34,x+\tfrac14,\tfrac34$	$\tfrac14,\bar{x}+\tfrac14,\tfrac14$	$x+\tfrac34,\tfrac14,\tfrac34$	$\bar{x}+\tfrac34,\tfrac34,\tfrac14$	$\tfrac34,\tfrac14,\bar{x}+\tfrac34$	$\tfrac14,\tfrac34,x+\tfrac34$

32 e .3m — no extra conditions

x,x,x	$\bar{x},\bar{x}+\tfrac12,x+\tfrac12$
$\bar{x}+\tfrac12,x+\tfrac12,\bar{x}$	$x+\tfrac12,\bar{x},\bar{x}+\tfrac12$
$x+\tfrac34,x+\tfrac14,\bar{x}+\tfrac34$	$\bar{x}+\tfrac14,\bar{x}+\tfrac14,\bar{x}+\tfrac14$
$x+\tfrac14,\bar{x}+\tfrac34,x+\tfrac34$	$\bar{x}+\tfrac34,x+\tfrac34,x+\tfrac14$

16 d .$\bar{3}m$ and **16 c .$\bar{3}m$** — hkl : $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$

16 d	$.\bar{3}m$	$\tfrac58,\tfrac58,\tfrac58$	$\tfrac38,\tfrac78,\tfrac18$	$\tfrac78,\tfrac18,\tfrac38$	$\tfrac18,\tfrac38,\tfrac78$
16 c	$.\bar{3}m$	$\tfrac18,\tfrac18,\tfrac18$	$\tfrac78,\tfrac38,\tfrac58$	$\tfrac38,\tfrac58,\tfrac78$	$\tfrac58,\tfrac78,\tfrac38$

8 b $\bar{4}3m$ and **8 a $\bar{4}3m$** — hkl : $h=2n+1$ or $h+k+l=4n$

8 b	$\bar{4}3m$	$\tfrac12,\tfrac12,\tfrac12$	$\tfrac14,\tfrac34,\tfrac14$
8 a	$\bar{4}3m$	$0,0,0$	$\tfrac34,\tfrac14,\tfrac34$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\tfrac14(\mathbf{a}-\mathbf{b})$ $\quad\mathbf{b}'=\tfrac14(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}'=\tfrac16(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\quad\mathbf{b}'=\tfrac16(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c2mm$
$\mathbf{a}'=\tfrac12(-\mathbf{a}+\mathbf{b})$ $\quad\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\tfrac18$

ORIGIN CHOICE 1

Maximal non-isomorphic subgroups

I	[2] $F\bar{4}3m$ (216)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+
	[2] $F4_132$ (210)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+
	[2] $Fd\bar{3}1$ ($Fd\bar{3}$, 203)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+
	[3] $F4_1/d12/m$ ($I4_1/amd$, 141)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
	[3] $F4_1/d12/m$ ($I4_1/amd$, 141)	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
	[3] $F4_1/d12/m$ ($I4_1/amd$, 141)	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
	[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
	[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
	[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
	[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $Fd\bar{3}m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (227)

Minimal non-isomorphic supergroups

I none

II [2] $Pn\bar{3}m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (224)

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\quad 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\quad x,0,\frac{1}{4}$
(5) $3^{+}\ x,x,x$	(6) $3^{+}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$	(7) $3^{+}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$	(8) $3^{+}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^{-}\ x,x,x$	(10) $3^{-}\ x,\bar{x}+\frac{1}{2},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{1}{2},\bar{x},x$	(12) $3^{-}\ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x-\frac{1}{4},\frac{3}{8}$	(14) $2\quad x,\bar{x}+\frac{1}{4},\frac{1}{8}$	(15) $4^{-}(0,0,\frac{3}{4})\quad \frac{1}{2},\frac{1}{4},z$	(16) $4^{+}(0,0,\frac{1}{4})\quad 0,\frac{3}{4},z$
(17) $4^{-}(\frac{3}{4},0,0)\quad x,\frac{1}{2},\frac{1}{4}$	(18) $2(0,\frac{1}{2},\frac{1}{2})\quad \frac{3}{8},y+\frac{1}{4},y$	(19) $2\quad \frac{1}{8},y+\frac{1}{4},\bar{y}$	(20) $4^{+}(\frac{1}{4},0,0)\quad x,0,\frac{3}{4}$
(21) $4^{+}(0,\frac{1}{4},0)\quad \frac{3}{4},y,0$	(22) $2(\frac{1}{2},0,\frac{1}{2})\quad x-\frac{1}{4},\frac{3}{8},x$	(23) $4^{-}(0,\frac{3}{4},0)\quad \frac{1}{4},y,\frac{1}{2}$	(24) $2\quad \bar{x}+\frac{1}{4},\frac{1}{8},x$
(25) $\bar{1}\quad \frac{1}{8},\frac{1}{8},\frac{1}{8}$	(26) $d(\frac{1}{4},\frac{3}{4},0)\quad x,y,\frac{3}{8}$	(27) $d(\frac{3}{4},0,\frac{1}{4})\quad x,\frac{3}{8},z$	(28) $d(0,\frac{1}{4},\frac{3}{4})\quad \frac{3}{8},y,z$
(29) $\bar{3}^{+}\ x,x,x;\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$	(30) $\bar{3}^{+}\ \bar{x}-1,x+1,\bar{x};\ -\frac{1}{8},\frac{1}{8},\frac{7}{8}$	(31) $\bar{3}^{+}\ x,\bar{x}+1,\bar{x};\ \frac{1}{8},\frac{7}{8},-\frac{1}{8}$	(32) $\bar{3}^{+}\ \bar{x}+1,\bar{x},x;\ \frac{7}{8},-\frac{1}{8},\frac{1}{8}$
(33) $\bar{3}^{-}\ x,x,x;\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$	(34) $\bar{3}^{-}\ x+\frac{3}{2},\bar{x}-1,\bar{x};\ \frac{5}{8},-\frac{1}{8},\frac{7}{8}$	(35) $\bar{3}^{-}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{3}{2},x;\ -\frac{1}{8},\frac{7}{8},\frac{5}{8}$	(36) $\bar{3}^{-}\ \bar{x}+1,x+\frac{1}{2},\bar{x};\ \frac{7}{8},\frac{5}{8},-\frac{1}{8}$
(37) $g(\frac{1}{4},-\frac{1}{4},\frac{1}{2})\quad x+\frac{1}{4},\bar{x},z$	(38) $m\quad x,x,z$	(39) $\bar{4}^{-}\ -\frac{1}{4},\frac{1}{4},z;\ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(40) $\bar{4}^{+}\ \frac{1}{2},0,z;\ \frac{1}{2},0,0$
(41) $\bar{4}^{-}\ x,-\frac{1}{4},\frac{1}{4};\ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$	(42) $g(\frac{1}{2},\frac{1}{4},-\frac{1}{4})\quad x,y+\frac{1}{4},\bar{y}$	(43) $m\quad x,y,y$	(44) $\bar{4}^{+}\ x,\frac{1}{2},0;\ 0,\frac{1}{2},0$
(45) $\bar{4}^{+}\ 0,y,\frac{1}{2};\ 0,0,\frac{1}{2}$	(46) $g(-\frac{1}{4},\frac{1}{2},\frac{1}{4})\quad \bar{x}+\frac{1}{4},y,x$	(47) $\bar{4}^{-}\ \frac{1}{4},y,-\frac{1}{4};\ \frac{1}{4},\frac{1}{4},-\frac{1}{4}$	(48) $m\quad x,y,x$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2\quad 0,0,z$	(3) $2\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{3},x-\frac{1}{6},x$	(6) $3^{+}\ \bar{x}+\frac{1}{2},x,\bar{x}$	(7) $3^{+}\ x,\bar{x},\bar{x}$	(8) $3^{+}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x+\frac{1}{6},x$	(10) $3^{-}\ x+\frac{1}{2},\bar{x},\bar{x}$	(11) $3^{-}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^{-}\ \bar{x},x,\bar{x}$
(13) $2(\frac{3}{4},\frac{3}{4},0)\quad x,x,\frac{1}{8}$	(14) $2(-\frac{1}{4},\frac{1}{4},0)\quad x,\bar{x}+\frac{1}{2},\frac{3}{8}$	(15) $4^{-}(0,0,\frac{1}{4})\quad \frac{1}{4},0,z$	(16) $4^{+}(0,0,\frac{3}{4})\quad \frac{1}{4},\frac{1}{2},z$
(17) $4^{-}(\frac{3}{4},0,0)\quad x,\frac{1}{2},-\frac{1}{4}$	(18) $2(0,\frac{1}{2},\frac{1}{2})\quad \frac{3}{8},y-\frac{1}{4},y$	(19) $2\quad \frac{1}{8},y+\frac{3}{4},\bar{y}$	(20) $4^{+}(\frac{1}{4},0,0)\quad x,0,\frac{1}{4}$
(21) $4^{+}(0,\frac{3}{4},0)\quad \frac{1}{2},y,-\frac{1}{4}$	(22) $2(\frac{1}{4},0,\frac{1}{4})\quad x,\frac{1}{8},x$	(23) $4^{-}(0,\frac{1}{4},0)\quad 0,y,\frac{3}{4}$	(24) $2(-\frac{1}{4},0,\frac{1}{4})\quad \bar{x}+\frac{1}{2},\frac{3}{8},x$
(25) $\bar{1}\quad \frac{1}{8},\frac{3}{8},\frac{3}{8}$	(26) $d(\frac{1}{4},\frac{1}{4},0)\quad x,y,\frac{1}{8}$	(27) $d(\frac{3}{4},0,\frac{3}{4})\quad x,\frac{1}{8},z$	(28) $d(0,\frac{3}{4},\frac{1}{4})\quad \frac{3}{8},y,z$
(29) $\bar{3}^{+}\ x,x+\frac{1}{2},x;\ \frac{1}{8},\frac{5}{8},\frac{1}{8}$	(30) $\bar{3}^{+}\ \bar{x}-1,x+\frac{3}{2},\bar{x};\ -\frac{1}{8},\frac{5}{8},\frac{7}{8}$	(31) $\bar{3}^{+}\ x,\bar{x}+\frac{1}{2},\bar{x};\ \frac{1}{8},\frac{3}{8},-\frac{1}{8}$	(32) $\bar{3}^{+}\ \bar{x}+1,\bar{x}-\frac{1}{2},x;\ \frac{7}{8},-\frac{5}{8},\frac{1}{8}$
(33) $\bar{3}^{-}\ x-\frac{1}{2},x-\frac{1}{2},x;\ \frac{1}{8},\frac{1}{8},\frac{5}{8}$	(34) $\bar{3}^{-}\ x+1,\bar{x}-\frac{3}{2},\bar{x};\ \frac{1}{8},-\frac{5}{8},\frac{7}{8}$	(35) $\bar{3}^{-}\ \bar{x},\bar{x}+1,x;\ -\frac{1}{8},\frac{7}{8},\frac{1}{8}$	(36) $\bar{3}^{-}\ \bar{x}+\frac{1}{2},x,\bar{x};\ \frac{3}{8},\frac{1}{8},-\frac{1}{8}$
(37) $m\quad x+\frac{1}{2},\bar{x},z$	(38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})\quad x-\frac{1}{4},x,z$	(39) $\bar{4}^{-}\ 0,0,z;\ 0,0,0$	(40) $\bar{4}^{+}\ \frac{1}{4},-\frac{1}{4},z;\ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$
(41) $\bar{4}^{-}\ x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(42) $g(\frac{1}{2},-\frac{1}{4},\frac{1}{4})\quad x,y+\frac{1}{4},\bar{y}$	(43) $g(0,\frac{1}{2},\frac{1}{2})\quad x,y,y$	(44) $\bar{4}^{+}\ x,0,0;\ 0,0,0$
(45) $\bar{4}^{+}\ \frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(46) $m\quad \bar{x},y,x$	(47) $\bar{4}^{-}\ \frac{1}{2},y,0;\ \frac{1}{2},0,0$	(48) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})\quad x-\frac{1}{4},y,x$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2\quad x,0,0$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x-\frac{1}{6},x$	(6) $3^{+}\ \bar{x},x,\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x-\frac{1}{3},x$	(10) $3^{-}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^{-}\ \bar{x},\bar{x},x$	(12) $3^{-}\ \bar{x},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)\quad x,x,\frac{1}{8}$	(14) $2(\frac{1}{4},-\frac{1}{4},0)\quad x,\bar{x}+\frac{1}{2},\frac{3}{8}$	(15) $4^{-}(0,0,\frac{1}{4})\quad \frac{3}{4},0,z$	(16) $4^{+}(0,0,\frac{3}{4})\quad -\frac{1}{4},\frac{1}{2},z$
(17) $4^{-}(\frac{1}{4},0,0)\quad x,\frac{1}{4},0$	(18) $2(0,\frac{3}{4},\frac{3}{4})\quad \frac{1}{8},y,y$	(19) $2(0,-\frac{1}{4},\frac{1}{4})\quad \frac{3}{8},y+\frac{1}{2},\bar{y}$	(20) $4^{+}(\frac{3}{4},0,0)\quad x,\frac{1}{4},\frac{1}{2}$
(21) $4^{+}(0,\frac{1}{4},0)\quad \frac{1}{4},y,0$	(22) $2(\frac{1}{2},0,\frac{1}{2})\quad x+\frac{1}{4},\frac{3}{8},x$	(23) $4^{-}(0,\frac{3}{4},0)\quad -\frac{1}{4},y,\frac{1}{2}$	(24) $2\quad \bar{x}+\frac{3}{4},\frac{1}{8},x$
(25) $\bar{1}\quad \frac{3}{8},\frac{1}{8},\frac{3}{8}$	(26) $d(\frac{3}{4},\frac{3}{4},0)\quad x,y,\frac{1}{8}$	(27) $d(\frac{1}{4},0,\frac{3}{4})\quad x,\frac{3}{8},z$	(28) $d(0,\frac{1}{4},\frac{1}{4})\quad \frac{1}{8},y,z$
(29) $\bar{3}^{+}\ x-\frac{1}{2},x-\frac{1}{2},x;\ \frac{1}{8},\frac{1}{8},\frac{5}{8}$	(30) $\bar{3}^{+}\ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x};\ -\frac{1}{8},\frac{1}{8},\frac{3}{8}$	(31) $\bar{3}^{+}\ x-\frac{1}{2},\bar{x}+\frac{3}{2},\bar{x};\ \frac{1}{8},\frac{7}{8},-\frac{5}{8}$	(32) $\bar{3}^{+}\ \bar{x}+\frac{3}{2},\bar{x}+\frac{1}{2},x;\ \frac{7}{8},-\frac{1}{8},\frac{5}{8}$
(33) $\bar{3}^{-}\ x+\frac{1}{2},x,x;\ \frac{5}{8},\frac{1}{8},\frac{1}{8}$	(34) $\bar{3}^{-}\ x+1,\bar{x}-1,\bar{x};\ \frac{1}{8},-\frac{1}{8},\frac{7}{8}$	(35) $\bar{3}^{-}\ \bar{x},\bar{x}+\frac{1}{2},x;\ -\frac{1}{8},\frac{3}{8},\frac{1}{8}$	(36) $\bar{3}^{-}\ \bar{x}+\frac{3}{2},x-\frac{1}{2},\bar{x};\ \frac{7}{8},\frac{1}{8},-\frac{5}{8}$
(37) $m\quad x,\bar{x},z$	(38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})\quad x+\frac{1}{4},x,z$	(39) $\bar{4}^{-}\ 0,\frac{1}{2},z;\ 0,\frac{1}{2},0$	(40) $\bar{4}^{+}\ \frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(41) $\bar{4}^{-}\ x,0,0;\ 0,0,0$	(42) $m\quad x,y+\frac{1}{2},\bar{y}$	(43) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})\quad x,y-\frac{1}{4},y$	(44) $\bar{4}^{+}\ x,\frac{1}{4},-\frac{1}{4};\ \frac{1}{4},\frac{1}{4},-\frac{1}{4}$
(45) $\bar{4}^{+}\ 0,y,0;\ 0,0,0$	(46) $g(\frac{1}{4},\frac{1}{2},-\frac{1}{4})\quad \bar{x}+\frac{1}{4},y,x$	(47) $\bar{4}^{-}\ \frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(48) $g(\frac{1}{2},0,\frac{1}{2})\quad x,y,x$

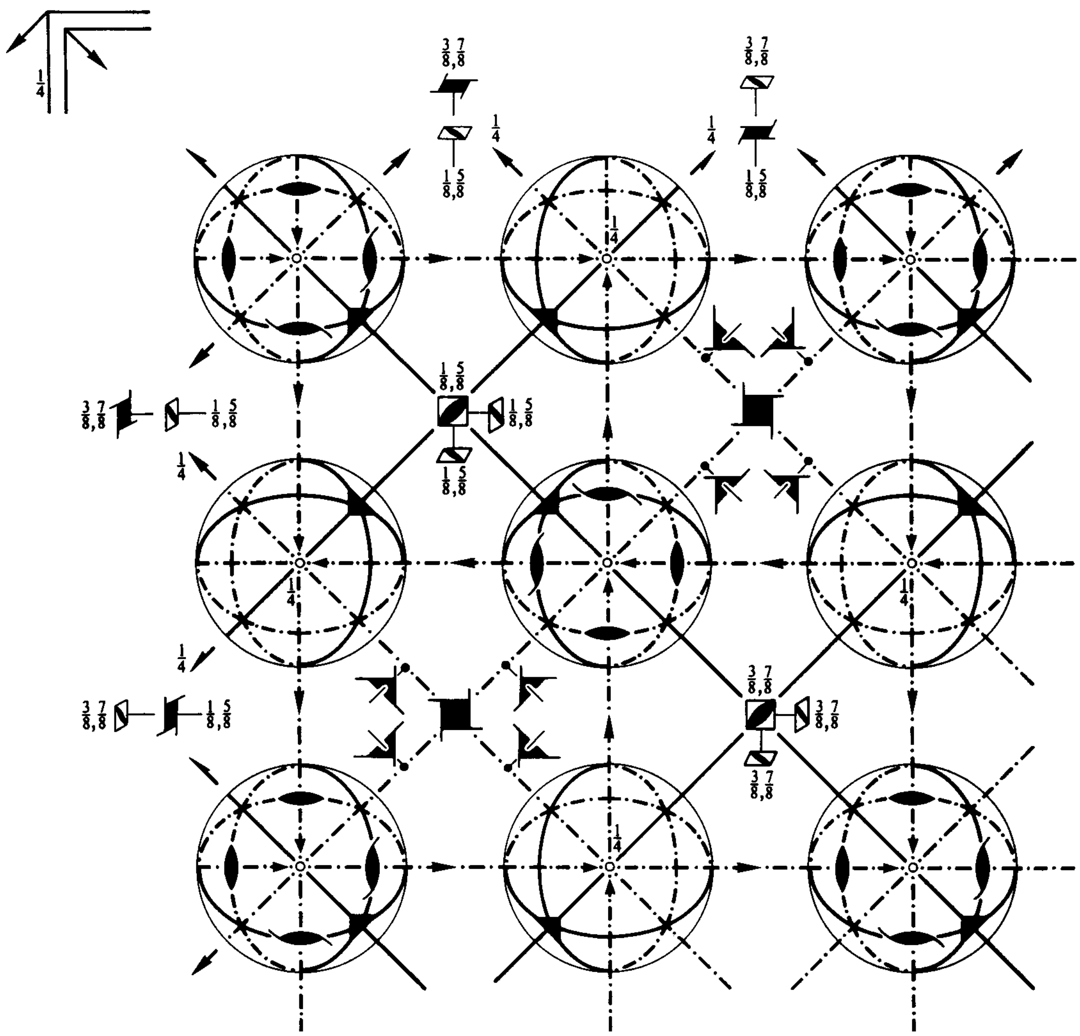
For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,\frac{1}{4},\frac{1}{4}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x+\frac{1}{3},x$	(6) $3^{+}\ \bar{x},x+\frac{1}{2},\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{3},x+\frac{1}{6},x$	(10) $3^{-}\ x,\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) $3^{-}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x+\frac{1}{4},\frac{3}{8}$	(14) $2\quad x,\bar{x}+\frac{3}{4},\frac{1}{8}$	(15) $4^{-}(0,0,\frac{3}{4})\quad \frac{1}{2},-\frac{1}{4},z$	(16) $4^{+}(0,0,\frac{1}{4})\quad 0,\frac{1}{4},z$
(17) $4^{-}(\frac{1}{4},0,0)\quad x,\frac{3}{4},0$	(18) $2(0,\frac{1}{4},\frac{1}{4})\quad \frac{1}{8},y,y$	(19) $2(0,\frac{1}{4},-\frac{1}{4})\quad \frac{3}{8},y+\frac{1}{2},\bar{y}$	(20) $4^{+}(\frac{3}{4},0,0)\quad x,-\frac{1}{4},\frac{1}{2}$
(21) $4^{+}(0,\frac{3}{4},0)\quad \frac{1}{2},y,\frac{1}{4}$	(22) $2(\frac{3}{4},0,\frac{3}{4})\quad x,\frac{1}{8},x$	(23) $4^{-}(0,\frac{1}{4},0)\quad 0,y,\frac{1}{4}$	(24) $2(\frac{1}{4},0,-\frac{1}{4})\quad \bar{x}+\frac{1}{2},\frac{3}{8},x$
(25) $\bar{1}\quad \frac{3}{8},\frac{3}{8},\frac{1}{8}$	(26) $d(\frac{3}{4},\frac{1}{4},0)\quad x,y,\frac{3}{8}$	(27) $d(\frac{1}{4},0,\frac{1}{4})\quad x,\frac{1}{8},z$	(28) $d(0,\frac{3}{4},\frac{3}{4})\quad \frac{1}{8},y,z$
(29) $\bar{3}^{+}\ x+\frac{1}{2},x,x;\ \frac{5}{8},\frac{1}{8},\frac{1}{8}$	(30) $\bar{3}^{+}\ \bar{x}-\frac{3}{2},x+1,\bar{x};\ -\frac{5}{8},\frac{1}{8},\frac{7}{8}$	(31) $\bar{3}^{+}\ x+\frac{1}{2},\bar{x}+1,\bar{x};\ \frac{5}{8},\frac{7}{8},-\frac{1}{8}$	(32) $\bar{3}^{+}\ \bar{x}+\frac{1}{2},\bar{x},x;\ \frac{3}{8},-\frac{1}{8},\frac{1}{8}$
(33) $\bar{3}^{-}\ x,x+\frac{1}{2},x;\ \frac{1}{8},\frac{5}{8},\frac{1}{8}$	(34) $\bar{3}^{-}\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};\ \frac{1}{8},-\frac{1}{8},\frac{3}{8}$	(35) $\bar{3}^{-}\ \bar{x}-\frac{1}{2},\bar{x}+1,x;\ -\frac{5}{8},\frac{7}{8},\frac{1}{8}$	(36) $\bar{3}^{-}\ \bar{x}+1,x,\bar{x};\ \frac{7}{8},\frac{1}{8},-\frac{1}{8}$
(37) $g(-\frac{1}{4},\frac{1}{4},\frac{1}{2})\quad x+\frac{1}{4},\bar{x},z$	(38) $g(\frac{1}{2},\frac{1}{2},0)\quad x,x,z$	(39) $\bar{4}^{-}\ \frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(40) $\bar{4}^{+}\ 0,0,z;\ 0,0,0$
(41) $\bar{4}^{-}\ x,0,\frac{1}{2};\ 0,0,\frac{1}{2}$	(42) $m\quad x,y,\bar{y}$	(43) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})\quad x,y+\frac{1}{4},y$	(44) $\bar{4}^{+}\ x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(45) $\bar{4}^{+}\ -\frac{1}{4},y,\frac{1}{4};\ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(46) $m\quad \bar{x}+\frac{1}{2},y,x$	(47) $\bar{4}^{-}\ 0,y,0;\ 0,0,0$	(48) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})\quad x+\frac{1}{4},y,x$

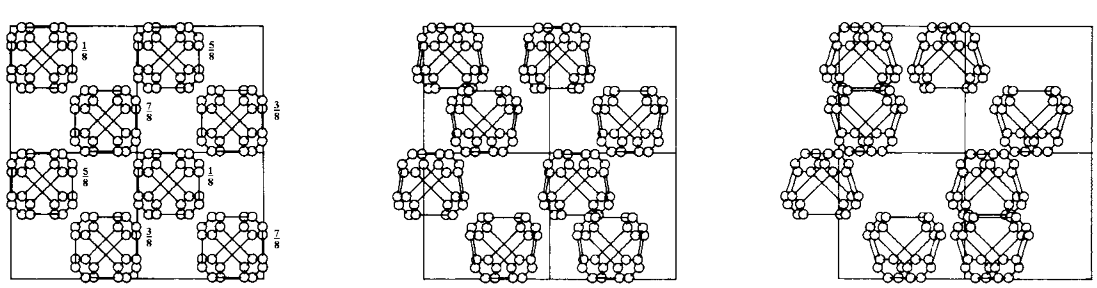
$F\,d\bar{3}m$ $\quad O_h^7$ $\quad m\bar{3}m$ $\quad$ Cubic

No. 227 $\quad F\ 4_1/d\ \bar{3}\ 2/m$ $\quad$ Patterson symmetry $F\,m\bar{3}m$

ORIGIN CHOICE 2



Upper left quadrant only



Origin at centre ($\bar{3}m$), at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ from $\bar{4}3m$

Asymmetric unit $\quad -\frac{1}{8} \le x \le \frac{3}{8};\quad -\frac{1}{8} \le y \le 0;\quad -\frac{1}{4} \le z \le 0;\quad y \le \min(\frac{1}{4}-x,x);\quad -y-\frac{1}{4} \le z \le y$

Vertices $\quad -\frac{1}{8},-\frac{1}{8},-\frac{1}{8} \quad \frac{3}{8},-\frac{1}{8},-\frac{1}{8} \quad \frac{1}{4},0,0 \quad 0,0,0 \quad \frac{1}{4},0,-\frac{1}{4} \quad 0,0,-\frac{1}{4}$

Symmetry operations

(*given on page* 703)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

$(0,0,0)+\quad(0,\frac{1}{2},\frac{1}{2})+\quad(\frac{1}{2},0,\frac{1}{2})+\quad(\frac{1}{2},\frac{1}{2},0)+$

Reflection conditions: h,k,l permutable

General:

192	i	1	(1) x,y,z	(2) $\bar{x}+\frac{3}{4},\bar{y}+\frac{1}{4},z+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{4},y+\frac{1}{2},\bar{z}+\frac{3}{4}$	(4) $x+\frac{1}{2},\bar{y}+\frac{3}{4},\bar{z}+\frac{1}{4}$	hkl : $h+k=2n$ and $h+l,k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{y}+\frac{1}{4}$	(7) $\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4},y+\frac{1}{2}$	(8) $\bar{z}+\frac{1}{4},x+\frac{1}{2},\bar{y}+\frac{3}{4}$	$0kl$: $k+l=4n$ and $k,l=2n$
			(9) y,z,x	(10) $\bar{y}+\frac{1}{4},z+\frac{1}{2},\bar{x}+\frac{3}{4}$	(11) $y+\frac{1}{2},\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4}$	(12) $\bar{y}+\frac{3}{4},\bar{z}+\frac{1}{4},x+\frac{1}{2}$	hhl : $h+l=2n$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{2}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y+\frac{1}{4},\bar{x}+\frac{1}{2},z+\frac{3}{4}$	(16) $\bar{y}+\frac{1}{2},x+\frac{3}{4},z+\frac{1}{4}$	$h00$: $h=4n$
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x+\frac{1}{4},\bar{z}+\frac{1}{2},y+\frac{3}{4}$	
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{2}$	(22) $z+\frac{1}{4},\bar{y}+\frac{1}{2},x+\frac{3}{4}$	(23) $\bar{z}+\frac{1}{2},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z},\bar{y},\bar{x}$	
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{1}{4},y+\frac{3}{4},\bar{z}+\frac{1}{2}$	(27) $x+\frac{3}{4},\bar{y}+\frac{1}{2},z+\frac{1}{4}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{4},z+\frac{3}{4}$	
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{4},y+\frac{3}{4}$	(31) $z+\frac{1}{4},x+\frac{3}{4},\bar{y}+\frac{1}{2}$	(32) $z+\frac{3}{4},\bar{x}+\frac{1}{2},y+\frac{1}{4}$	
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y+\frac{3}{4},\bar{z}+\frac{1}{2},x+\frac{1}{4}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{4},x+\frac{3}{4}$	(36) $y+\frac{1}{4},z+\frac{3}{4},\bar{x}+\frac{1}{2}$	
			(37) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{1}{2}$	(38) y,x,z	(39) $\bar{y}+\frac{3}{4},x+\frac{1}{2},\bar{z}+\frac{1}{4}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$	
			(41) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$	(43) x,z,y	(44) $\bar{x}+\frac{3}{4},z+\frac{1}{2},\bar{y}+\frac{1}{4}$	
			(45) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{1}{2}$	(46) $\bar{z}+\frac{3}{4},y+\frac{1}{2},\bar{x}+\frac{1}{4}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(48) z,y,x	

Special: as above, plus

96	h	$..2$	$0,y,\bar{y}$	$\frac{3}{4},\bar{y}+\frac{1}{4},\bar{y}+\frac{1}{2}$	$\frac{1}{4},y+\frac{1}{2},y+\frac{3}{4}$	$\frac{1}{2},\bar{y}+\frac{3}{4},y+\frac{1}{4}$	no extra conditions
			$\bar{y},0,y$	$\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}+\frac{1}{4}$	$y+\frac{3}{4},\frac{1}{4},y+\frac{1}{2}$	$y+\frac{1}{4},\frac{1}{2},\bar{y}+\frac{3}{4}$	
			$y,\bar{y},0$	$\bar{y}+\frac{1}{4},\bar{y}+\frac{1}{2},\frac{3}{4}$	$y+\frac{1}{2},y+\frac{3}{4},\frac{1}{4}$	$\bar{y}+\frac{3}{4},y+\frac{1}{4},\frac{1}{2}$	
			$0,\bar{y},y$	$\frac{1}{4},y+\frac{3}{4},y+\frac{1}{2}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{4}$	$\frac{1}{2},y+\frac{1}{4},\bar{y}+\frac{3}{4}$	
			$y,0,\bar{y}$	$y+\frac{1}{2},\frac{1}{4},y+\frac{3}{4}$	$\bar{y}+\frac{1}{4},\frac{3}{4},\bar{y}+\frac{1}{2}$	$\bar{y}+\frac{3}{4},\frac{1}{2},y+\frac{1}{4}$	
			$\bar{y},y,0$	$y+\frac{3}{4},y+\frac{1}{2},\frac{1}{4}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{4},\frac{3}{4}$	$y+\frac{1}{4},\bar{y}+\frac{3}{4},\frac{1}{2}$	
96	g	$..m$	x,x,z	$\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},z+\frac{1}{2}$	$\bar{x}+\frac{1}{4},x+\frac{1}{2},\bar{z}+\frac{3}{4}$	$x+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{z}+\frac{1}{4}$	no extra conditions
			z,x,x	$z+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4}$	$\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4},x+\frac{1}{2}$	$\bar{z}+\frac{1}{4},x+\frac{1}{2},\bar{x}+\frac{3}{4}$	
			x,z,x	$\bar{x}+\frac{1}{4},z+\frac{1}{2},\bar{x}+\frac{3}{4}$	$x+\frac{1}{2},\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4}$	$\bar{x}+\frac{3}{4},\bar{z}+\frac{1}{4},x+\frac{1}{2}$	
			$x+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{2}$	$\bar{x},\bar{x},\bar{z}$	$x+\frac{1}{4},\bar{x}+\frac{1}{2},z+\frac{3}{4}$	$\bar{x}+\frac{1}{2},x+\frac{3}{4},z+\frac{1}{4}$	
			$x+\frac{3}{4},z+\frac{1}{4},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},z+\frac{3}{4},x+\frac{1}{4}$	$\bar{x},\bar{z},\bar{x}$	$x+\frac{1}{4},\bar{z}+\frac{1}{2},x+\frac{3}{4}$	
			$z+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{2}$	$z+\frac{1}{4},\bar{x}+\frac{1}{2},x+\frac{3}{4}$	$\bar{z}+\frac{1}{2},x+\frac{3}{4},x+\frac{1}{4}$	$\bar{z},\bar{x},\bar{x}$	

48	f	$2.mm$	$x,\frac{1}{8},\frac{1}{8}$	$\bar{x}+\frac{3}{4},\frac{1}{8},\frac{5}{8}$	$\frac{1}{8},x,\frac{1}{8}$	$\frac{5}{8},\bar{x}+\frac{3}{4},\frac{1}{8}$	$\frac{1}{8},\frac{1}{8},x$	$\frac{1}{8},\frac{5}{8},\bar{x}+\frac{3}{4}$	hkl : $h=2n+1$ or $h+k+l=4n$
			$\frac{7}{8},x+\frac{1}{4},\frac{3}{8}$	$\frac{7}{8},\bar{x},\frac{7}{8}$	$x+\frac{3}{4},\frac{3}{8},\frac{3}{8}$	$\bar{x}+\frac{1}{2},\frac{7}{8},\frac{3}{8}$	$\frac{7}{8},\frac{3}{8},\bar{x}+\frac{1}{2}$	$\frac{3}{8},\frac{3}{8},x+\frac{3}{4}$	

32	e	$.3m$	x,x,x	$\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},x+\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{4},x+\frac{1}{2},\bar{x}+\frac{3}{4}$	$x+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4}$	
			$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{2}$	$\bar{x},\bar{x},\bar{x}$	
			$x+\frac{1}{4},\bar{x}+\frac{1}{2},x+\frac{3}{4}$	$\bar{x}+\frac{1}{2},x+\frac{3}{4},x+\frac{1}{4}$	

16	d	$.\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},0,\frac{1}{4}$	$0,\frac{1}{4},\frac{3}{4}$	hkl : $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16	c	$.\bar{3}m$	$0,0,0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$	

8	b	$\bar{4}3m$	$\frac{3}{8},\frac{3}{8},\frac{3}{8}$	$\frac{1}{8},\frac{5}{8},\frac{1}{8}$	hkl : $h=2n+1$ or $h+k+l=4n$
8	a	$\bar{4}3m$	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{3}{8},\frac{3}{8}$	

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{4}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{4}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{8},\frac{3}{8},z$

Along [111] $p6mm$
$\mathbf{a}'=\frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $F\bar{4}3m$ (216)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+
	[2] $F4_132$ (210)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+
	[2] $Fd\bar{3}1$ ($Fd\bar{3}$, 203)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+
	[3] $F4_1/d12/m$ ($I4_1/amd$, 141)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
	[3] $F4_1/d12/m$ ($I4_1/amd$, 141)	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
	[3] $F4_1/d12/m$ ($I4_1/amd$, 141)	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
	[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
	[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
	[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
	[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+
IIa	none	
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $Fd\bar{3}m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (227)

Minimal non-isomorphic supergroups

I none

II [2] $Pn\bar{3}m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (224)

CONTINUED
(*from page* 700)

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{3}{8},\frac{1}{8},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{8},y,\frac{3}{8}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{3}{8},\frac{1}{8}$
(5) $3^{+}\ x,x,x$	(6) $3^{+}\ \bar{x}+\frac{1}{2},x+\frac{1}{4},\bar{x}$	(7) $3^{+}\ x+\frac{3}{4},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^{+}\ \bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x$
(9) $3^{-}\ x,x,x$	(10) $3^{-}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{5}{12},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^{-}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{7}{12},\bar{x}+\frac{5}{12},x$	(12) $3^{-}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}-\frac{1}{6},x+\frac{7}{12},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x-\frac{1}{4},\frac{1}{4}$	(14) $2\quad x,\bar{x},0$	(15) $4^{-}(0,0,\frac{3}{4})\quad \frac{3}{8},\frac{1}{8},z$	(16) $4^{+}(0,0,\frac{1}{4})\quad -\frac{1}{8},\frac{5}{8},z$
(17) $4^{-}(\frac{3}{4},0,0)\quad x,\frac{3}{8},\frac{1}{8}$	(18) $2(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y+\frac{1}{4},y$	(19) $2\quad 0,y,\bar{y}$	(20) $4^{+}(\frac{1}{4},0,0)\quad x,-\frac{1}{8},\frac{5}{8}$
(21) $4^{+}(0,\frac{1}{4},0)\quad \frac{5}{8},y,-\frac{1}{8}$	(22) $2(\frac{1}{2},0,\frac{1}{2})\quad x-\frac{1}{4},\frac{1}{4},x$	(23) $4^{-}(0,\frac{3}{4},0)\quad \frac{1}{8},y,\frac{3}{8}$	(24) $2\quad \bar{x},0,x$
(25) $\bar{1}\quad 0,0,0$	(26) $d(\frac{1}{4},\frac{3}{4},0)\quad x,y,\frac{1}{4}$	(27) $d(\frac{3}{4},0,\frac{1}{4})\quad x,\frac{1}{4},z$	(28) $d(0,\frac{1}{4},\frac{3}{4})\quad \frac{1}{4},y,z$
(29) $\bar{3}^{+}\ x,x,x;\ 0,0,0$	(30) $\bar{3}^{+}\ \bar{x}-1,x+\frac{3}{4},\bar{x};\ -\frac{1}{4},0,\frac{3}{4}$	(31) $\bar{3}^{+}\ x-\frac{1}{4},\bar{x}+1,\bar{x};\ 0,\frac{3}{4},-\frac{1}{4}$	(32) $\bar{3}^{+}\ \bar{x}+\frac{3}{4},\bar{x}-\frac{1}{4},x;\ \frac{3}{4},-\frac{1}{4},0$
(33) $\bar{3}^{-}\ x,x,x;\ 0,0,0$	(34) $\bar{3}^{-}\ x+\frac{5}{4},\bar{x}-1,\bar{x};\ \frac{1}{2},-\frac{1}{4},\frac{3}{4}$	(35) $\bar{3}^{-}\ \bar{x}+\frac{1}{4},\bar{x}+\frac{5}{4},x;\ -\frac{1}{4},\frac{3}{4},\frac{1}{2}$	(36) $\bar{3}^{-}\ \bar{x}+1,x+\frac{1}{4},\bar{x};\ \frac{3}{4},\frac{1}{2},-\frac{1}{4}$
(37) $g(-\frac{1}{4},\frac{1}{4},\frac{1}{2})\quad x+\frac{1}{2},\bar{x},z$	(38) $m\quad x,x,z$	(39) $\bar{4}^{-}\ \frac{1}{8},\frac{5}{8},z;\ \frac{1}{8},\frac{5}{8},\frac{1}{8}$	(40) $\bar{4}^{+}\ \frac{3}{8},-\frac{1}{8},z;\ \frac{3}{8},-\frac{1}{8},\frac{3}{8}$
(41) $\bar{4}^{-}\ x,\frac{1}{8},\frac{5}{8};\ \frac{1}{8},\frac{1}{8},\frac{5}{8}$	(42) $g(\frac{1}{2},-\frac{1}{4},\frac{1}{4})\quad x,y+\frac{1}{2},\bar{y}$	(43) $m\quad x,y,y$	(44) $\bar{4}^{+}\ x,\frac{3}{8},-\frac{1}{8};\ \frac{3}{8},\frac{3}{8},-\frac{1}{8}$
(45) $\bar{4}^{+}\ -\frac{1}{8},y,\frac{3}{8};\ -\frac{1}{8},\frac{3}{8},\frac{3}{8}$	(46) $g(\frac{1}{4},\frac{1}{2},-\frac{1}{4})\quad \bar{x}+\frac{1}{2},y,x$	(47) $\bar{4}^{-}\ \frac{5}{8},y,\frac{1}{8};\ \frac{5}{8},\frac{1}{8},\frac{1}{8}$	(48) $m\quad x,y,x$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2\quad \frac{3}{8},\frac{3}{8},z$	(3) $2\quad \frac{1}{8},y,\frac{1}{8}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{8},\frac{3}{8}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{3},x-\frac{1}{6},x$	(6) $3^{+}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}+\frac{1}{6},x+\frac{5}{12},\bar{x}$	(7) $3^{+}\ x+\frac{3}{4},\bar{x},\bar{x}$	(8) $3^{+}\ \bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x+\frac{1}{6},x$	(10) $3^{-}\ x+\frac{1}{4},\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},x$	(12) $3^{-}\ \bar{x},x+\frac{3}{4},\bar{x}$
(13) $2(\frac{3}{4},\frac{3}{4},0)\quad x,x,0$	(14) $2(-\frac{1}{4},\frac{1}{4},0)\quad x,\bar{x}+\frac{1}{4},\frac{1}{4}$	(15) $4^{-}(0,0,\frac{1}{4})\quad \frac{1}{8},-\frac{1}{8},z$	(16) $4^{+}(0,0,\frac{3}{4})\quad \frac{1}{8},\frac{3}{8},z$
(17) $4^{-}(\frac{3}{4},0,0)\quad x,\frac{3}{8},-\frac{3}{8}$	(18) $2(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y-\frac{1}{4},y$	(19) $2\quad 0,y+\frac{1}{2},\bar{y}$	(20) $4^{+}(\frac{1}{4},0,0)\quad x,-\frac{1}{8},\frac{1}{8}$
(21) $4^{+}(0,\frac{3}{4},0)\quad \frac{3}{8},y,-\frac{3}{8}$	(22) $2(\frac{1}{4},0,\frac{1}{4})\quad x,0,x$	(23) $4^{-}(0,\frac{1}{4},0)\quad -\frac{1}{8},y,\frac{5}{8}$	(24) $2(-\frac{1}{4},0,\frac{1}{4})\quad \bar{x}+\frac{1}{4},\frac{1}{4},x$
(25) $\bar{1}\quad 0,\frac{1}{4},\frac{1}{4}$	(26) $d(\frac{1}{4},\frac{1}{4},0)\quad x,y,0$	(27) $d(\frac{3}{4},0,\frac{3}{4})\quad x,0,z$	(28) $d(0,\frac{3}{4},\frac{1}{4})\quad \frac{1}{4},y,z$
(29) $\bar{3}^{+}\ x,x+\frac{1}{2},x;\ 0,\frac{1}{2},0$	(30) $\bar{3}^{+}\ \bar{x}-1,x+\frac{5}{4},\bar{x};\ -\frac{1}{4},\frac{1}{2},\frac{3}{4}$	(31) $\bar{3}^{+}\ x-\frac{1}{4},\bar{x}+\frac{1}{2},\bar{x};\ 0,\frac{1}{4},-\frac{1}{4}$	(32) $\bar{3}^{+}\ \bar{x}+\frac{3}{4},\bar{x}-\frac{3}{4},x;\ \frac{3}{4},-\frac{3}{4},0$
(33) $\bar{3}^{-}\ x-\frac{1}{2},x-\frac{1}{2},x;\ 0,0,\frac{1}{2}$	(34) $\bar{3}^{-}\ x+\frac{3}{4},\bar{x}-\frac{3}{2},\bar{x};\ 0,-\frac{3}{4},\frac{3}{4}$	(35) $\bar{3}^{-}\ \bar{x}-\frac{1}{4},\bar{x}+\frac{3}{4},x;\ -\frac{1}{4},\frac{3}{4},0$	(36) $\bar{3}^{-}\ \bar{x}+\frac{1}{2},x-\frac{1}{4},\bar{x};\ \frac{1}{4},0,-\frac{1}{4}$
(37) $m\quad x+\frac{1}{4},\bar{x},z$	(38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})\quad x-\frac{1}{4},x,z$	(39) $\bar{4}^{-}\ \frac{3}{8},\frac{3}{8},z;\ \frac{3}{8},\frac{3}{8},\frac{3}{8}$	(40) $\bar{4}^{+}\ \frac{5}{8},\frac{1}{8},z;\ \frac{5}{8},\frac{1}{8},\frac{1}{8}$
(41) $\bar{4}^{-}\ x,\frac{1}{8},\frac{1}{8};\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$	(42) $g(\frac{1}{2},\frac{1}{4},-\frac{1}{4})\quad x,y+\frac{1}{2},\bar{y}$	(43) $g(0,\frac{1}{2},\frac{1}{2})\quad x,y,y$	(44) $\bar{4}^{+}\ x,\frac{3}{8},\frac{3}{8};\ \frac{3}{8},\frac{3}{8},\frac{3}{8}$
(45) $\bar{4}^{+}\ \frac{1}{8},y,\frac{1}{8};\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$	(46) $m\quad \bar{x}+\frac{3}{4},y,x$	(47) $\bar{4}^{-}\ \frac{3}{8},y,-\frac{1}{8};\ \frac{3}{8},\frac{3}{8},-\frac{1}{8}$	(48) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})\quad x-\frac{1}{4},y,x$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2\quad \frac{1}{8},\frac{1}{8},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{3}{8},y,\frac{1}{8}$	(4) $2\quad x,\frac{3}{8},\frac{3}{8}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x-\frac{1}{6},x$	(6) $3^{+}\ \bar{x},x+\frac{3}{4},\bar{x}$	(7) $3^{+}\ x+\frac{1}{4},\bar{x},\bar{x}$	(8) $3^{+}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{5}{12},\bar{x}+\frac{7}{12},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x-\frac{1}{3},x$	(10) $3^{-}\ x+\frac{1}{4},\bar{x}+\frac{1}{2},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},x$	(12) $3^{-}\ \bar{x},x+\frac{1}{4},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)\quad x,x,0$	(14) $2(\frac{1}{4},-\frac{1}{4},0)\quad x,\bar{x}+\frac{1}{4},\frac{1}{4}$	(15) $4^{-}(0,0,\frac{1}{4})\quad \frac{5}{8},-\frac{1}{8},z$	(16) $4^{+}(0,0,\frac{3}{4})\quad -\frac{3}{8},\frac{3}{8},z$
(17) $4^{-}(\frac{1}{4},0,0)\quad x,\frac{1}{8},-\frac{1}{8}$	(18) $2(0,\frac{3}{4},\frac{3}{4})\quad 0,y,y$	(19) $2(0,-\frac{1}{4},\frac{1}{4})\quad \frac{1}{4},y+\frac{1}{4},\bar{y}$	(20) $4^{+}(\frac{3}{4},0,0)\quad x,\frac{1}{8},\frac{3}{8}$
(21) $4^{+}(0,\frac{1}{4},0)\quad \frac{1}{8},y,-\frac{1}{8}$	(22) $2(\frac{1}{2},0,\frac{1}{2})\quad x+\frac{1}{4},\frac{1}{4},x$	(23) $4^{-}(0,\frac{3}{4},0)\quad -\frac{3}{8},y,\frac{3}{8}$	(24) $2\quad \bar{x}+\frac{1}{2},0,x$
(25) $\bar{1}\quad \frac{1}{4},0,\frac{1}{4}$	(26) $d(\frac{3}{4},\frac{3}{4},0)\quad x,y,0$	(27) $d(\frac{1}{4},0,\frac{3}{4})\quad x,\frac{1}{4},z$	(28) $d(0,\frac{1}{4},\frac{1}{4})\quad 0,y,z$
(29) $\bar{3}^{+}\ x-\frac{1}{2},x-\frac{1}{2},x;\ 0,0,\frac{1}{2}$	(30) $\bar{3}^{+}\ \bar{x}-\frac{1}{2},x+\frac{1}{4},\bar{x};\ -\frac{1}{4},0,\frac{1}{4}$	(31) $\bar{3}^{+}\ x-\frac{3}{4},\bar{x}+\frac{3}{2},\bar{x};\ 0,\frac{3}{4},-\frac{3}{4}$	(32) $\bar{3}^{+}\ \bar{x}+\frac{5}{4},\bar{x}+\frac{1}{4},x;\ \frac{3}{4},-\frac{1}{4},\frac{1}{2}$
(33) $\bar{3}^{-}\ x+\frac{1}{2},x,x;\ \frac{1}{2},0,0$	(34) $\bar{3}^{-}\ x+\frac{3}{4},\bar{x}-1,\bar{x};\ 0,-\frac{1}{4},\frac{3}{4}$	(35) $\bar{3}^{-}\ \bar{x}-\frac{1}{4},\bar{x}+\frac{1}{4},x;\ -\frac{1}{4},\frac{1}{4},0$	(36) $\bar{3}^{-}\ \bar{x}+\frac{3}{2},x-\frac{3}{4},\bar{x};\ \frac{3}{4},0,-\frac{3}{4}$
(37) $m\quad x+\frac{3}{4},\bar{x},z$	(38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})\quad x+\frac{1}{4},x,z$	(39) $\bar{4}^{-}\ -\frac{1}{8},\frac{3}{8},z;\ -\frac{1}{8},\frac{3}{8},\frac{3}{8}$	(40) $\bar{4}^{+}\ \frac{1}{8},\frac{1}{8},z;\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$
(41) $\bar{4}^{-}\ x,\frac{3}{8},\frac{3}{8};\ \frac{3}{8},\frac{3}{8},\frac{3}{8}$	(42) $m\quad x,y+\frac{1}{4},\bar{y}$	(43) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})\quad x,y-\frac{1}{4},y$	(44) $\bar{4}^{+}\ x,\frac{5}{8},\frac{1}{8};\ \frac{1}{8},\frac{5}{8},\frac{1}{8}$
(45) $\bar{4}^{+}\ \frac{3}{8},y,\frac{3}{8};\ \frac{3}{8},\frac{3}{8},\frac{3}{8}$	(46) $g(-\frac{1}{4},\frac{1}{2},\frac{1}{4})\quad \bar{x}+\frac{1}{2},y,x$	(47) $\bar{4}^{-}\ \frac{1}{8},y,\frac{1}{8};\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$	(48) $g(\frac{1}{2},0,\frac{1}{2})\quad x,y,x$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

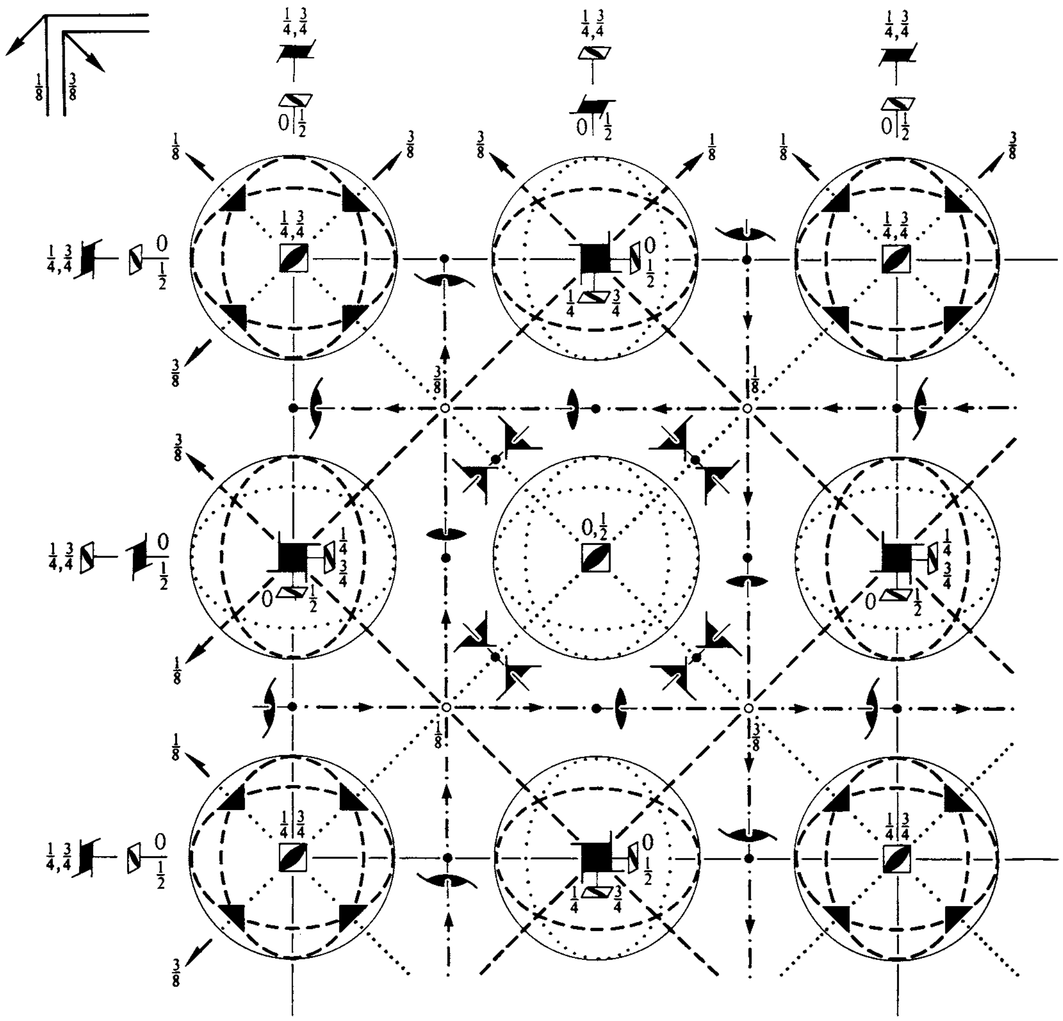
(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{8},\frac{3}{8},z$	(3) $2\quad \frac{3}{8},y,\frac{3}{8}$	(4) $2\quad x,\frac{1}{8},\frac{1}{8}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x+\frac{1}{3},x$	(6) $3^{+}\ \bar{x},x+\frac{1}{4},\bar{x}$	(7) $3^{+}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{7}{12},\bar{x}-\frac{1}{6},\bar{x}$	(8) $3^{+}\ \bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{3},x+\frac{1}{6},x$	(10) $3^{-}\ x+\frac{3}{4},\bar{x},\bar{x}$	(11) $3^{-}\ \bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},x$	(12) $3^{-}\ \bar{x}-\frac{1}{2},x+\frac{3}{4},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x+\frac{1}{4},\frac{1}{4}$	(14) $2\quad x,\bar{x}+\frac{1}{2},0$	(15) $4^{-}(0,0,\frac{3}{4})\quad \frac{3}{8},-\frac{3}{8},z$	(16) $4^{+}(0,0,\frac{1}{4})\quad -\frac{1}{8},\frac{1}{8},z$
(17) $4^{-}(\frac{1}{4},0,0)\quad x,\frac{5}{8},-\frac{1}{8}$	(18) $2(0,\frac{1}{4},\frac{1}{4})\quad 0,y,y$	(19) $2(0,\frac{1}{4},-\frac{1}{4})\quad \frac{1}{4},y+\frac{1}{4},\bar{y}$	(20) $4^{+}(\frac{3}{4},0,0)\quad x,-\frac{3}{8},\frac{3}{8}$
(21) $4^{+}(0,\frac{3}{4},0)\quad \frac{3}{8},y,\frac{1}{8}$	(22) $2(\frac{3}{4},0,\frac{3}{4})\quad x,0,x$	(23) $4^{-}(0,\frac{1}{4},0)\quad -\frac{1}{8},y,\frac{1}{8}$	(24) $2(\frac{1}{4},0,-\frac{1}{4})\quad \bar{x}+\frac{1}{4},\frac{1}{4},x$
(25) $\bar{1}\quad \frac{1}{4},\frac{1}{4},0$	(26) $d(\frac{3}{4},\frac{1}{4},0)\quad x,y,\frac{1}{4}$	(27) $d(\frac{1}{4},0,\frac{1}{4})\quad x,0,z$	(28) $d(0,\frac{3}{4},\frac{3}{4})\quad 0,y,z$
(29) $\bar{3}^{+}\ x+\frac{1}{2},x,x;\ \frac{1}{2},0,0$	(30) $\bar{3}^{+}\ \bar{x}-\frac{3}{2},x+\frac{3}{4},\bar{x};\ -\frac{3}{4},0,\frac{3}{4}$	(31) $\bar{3}^{+}\ x+\frac{1}{4},\bar{x}+1,\bar{x};\ \frac{1}{2},\frac{3}{4},-\frac{1}{4}$	(32) $\bar{3}^{+}\ \bar{x}+\frac{1}{4},\bar{x}-\frac{1}{4},x;\ \frac{1}{4},-\frac{1}{4},0$
(33) $\bar{3}^{-}\ x,x+\frac{1}{2},x;\ 0,\frac{1}{2},0$	(34) $\bar{3}^{-}\ x+\frac{1}{4},\bar{x}-\frac{1}{2},\bar{x};\ 0,-\frac{1}{4},\frac{1}{4}$	(35) $\bar{3}^{-}\ \bar{x}-\frac{3}{4},\bar{x}+\frac{3}{4},x;\ -\frac{3}{4},\frac{3}{4},0$	(36) $\bar{3}^{-}\ \bar{x}+1,x-\frac{1}{4},\bar{x};\ \frac{3}{4},0,-\frac{1}{4}$
(37) $g(\frac{1}{4},-\frac{1}{4},\frac{1}{2})\quad x+\frac{1}{2},\bar{x},z$	(38) $g(\frac{1}{2},\frac{1}{2},0)\quad x,x,z$	(39) $\bar{4}^{-}\ \frac{1}{8},\frac{1}{8},z;\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$	(40) $\bar{4}^{+}\ \frac{3}{8},\frac{3}{8},z;\ \frac{3}{8},\frac{3}{8},\frac{3}{8}$
(41) $\bar{4}^{-}\ x,-\frac{1}{8},\frac{3}{8};\ \frac{3}{8},-\frac{1}{8},\frac{3}{8}$	(42) $m\quad x,y+\frac{3}{4},\bar{y}$	(43) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})\quad x,y+\frac{1}{4},y$	(44) $\bar{4}^{+}\ x,\frac{1}{8},\frac{1}{8};\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$
(45) $\bar{4}^{+}\ \frac{1}{8},y,\frac{5}{8};\ \frac{1}{8},\frac{1}{8},\frac{5}{8}$	(46) $m\quad \bar{x}+\frac{1}{4},y,x$	(47) $\bar{4}^{-}\ \frac{3}{8},y,\frac{3}{8};\ \frac{3}{8},\frac{3}{8},\frac{3}{8}$	(48) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})\quad x+\frac{1}{4},y,x$

International Tables for Crystallography (2006). Vol. A, Space group 228, pp. 704–711.

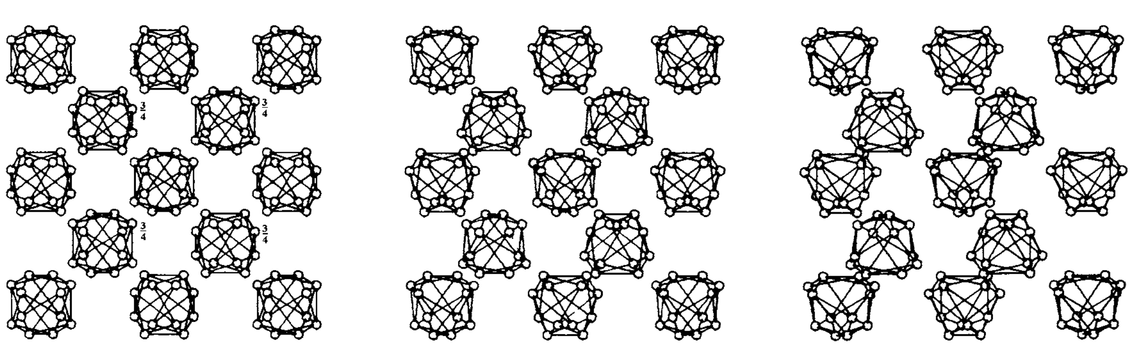
$Fd\bar{3}c$ $\quad O_h^8 \quad$ $m\bar{3}m$ $\quad$ Cubic

No. 228 $\quad F\,4_1/d\,\bar{3}\,2/c \quad$ Patterson symmetry $Fm\bar{3}m$

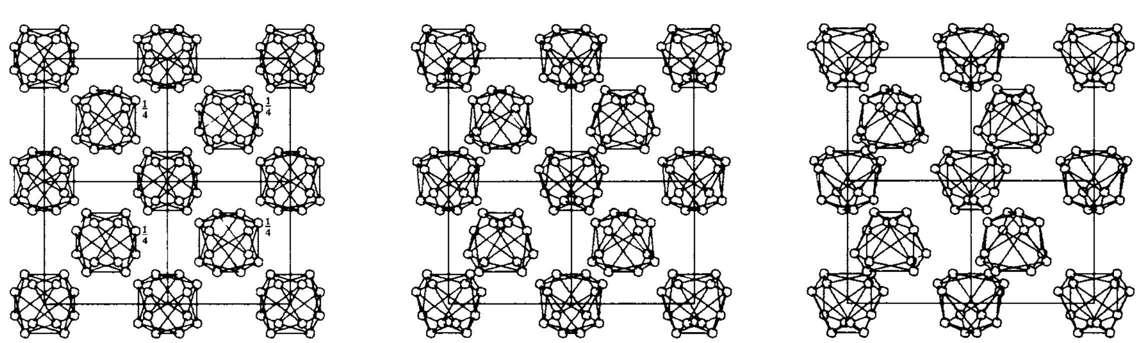
ORIGIN CHOICE 1



Upper left quadrant only



Upper half of unit cell



Lower half of unit cell

Origin at 23, at $-\frac{3}{8},-\frac{3}{8},-\frac{3}{8}$ from centre ($\bar{3}$)

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{8}$; $-\frac{1}{8} \le z \le \frac{1}{8}$; $y \le \min(\frac{1}{2}-x, x)$; $-y \le z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{3}{8},\frac{1}{8},\frac{1}{8}$ $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $\frac{3}{8},\frac{1}{8},-\frac{1}{8}$ $\frac{1}{8},\frac{1}{8},-\frac{1}{8}$

Symmetry operations

(*given on page* 707)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$

h,k,l permutable

General:

192 *h* 1

(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$
(5) z,x,y	(6) $z+\frac{1}{2},\bar{x},\bar{y}+\frac{1}{2}$	(7) $\bar{z},\bar{x}+\frac{1}{2},y+\frac{1}{2}$	(8) $\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{y}$
(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z+\frac{1}{2},\bar{x}$	(11) $y+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$	(12) $\bar{y},\bar{z}+\frac{1}{2},x+\frac{1}{2}$
(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{3}{4}$	(14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$
(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{3}{4}$	(18) $\bar{x}+\frac{3}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$
(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{3}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{3}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4}$
(25) $\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4}$	(26) $x+\frac{3}{4},y+\frac{1}{4},\bar{z}+\frac{1}{4}$	(27) $x+\frac{1}{4},\bar{y}+\frac{1}{4},z+\frac{3}{4}$	(28) $\bar{x}+\frac{1}{4},y+\frac{3}{4},z+\frac{1}{4}$
(29) $\bar{z}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(30) $\bar{z}+\frac{1}{4},x+\frac{3}{4},y+\frac{1}{4}$	(31) $z+\frac{3}{4},x+\frac{1}{4},\bar{y}+\frac{1}{4}$	(32) $z+\frac{1}{4},\bar{x}+\frac{1}{4},y+\frac{3}{4}$
(33) $\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4},\bar{x}+\frac{3}{4}$	(34) $y+\frac{1}{4},\bar{z}+\frac{1}{4},x+\frac{3}{4}$	(35) $\bar{y}+\frac{1}{4},z+\frac{3}{4},x+\frac{1}{4}$	(36) $y+\frac{3}{4},z+\frac{1}{4},\bar{x}+\frac{1}{4}$
(37) $\bar{y},\bar{x}+\frac{1}{2},z$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y}+\frac{1}{2},x,\bar{z}$	(40) $y,\bar{x},\bar{z}+\frac{1}{2}$
(41) $\bar{x},\bar{z}+\frac{1}{2},y$	(42) $x,\bar{z},\bar{y}+\frac{1}{2}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x}+\frac{1}{2},z,\bar{y}$
(45) $\bar{z},\bar{y}+\frac{1}{2},x$	(46) $\bar{z}+\frac{1}{2},y,\bar{x}$	(47) $z,\bar{y},\bar{x}+\frac{1}{2}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$

Reflection conditions:
hkl : $h+k=2n$ and $h+l, k+l=2n$
$0kl$: $k+l=4n$ and $k,l=2n$
hhl : $h,l=2n$
$h00$: $h=4n$

Special: as above, plus

96 *g* ..2 — no extra conditions

$\frac{1}{8},y,\bar{y}+\frac{1}{4}$	$\frac{7}{8},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$	$\frac{3}{8},y+\frac{1}{2},y+\frac{3}{4}$	$\frac{5}{8},\bar{y},y+\frac{1}{4}$
$\bar{y}+\frac{1}{4},\frac{1}{8},y$	$\bar{y}+\frac{3}{4},\frac{7}{8},\bar{y}+\frac{1}{2}$	$y+\frac{3}{4},\frac{3}{8},y+\frac{1}{2}$	$y+\frac{1}{4},\frac{5}{8},\bar{y}$
$y,\bar{y}+\frac{1}{4},\frac{1}{8}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{7}{8}$	$y+\frac{1}{2},y+\frac{3}{4},\frac{3}{8}$	$\bar{y},y+\frac{1}{4},\frac{5}{8}$
$\frac{5}{8},\bar{y}+\frac{3}{4},y+\frac{1}{2}$	$\frac{7}{8},y+\frac{1}{4},y$	$\frac{3}{8},\bar{y}+\frac{1}{4},\bar{y}$	$\frac{1}{8},y+\frac{3}{4},\bar{y}+\frac{1}{2}$
$y+\frac{1}{2},\frac{5}{8},\bar{y}+\frac{3}{4}$	$y,\frac{7}{8},y+\frac{1}{4}$	$\bar{y},\frac{3}{8},\bar{y}+\frac{1}{4}$	$\bar{y}+\frac{1}{2},\frac{1}{8},y+\frac{3}{4}$
$\bar{y}+\frac{3}{4},y+\frac{1}{2},\frac{5}{8}$	$y+\frac{1}{4},y,\frac{7}{8}$	$\bar{y}+\frac{1}{4},\bar{y},\frac{3}{8}$	$y+\frac{3}{4},\bar{y}+\frac{1}{2},\frac{1}{8}$

96 *f* 2.. — *hkl* : $h+k+l=4n$

$x,0,0$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$0,x,0$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$0,0,x$	$\frac{1}{2},\frac{1}{2},\bar{x}$
$\frac{3}{4},x+\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{4},\frac{1}{4}$	$x+\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\bar{x}+\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\bar{x}+\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},x+\frac{3}{4}$
$\bar{x}+\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$x+\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\bar{x}+\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},x+\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\bar{x}+\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x+\frac{3}{4}$
$0,\bar{x}+\frac{1}{2},0$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},0$	$x,0,\frac{1}{2}$	$0,\frac{1}{2},x$	$\frac{1}{2},0,\bar{x}$

64 *e* .3. — *hkl* : $h=2n$

x,x,x	$\bar{x},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}$	$x+\frac{1}{2},\bar{x},\bar{x}+\frac{1}{2}$
$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{3}{4}$	$\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4}$	$x+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$	$\bar{x}+\frac{3}{4},x+\frac{3}{4},x+\frac{1}{4}$
$\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4}$	$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{4}$	$x+\frac{1}{4},\bar{x}+\frac{1}{4},x+\frac{3}{4}$	$\bar{x}+\frac{1}{4},x+\frac{3}{4},x+\frac{1}{4}$
$\bar{x},\bar{x}+\frac{1}{2},x$	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,\bar{x}$	$x,\bar{x},\bar{x}+\frac{1}{2}$

48 *d* $\bar{4}$.. — *hkl* : $h+k+l=4n$

$\frac{1}{4},0,0$	$\frac{3}{4},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},\frac{1}{2}$	$0,0,\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$
$\frac{3}{4},\frac{1}{2},\frac{3}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$0,\frac{1}{4},\frac{3}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$

32 *c* .$\bar{3}$. $\frac{3}{8},\frac{3}{8},\frac{3}{8}$ $\frac{5}{8},\frac{1}{8},\frac{7}{8}$ $\frac{1}{8},\frac{7}{8},\frac{5}{8}$ $\frac{7}{8},\frac{5}{8},\frac{1}{8}$ $\frac{1}{8},\frac{5}{8},\frac{3}{8}$ $\frac{7}{8},\frac{7}{8},\frac{7}{8}$ $\frac{5}{8},\frac{3}{8},\frac{1}{8}$ $\frac{3}{8},\frac{1}{8},\frac{5}{8}$ — *hkl* : $h,k,l=4n+2$ or $h,k,l=4n$

32 *b* .32 $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $\frac{7}{8},\frac{3}{8},\frac{5}{8}$ $\frac{3}{8},\frac{5}{8},\frac{7}{8}$ $\frac{5}{8},\frac{7}{8},\frac{3}{8}$ $\frac{5}{8},\frac{5}{8},\frac{5}{8}$ $\frac{7}{8},\frac{3}{8},\frac{1}{8}$ $\frac{3}{8},\frac{1}{8},\frac{7}{8}$ $\frac{1}{8},\frac{7}{8},\frac{3}{8}$ — *hkl* : $h,k,l=4n+2$ or $h,k,l=4n$

16 *a* 23. $0,0,0$ $\frac{3}{4},\frac{1}{4},\frac{3}{4}$ $\frac{1}{4},\frac{3}{4},\frac{3}{4}$ $0,\frac{1}{2},0$ — *hkl* : $h+k+l=4n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{4}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{4}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{4}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,\frac{1}{8}$

Maximal non-isomorphic subgroups

I	[2] $F\bar{4}3c$ (219)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+
	[2] $F4_132$ (210)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+
	[2] $Fd\bar{3}1$ ($Fd\bar{3}$, 203)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+
	[3] $F4_1/d12/c$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
	[3] $F4_1/d12/c$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
	[3] $F4_1/d12/c$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
	[4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
	[4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
	[4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
	[4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $Fd\bar{3}c$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (228)

Minimal non-isomorphic supergroups

I none

II [2] $Pn\bar{3}m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (224)

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$
(5) 3^{+} x,x,x	(6) $3^{+}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$	(7) $3^{+}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$	(8) $3^{+}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) 3^{-} x,x,x	(10) 3^{-} $x,\bar{x}+\frac{1}{2},\bar{x}$	(11) 3^{-} $\bar{x}+\frac{1}{2},\bar{x},x$	(12) 3^{-} $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{3}{8}$	(14) 2 $x,\bar{x}+\frac{1}{4},\frac{1}{8}$	(15) $4^{-}(0,0,\frac{3}{4})$ $\frac{1}{2},\frac{1}{4},z$	(16) $4^{+}(0,0,\frac{1}{4})$ $0,\frac{3}{4},z$
(17) $4^{-}(\frac{3}{4},0,0)$ $x,\frac{1}{2},\frac{1}{4}$	(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{3}{8},y+\frac{1}{4},y$	(19) 2 $\frac{1}{8},y+\frac{1}{4},\bar{y}$	(20) $4^{+}(\frac{1}{4},0,0)$ $x,0,\frac{3}{4}$
(21) $4^{+}(0,\frac{1}{4},0)$ $\frac{3}{4},y,0$	(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x-\frac{1}{4},\frac{3}{8},x$	(23) $4^{-}(0,\frac{3}{4},0)$ $\frac{1}{4},y,\frac{1}{2}$	(24) 2 $\bar{x}+\frac{1}{4},\frac{1}{8},x$
(25) $\bar{1}$ $\frac{3}{8},\frac{3}{8},\frac{3}{8}$	(26) $d(\frac{3}{4},\frac{1}{4},0)$ $x,y,\frac{1}{8}$	(27) $d(\frac{1}{4},0,\frac{3}{4})$ $x,\frac{1}{8},z$	(28) $d(0,\frac{3}{4},\frac{1}{4})$ $\frac{1}{8},y,z$
(29) $\bar{3}^{+}$ x,x,x; $\frac{3}{8},\frac{3}{8},\frac{3}{8}$	(30) $\bar{3}^{+}$ $\bar{x}-1,x+1,\bar{x}$; $-\frac{3}{8},\frac{3}{8},\frac{5}{8}$	(31) $\bar{3}^{+}$ $x,\bar{x}+1,\bar{x}$; $\frac{3}{8},\frac{5}{8},-\frac{3}{8}$	(32) $\bar{3}^{+}$ $\bar{x}+1,\bar{x},x$; $\frac{5}{8},-\frac{3}{8},\frac{3}{8}$
(33) $\bar{3}^{-}$ x,x,x; $\frac{3}{8},\frac{3}{8},\frac{3}{8}$	(34) $\bar{3}^{-}$ $x+\frac{1}{2},\bar{x}-1,\bar{x}$; $-\frac{1}{8},-\frac{3}{8},\frac{5}{8}$	(35) $\bar{3}^{-}$ $\bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x$; $-\frac{3}{8},\frac{5}{8},-\frac{1}{8}$	(36) $\bar{3}^{-}$ $\bar{x}+1,x-\frac{1}{2},\bar{x}$; $\frac{5}{8},-\frac{1}{8},-\frac{3}{8}$
(37) $g(-\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{4},\bar{x},z$	(38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z	(39) $\bar{4}^{-}$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},0$	(40) $\bar{4}^{+}$ $0,0,z$; $0,0,\frac{1}{4}$
(41) $\bar{4}^{-}$ $x,\frac{1}{4},\frac{1}{4}$; $0,\frac{1}{4},\frac{1}{4}$	(42) $g(0,-\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$	(43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y	(44) $\bar{4}^{+}$ $x,0,0$; $\frac{1}{4},0,0$
(45) $\bar{4}^{+}$ $0,y,0$; $0,\frac{1}{4},0$	(46) $g(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$	(47) $\bar{4}^{-}$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},0,\frac{1}{4}$	(48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) 2 $0,0,z$	(3) 2 $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{3},x-\frac{1}{6},x$	(6) 3^{+} $\bar{x}+\frac{1}{2},x,\bar{x}$	(7) 3^{+} $x,\bar{x},\bar{x}$	(8) 3^{+} $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x+\frac{1}{6},x$	(10) 3^{-} $x+\frac{1}{2},\bar{x},\bar{x}$	(11) $3^{-}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) 3^{-} $\bar{x},x,\bar{x}$
(13) $2(\frac{3}{4},\frac{3}{4},0)$ $x,x,\frac{1}{8}$	(14) $2(-\frac{1}{4},\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{2},\frac{3}{8}$	(15) $4^{-}(0,0,\frac{1}{4})$ $\frac{1}{4},0,z$	(16) $4^{+}(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{2},z$
(17) $4^{-}(\frac{3}{4},0,0)$ $x,\frac{1}{2},-\frac{1}{4}$	(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{3}{8},y-\frac{1}{4},y$	(19) 2 $\frac{1}{8},y+\frac{3}{4},\bar{y}$	(20) $4^{+}(\frac{1}{4},0,0)$ $x,0,\frac{1}{4}$
(21) $4^{+}(0,\frac{3}{4},0)$ $\frac{1}{2},y,-\frac{1}{4}$	(22) $2(\frac{1}{4},0,\frac{1}{4})$ $x,\frac{1}{8},x$	(23) $4^{-}(0,\frac{1}{4},0)$ $0,y,\frac{3}{4}$	(24) $2(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{2},\frac{3}{8},x$
(25) $\bar{1}$ $\frac{3}{8},\frac{1}{8},\frac{1}{8}$	(26) $d(\frac{3}{4},\frac{3}{4},0)$ $x,y,\frac{3}{8}$	(27) $d(\frac{1}{4},0,\frac{1}{4})$ $x,\frac{3}{8},z$	(28) $d(0,\frac{1}{4},\frac{3}{4})$ $\frac{1}{8},y,z$
(29) $\bar{3}^{+}$ $x,x-\frac{1}{2},x$; $\frac{3}{8},-\frac{1}{8},\frac{3}{8}$	(30) $\bar{3}^{+}$ $\bar{x}-1,x+\frac{1}{2},\bar{x}$; $-\frac{3}{8},-\frac{1}{8},\frac{5}{8}$	(31) $\bar{3}^{+}$ $x,\bar{x}+\frac{3}{2},\bar{x}$; $\frac{3}{8},\frac{9}{8},-\frac{3}{8}$	(32) $\bar{3}^{+}$ $\bar{x}+1,\bar{x}+\frac{1}{2},x$; $\frac{5}{8},\frac{1}{8},\frac{3}{8}$
(33) $\bar{3}^{-}$ $x+\frac{1}{2},x+\frac{1}{2},x$; $\frac{3}{8},\frac{3}{8},-\frac{1}{8}$	(34) $\bar{3}^{-}$ $x+1,\bar{x}-\frac{1}{2},\bar{x}$; $\frac{3}{8},\frac{1}{8},\frac{5}{8}$	(35) $\bar{3}^{-}$ $\bar{x},\bar{x}+1,x$; $-\frac{3}{8},\frac{5}{8},\frac{3}{8}$	(36) $\bar{3}^{-}$ $\bar{x}+\frac{3}{2},x,\bar{x}$; $\frac{9}{8},\frac{3}{8},-\frac{3}{8}$
(37) c $x,\bar{x},z$	(38) $g(\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{4},x,z$	(39) $\bar{4}^{-}$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$	(40) $\bar{4}^{+}$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},0$
(41) $\bar{4}^{-}$ $x,-\frac{1}{4},\frac{1}{4}$; $0,-\frac{1}{4},\frac{1}{4}$	(42) $g(0,\frac{1}{4},-\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$	(43) a x,y,y	(44) $\bar{4}^{+}$ $x,\frac{1}{2},0$; $\frac{1}{4},\frac{1}{2},0$
(45) $\bar{4}^{+}$ $-\frac{1}{4},y,\frac{1}{4}$; $-\frac{1}{4},0,\frac{1}{4}$	(46) b $\bar{x}+\frac{1}{2},y,x$	(47) $\bar{4}^{-}$ $0,y,0$; $0,\frac{1}{4},0$	(48) $g(\frac{1}{4},0,\frac{1}{4})$ $x+\frac{1}{4},y,x$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) 2 $x,0,0$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x-\frac{1}{6},x$	(6) 3^{+} $\bar{x},x,\bar{x}$	(7) 3^{+} $x+\frac{1}{2},\bar{x},\bar{x}$	(8) 3^{+} $\bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x-\frac{1}{3},x$	(10) $3^{-}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) 3^{-} $\bar{x},\bar{x},x$	(12) 3^{-} $\bar{x},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)$ $x,x,\frac{1}{8}$	(14) $2(\frac{1}{4},-\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{2},\frac{3}{8}$	(15) $4^{-}(0,0,\frac{1}{4})$ $\frac{3}{4},0,z$	(16) $4^{+}(0,0,\frac{3}{4})$ $-\frac{1}{4},\frac{1}{2},z$
(17) $4^{-}(\frac{1}{4},0,0)$ $x,\frac{1}{4},0$	(18) $2(0,\frac{3}{4},\frac{3}{4})$ $\frac{1}{8},y,y$	(19) $2(0,-\frac{1}{4},\frac{1}{4})$ $\frac{3}{8},y+\frac{1}{2},\bar{y}$	(20) $4^{+}(\frac{3}{4},0,0)$ $x,\frac{1}{4},\frac{1}{2}$
(21) $4^{+}(0,\frac{1}{4},0)$ $\frac{1}{4},y,0$	(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x+\frac{1}{4},\frac{3}{8},x$	(23) $4^{-}(0,\frac{3}{4},0)$ $-\frac{1}{4},y,\frac{1}{2}$	(24) 2 $\bar{x}+\frac{3}{4},\frac{1}{8},x$
(25) $\bar{1}$ $\frac{1}{8},\frac{3}{8},\frac{1}{8}$	(26) $d(\frac{1}{4},\frac{1}{4},0)$ $x,y,\frac{3}{8}$	(27) $d(\frac{3}{4},0,\frac{1}{4})$ $x,\frac{1}{8},z$	(28) $d(0,\frac{3}{4},\frac{3}{4})$ $\frac{3}{8},y,z$
(29) $\bar{3}^{+}$ $x+\frac{1}{2},x+\frac{1}{2},x$; $\frac{3}{8},\frac{3}{8},-\frac{1}{8}$	(30) $\bar{3}^{+}$ $\bar{x}-\frac{3}{2},x+\frac{3}{2},\bar{x}$; $-\frac{3}{8},\frac{3}{8},\frac{9}{8}$	(31) $\bar{3}^{+}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$; $\frac{3}{8},\frac{5}{8},\frac{1}{8}$	(32) $\bar{3}^{+}$ $\bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x$; $\frac{5}{8},-\frac{3}{8},-\frac{1}{8}$
(33) $\bar{3}^{-}$ $x-\frac{1}{2},x,x$; $-\frac{1}{8},\frac{3}{8},\frac{3}{8}$	(34) $\bar{3}^{-}$ $x+1,\bar{x}-1,\bar{x}$; $\frac{3}{8},-\frac{3}{8},\frac{5}{8}$	(35) $\bar{3}^{-}$ $\bar{x},\bar{x}+\frac{3}{2},x$; $-\frac{3}{8},\frac{9}{8},\frac{3}{8}$	(36) $\bar{3}^{-}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}$; $\frac{5}{8},\frac{3}{8},\frac{1}{8}$
(37) c $x+\frac{1}{2},\bar{x},z$	(38) $g(\frac{1}{4},\frac{1}{4},0)$ $x-\frac{1}{4},x,z$	(39) $\bar{4}^{-}$ $0,0,z$; $0,0,\frac{1}{4}$	(40) $\bar{4}^{+}$ $\frac{1}{4},-\frac{1}{4},z$; $\frac{1}{4},-\frac{1}{4},0$
(41) $\bar{4}^{-}$ $x,0,\frac{1}{2}$; $\frac{1}{4},0,\frac{1}{2}$	(42) a $x,y,\bar{y}$	(43) $g(0,\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},y$	(44) $\bar{4}^{+}$ $x,\frac{1}{4},\frac{1}{4}$; $0,\frac{1}{4},\frac{1}{4}$
(45) $\bar{4}^{+}$ $0,y,\frac{1}{2}$; $0,\frac{1}{4},\frac{1}{2}$	(46) $g(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$	(47) $\bar{4}^{-}$ $\frac{1}{4},y,-\frac{1}{4}$; $\frac{1}{4},0,-\frac{1}{4}$	(48) b x,y,x

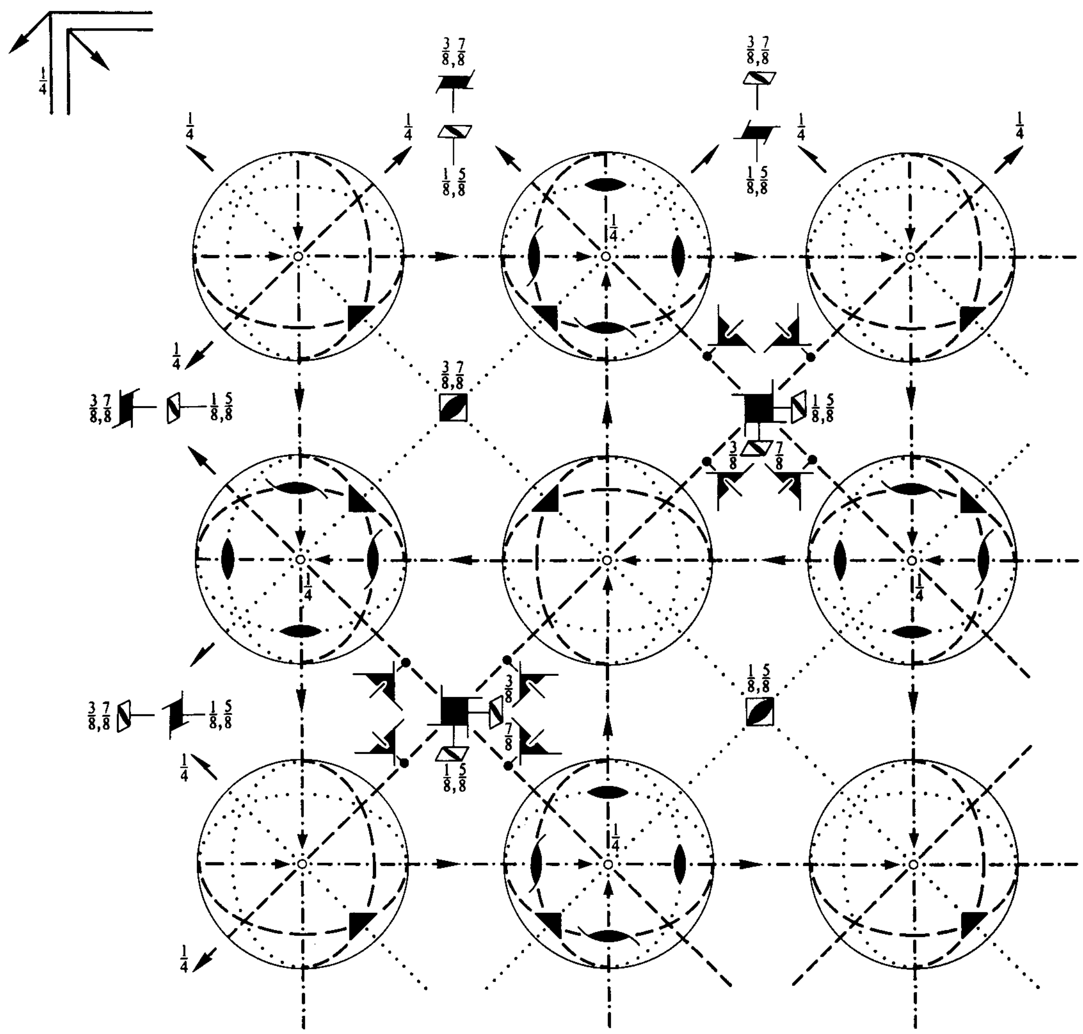
For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) 2 $0,y,0$	(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $3^{+}(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x+\frac{1}{3},x$	(6) 3^{+} $\bar{x},x+\frac{1}{2},\bar{x}$	(7) 3^{+} $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) 3^{+} $\bar{x},\bar{x},x$
(9) $3^{-}(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},x+\frac{1}{6},x$	(10) 3^{-} $x,\bar{x},\bar{x}$	(11) 3^{-} $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) $3^{-}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{3}{8}$	(14) 2 $x,\bar{x}+\frac{3}{4},\frac{1}{8}$	(15) $4^{-}(0,0,\frac{3}{4})$ $\frac{1}{2},-\frac{1}{4},z$	(16) $4^{+}(0,0,\frac{1}{4})$ $0,\frac{1}{4},z$
(17) $4^{-}(\frac{1}{4},0,0)$ $x,\frac{3}{4},0$	(18) $2(0,\frac{1}{4},\frac{1}{4})$ $\frac{1}{8},y,y$	(19) $2(0,\frac{1}{4},-\frac{1}{4})$ $\frac{3}{8},y+\frac{1}{2},\bar{y}$	(20) $4^{+}(\frac{3}{4},0,0)$ $x,-\frac{1}{4},\frac{1}{2}$
(21) $4^{+}(0,\frac{3}{4},0)$ $\frac{1}{2},y,\frac{1}{4}$	(22) $2(\frac{3}{4},0,\frac{3}{4})$ $x,\frac{1}{8},x$	(23) $4^{-}(0,\frac{1}{4},0)$ $0,y,\frac{1}{4}$	(24) $2(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{2},\frac{3}{8},x$
(25) $\bar{1}$ $\frac{1}{8},\frac{1}{8},\frac{3}{8}$	(26) $d(\frac{1}{4},\frac{3}{4},0)$ $x,y,\frac{1}{8}$	(27) $d(\frac{3}{4},0,\frac{3}{4})$ $x,\frac{3}{8},z$	(28) $d(0,\frac{1}{4},\frac{1}{4})$ $\frac{3}{8},y,z$
(29) $\bar{3}^{+}$ $x-\frac{1}{2},x,x$; $-\frac{1}{8},\frac{3}{8},\frac{3}{8}$	(30) $\bar{3}^{+}$ $\bar{x}-\frac{1}{2},x+1,\bar{x}$; $\frac{1}{8},\frac{3}{8},\frac{5}{8}$	(31) $\bar{3}^{+}$ $x-\frac{1}{2},\bar{x}+1,\bar{x}$; $-\frac{1}{8},\frac{5}{8},-\frac{3}{8}$	(32) $\bar{3}^{+}$ $\bar{x}+\frac{3}{2},\bar{x},x$; $\frac{9}{8},-\frac{3}{8},\frac{3}{8}$
(33) $\bar{3}^{-}$ $x,x-\frac{1}{2},x$; $\frac{3}{8},-\frac{1}{8},\frac{3}{8}$	(34) $\bar{3}^{-}$ $x+\frac{3}{2},\bar{x}-\frac{3}{2},\bar{x}$; $\frac{3}{8},-\frac{3}{8},\frac{9}{8}$	(35) $\bar{3}^{-}$ $\bar{x}+\frac{1}{2},\bar{x}+1,x$; $\frac{1}{8},\frac{5}{8},\frac{3}{8}$	(36) $\bar{3}^{-}$ $\bar{x}+1,x,\bar{x}$; $\frac{5}{8},\frac{3}{8},-\frac{3}{8}$
(37) $g(\frac{1}{4},-\frac{1}{4},0)$ $x+\frac{1}{4},\bar{x},z$	(38) c x,x,z	(39) $\bar{4}^{-}$ $-\frac{1}{4},\frac{1}{4},z$; $-\frac{1}{4},\frac{1}{4},0$	(40) $\bar{4}^{+}$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$
(41) $\bar{4}^{-}$ $x,0,0$; $\frac{1}{4},0,0$	(42) a $x,y+\frac{1}{2},\bar{y}$	(43) $g(0,\frac{1}{4},\frac{1}{4})$ $x,y-\frac{1}{4},y$	(44) $\bar{4}^{+}$ $x,\frac{1}{4},-\frac{1}{4}$; $0,\frac{1}{4},-\frac{1}{4}$
(45) $\bar{4}^{+}$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},0,\frac{1}{4}$	(46) b $\bar{x},y,x$	(47) $\bar{4}^{-}$ $\frac{1}{2},y,0$; $\frac{1}{2},\frac{1}{4},0$	(48) $g(\frac{1}{4},0,\frac{1}{4})$ $x-\frac{1}{4},y,x$

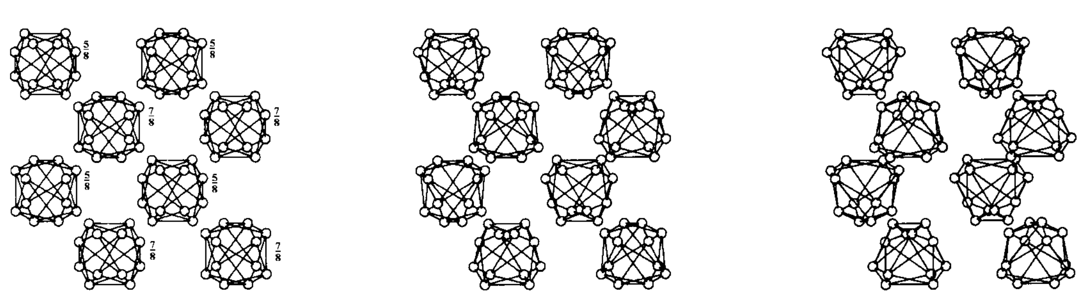
$F\,d\,\bar{3}\,c$ $\quad O_h^8$ $\quad m\bar{3}m$ $\quad$ Cubic

No. 228 $\quad F\ 4_1/d\ \bar{3}\ 2/c$ $\quad$ Patterson symmetry $F\,m\bar{3}m$

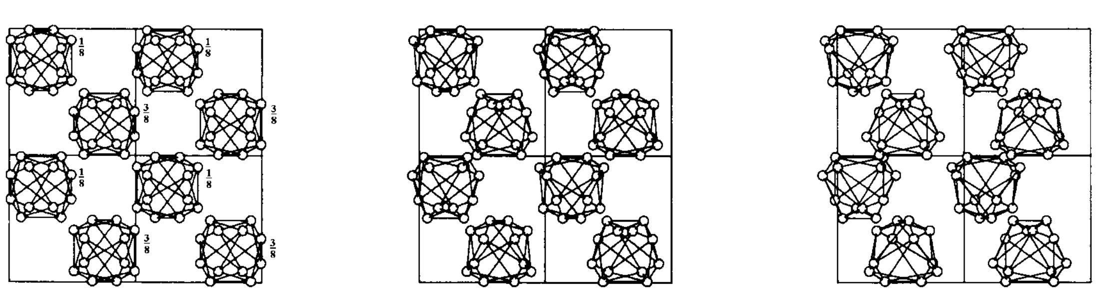
ORIGIN CHOICE 2



Upper left quadrant only



Upper half of unit cell



Lower half of unit cell

Origin at centre ($\bar{3}$), at $\frac{3}{8},\frac{3}{8},\frac{3}{8}$ from 23

Asymmetric unit $-\frac{1}{8} \le x \le \frac{3}{8}$; $-\frac{1}{8} \le y \le 0$; $-\frac{1}{4} \le z \le 0$; $y \le \min(\frac{1}{4}-x, x)$; $-y-\frac{1}{4} \le z \le y$

Vertices $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ $\frac{3}{8},-\frac{1}{8},-\frac{1}{8}$ $\frac{1}{4},0,0$ $0,0,0$ $\frac{1}{4},0,-\frac{1}{4}$ $0,0,-\frac{1}{4}$

Symmetry operations

(*given on page* 711)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$

h,k,l permutable

General:

192 *h* 1

(1) x,y,z	(2) $\bar{x}+\frac{1}{4},\bar{y}+\frac{3}{4},z+\frac{1}{2}$	(3) $\bar{x}+\frac{3}{4},y+\frac{1}{2},\bar{z}+\frac{1}{4}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{4},\bar{z}+\frac{3}{4}$
(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{4},\bar{y}+\frac{3}{4}$	(7) $\bar{z}+\frac{1}{4},\bar{x}+\frac{3}{4},y+\frac{1}{2}$	(8) $\bar{z}+\frac{3}{4},x+\frac{1}{2},\bar{y}+\frac{1}{4}$
(9) y,z,x	(10) $\bar{y}+\frac{3}{4},z+\frac{1}{2},\bar{x}+\frac{1}{4}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(12) $\bar{y}+\frac{1}{4},\bar{z}+\frac{3}{4},x+\frac{1}{2}$
(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y+\frac{1}{4},\bar{x},z+\frac{3}{4}$	(16) $\bar{y},x+\frac{3}{4},z+\frac{1}{4}$
(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}$	(18) $\bar{x},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x+\frac{1}{4},\bar{z},y+\frac{3}{4}$
(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}$	(22) $z+\frac{1}{4},\bar{y},x+\frac{3}{4}$	(23) $\bar{z},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$
(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{3}{4},y+\frac{1}{4},\bar{z}+\frac{1}{2}$	(27) $x+\frac{1}{4},\bar{y}+\frac{1}{2},z+\frac{3}{4}$	(28) $\bar{x}+\frac{1}{2},y+\frac{3}{4},z+\frac{1}{4}$
(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z}+\frac{1}{2},x+\frac{3}{4},y+\frac{1}{4}$	(31) $z+\frac{3}{4},x+\frac{1}{4},\bar{y}+\frac{1}{2}$	(32) $z+\frac{1}{4},\bar{x}+\frac{1}{2},y+\frac{3}{4}$
(33) $\bar{y},\bar{z},\bar{x}$	(34) $y+\frac{1}{4},\bar{z}+\frac{1}{2},x+\frac{3}{4}$	(35) $\bar{y}+\frac{1}{2},z+\frac{3}{4},x+\frac{1}{4}$	(36) $y+\frac{3}{4},z+\frac{1}{4},\bar{x}+\frac{1}{2}$
(37) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y}+\frac{3}{4},x,\bar{z}+\frac{1}{4}$	(40) $y,\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$
(41) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y$	(42) $x,\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x}+\frac{3}{4},z,\bar{y}+\frac{1}{4}$
(45) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x$	(46) $\bar{z}+\frac{3}{4},y,\bar{x}+\frac{1}{4}$	(47) $z,\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$

hkl : $h+k=2n$ and $h+l,k+l=2n$
$0kl$: $k+l=4n$ and $k,l=2n$
hhl : $h,l=2n$
$h00$: $h=4n$

Special: as above, plus

96 *g* ..2 — no extra conditions

$\frac{1}{4},y,\bar{y}$	$0,\bar{y}+\frac{3}{4},\bar{y}+\frac{1}{2}$	$\frac{1}{2},y+\frac{1}{2},y+\frac{1}{4}$	$\frac{3}{4},\bar{y}+\frac{1}{4},y+\frac{3}{4}$
$\bar{y},\frac{1}{4},y$	$\bar{y}+\frac{1}{2},0,\bar{y}+\frac{3}{4}$	$y+\frac{1}{4},\frac{1}{2},y+\frac{1}{2}$	$y+\frac{3}{4},\frac{3}{4},\bar{y}+\frac{1}{4}$
$y,\bar{y},\frac{1}{4}$	$\bar{y}+\frac{3}{4},\bar{y}+\frac{1}{2},0$	$y+\frac{1}{2},y+\frac{1}{4},\frac{1}{2}$	$\bar{y}+\frac{1}{4},y+\frac{3}{4},\frac{3}{4}$
$\frac{3}{4},\bar{y},y$	$0,y+\frac{1}{4},y+\frac{1}{2}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$	$\frac{1}{4},y+\frac{3}{4},\bar{y}+\frac{1}{4}$
$y,\frac{3}{4},\bar{y}$	$y+\frac{1}{2},0,y+\frac{1}{4}$	$\bar{y}+\frac{3}{4},\frac{1}{2},\bar{y}+\frac{1}{2}$	$\bar{y}+\frac{1}{4},\frac{1}{4},y+\frac{3}{4}$
$\bar{y},y,\frac{3}{4}$	$y+\frac{1}{4},y+\frac{1}{2},0$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{1}{2}$	$y+\frac{3}{4},\bar{y}+\frac{1}{4},\frac{1}{4}$

96 *f* 2.. — hkl : $h+k+l=4n$

$x,\frac{1}{8},\frac{1}{8}$	$\bar{x}+\frac{1}{4},\frac{5}{8},\frac{5}{8}$	$\frac{1}{8},x,\frac{1}{8}$	$\frac{5}{8},\bar{x}+\frac{1}{4},\frac{5}{8}$	$\frac{1}{8},\frac{1}{8},x$	$\frac{5}{8},\frac{5}{8},\bar{x}+\frac{1}{4}$
$\frac{7}{8},x+\frac{1}{4},\frac{7}{8}$	$\frac{3}{8},\bar{x}+\frac{1}{2},\frac{3}{8}$	$x+\frac{3}{4},\frac{3}{8},\frac{7}{8}$	$\bar{x},\frac{7}{8},\frac{3}{8}$	$\frac{7}{8},\frac{3}{8},\bar{x}$	$\frac{3}{8},\frac{7}{8},x+\frac{3}{4}$
$\bar{x},\frac{7}{8},\frac{7}{8}$	$x+\frac{3}{4},\frac{3}{8},\frac{3}{8}$	$\frac{7}{8},\bar{x},\frac{7}{8}$	$\frac{3}{8},x+\frac{3}{4},\frac{3}{8}$	$\frac{7}{8},\frac{7}{8},\bar{x}$	$\frac{3}{8},\frac{3}{8},x+\frac{3}{4}$
$\frac{1}{8},\bar{x}+\frac{3}{4},\frac{1}{8}$	$\frac{5}{8},x+\frac{1}{2},\frac{5}{8}$	$\bar{x}+\frac{1}{4},\frac{5}{8},\frac{1}{8}$	$x,\frac{1}{8},\frac{5}{8}$	$\frac{1}{8},\frac{5}{8},x$	$\frac{5}{8},\frac{1}{8},\bar{x}+\frac{1}{4}$

64 *e* .3. — hkl : $h=2n$

x,x,x	$\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{1}{2}$	$\bar{x}+\frac{3}{4},x+\frac{1}{2},\bar{x}+\frac{1}{4}$	$x+\frac{1}{2},\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4}$
$x+\frac{3}{4},x+\frac{1}{4},\bar{x}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{4},\bar{x},x+\frac{3}{4}$	$\bar{x},x+\frac{3}{4},x+\frac{1}{4}$
$\bar{x},\bar{x},\bar{x}$	$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{2}$	$x+\frac{1}{4},\bar{x}+\frac{1}{2},x+\frac{3}{4}$	$\bar{x}+\frac{1}{2},x+\frac{3}{4},x+\frac{1}{4}$
$\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x$	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{3}{4},x,\bar{x}+\frac{1}{4}$	$x,\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4}$

48 *d* $\bar{4}$.. — hkl : $h+k+l=4n$

$\frac{7}{8},\frac{1}{8},\frac{1}{8}$	$\frac{3}{8},\frac{5}{8},\frac{5}{8}$	$\frac{1}{8},\frac{7}{8},\frac{1}{8}$	$\frac{5}{8},\frac{3}{8},\frac{5}{8}$	$\frac{1}{8},\frac{1}{8},\frac{7}{8}$	$\frac{5}{8},\frac{5}{8},\frac{3}{8}$
$\frac{7}{8},\frac{1}{8},\frac{7}{8}$	$\frac{3}{8},\frac{5}{8},\frac{3}{8}$	$\frac{5}{8},\frac{3}{8},\frac{7}{8}$	$\frac{1}{8},\frac{7}{8},\frac{3}{8}$	$\frac{7}{8},\frac{3}{8},\frac{1}{8}$	$\frac{3}{8},\frac{7}{8},\frac{5}{8}$

32 *c* .$\bar{3}$. — $0,0,0$ $\frac{1}{4},\frac{3}{4},\frac{1}{2}$ $\frac{3}{4},\frac{1}{2},\frac{1}{4}$ $\frac{1}{2},\frac{1}{4},\frac{3}{4}$ $\frac{3}{4},\frac{1}{4},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\frac{1}{4},0,\frac{3}{4}$ $0,\frac{3}{4},\frac{1}{4}$ — hkl : $h,k,l=4n+2$ or $h,k,l=4n$

32 *b* .32 — $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $0,\frac{1}{2},\frac{3}{4}$ $\frac{1}{2},\frac{3}{4},0$ $\frac{3}{4},0,\frac{1}{2}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$ $0,\frac{1}{2},\frac{1}{4}$ $\frac{1}{2},\frac{1}{4},0$ $\frac{1}{4},0,\frac{1}{2}$ — hkl : $h,k,l=4n+2$ or $h,k,l=4n$

16 *a* 23. — $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $\frac{7}{8},\frac{3}{8},\frac{7}{8}$ $\frac{7}{8},\frac{7}{8},\frac{7}{8}$ $\frac{1}{8},\frac{5}{8},\frac{1}{8}$ — hkl : $h+k+l=4n$

ORIGIN CHOICE 2

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{4}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{4}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{8}, \frac{3}{8}, z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{4}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $F\bar{4}3c$ (219)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+
	[2] $F4_132$ (210)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+
	[2] $Fd\bar{3}1$ ($Fd\bar{3}$, 203)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+
	[3] $F4_1/d12/c$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
	[3] $F4_1/d12/c$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
	[3] $F4_1/d12/c$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
	[4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
	[4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
	[4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
	[4] $F1\bar{3}2/c$ ($R\bar{3}c$, 167)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+
IIa	none	
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $Fd\bar{3}c$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (228)

Minimal non-isomorphic supergroups

I none

II [2] $Pn\bar{3}m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (224)

Symmetry operations

For (0,0,0)+ set

(1) 1
(2) $2(0,0,\frac12)\quad \frac18,\frac38,z$
(3) $2(0,\frac12,0)\quad \frac38,y,\frac18$
(4) $2(\frac12,0,0)\quad x,\frac18,\frac38$
(5) $3^{+}\ x,x,x$
(6) $3^{+}(\frac13,-\frac13,\frac13)\quad \bar{x}+\frac16,x+\frac{5}{12},\bar{x}$
(7) $3^{+}(-\frac13,\frac13,\frac13)\quad x+\frac{7}{12},\bar{x}-\frac16,\bar{x}$
(8) $3^{+}(\frac13,\frac13,-\frac13)\quad \bar{x}+\frac{5}{12},\bar{x}+\frac{7}{12},x$
(9) $3^{-}\ x,x,x$
(10) $3^{-}\ x+\frac14,\bar{x}+\frac12,\bar{x}$
(11) $3^{-}\ \bar{x}+\frac34,\bar{x}+\frac14,x$
(12) $3^{-}\ \bar{x}-\frac12,x+\frac34,\bar{x}$
(13) $2(\frac12,\frac12,0)\quad x,x-\frac14,0$
(14) $2\quad x,\bar{x}+\frac12,\frac14$
(15) $4^{-}(0,0,\frac34)\quad \frac18,-\frac18,z$
(16) $4^{+}(0,0,\frac14)\quad -\frac38,\frac38,z$
(17) $4^{-}(\frac34,0,0)\quad x,\frac18,-\frac18$
(18) $2(0,\frac12,\frac12)\quad 0,y+\frac14,y$
(19) $2\quad \frac14,y+\frac12,\bar{y}$
(20) $4^{+}(\frac14,0,0)\quad x,-\frac38,\frac38$
(21) $4^{+}(0,\frac14,0)\quad \frac38,y,-\frac38$
(22) $2(\frac12,0,\frac12)\quad x-\frac14,0,x$
(23) $4^{-}(0,\frac34,0)\quad -\frac18,y,\frac18$
(24) $2\quad \bar{x}+\frac12,\frac14,x$
(25) $\bar{1}\quad 0,0,0$
(26) $d(\frac34,\frac14,0)\quad x,y,\frac14$
(27) $d(\frac14,0,\frac34)\quad x,\frac14,z$
(28) $d(0,\frac34,\frac14)\quad \frac14,y,z$
(29) $\bar{3}^{+}\ x,x,x;\ 0,0,0$
(30) $\bar{3}^{+}\ \bar{x}-1,x+\frac54,\bar{x};\ -\frac14,\frac12,\frac34$
(31) $\bar{3}^{+}\ x+\frac14,\bar{x}+1,\bar{x};\ \frac12,\frac34,-\frac14$
(32) $\bar{3}^{+}\ \bar{x}+\frac54,\bar{x}+\frac14,x;\ \frac34,-\frac14,\frac12$
(33) $\bar{3}^{-}\ x,x,x;\ 0,0,0$
(34) $\bar{3}^{-}\ x+\frac34,\bar{x}-1,\bar{x};\ 0,-\frac14,\frac34$
(35) $\bar{3}^{-}\ \bar{x}-\frac14,\bar{x}+\frac34,x;\ -\frac14,\frac34,0$
(36) $\bar{3}^{-}\ \bar{x}+1,x-\frac14,\bar{x};\ \frac34,0,-\frac14$
(37) $g(-\frac14,\frac14,0)\quad x+\frac12,\bar{x},z$
(38) $n(\frac12,\frac12,\frac12)\quad x,x,z$
(39) $\bar{4}^{-}\ \frac38,\frac38,z;\ \frac38,\frac38,\frac18$
(40) $\bar{4}^{+}\ \frac18,\frac18,z;\ \frac18,\frac18,\frac38$
(41) $\bar{4}^{-}\ x,\frac38,\frac38;\ \frac18,\frac38,\frac38$
(42) $g(0,-\frac14,\frac14)\quad x,y+\frac12,\bar{y}$
(43) $n(\frac12,\frac12,\frac12)\quad x,y,y$
(44) $\bar{4}^{+}\ x,\frac18,\frac18;\ \frac38,\frac18,\frac18$
(45) $\bar{4}^{+}\ \frac18,y,\frac18;\ \frac18,\frac38,\frac18$
(46) $g(\frac14,0,-\frac14)\quad \bar{x}+\frac12,y,x$
(47) $\bar{4}^{-}\ \frac38,y,\frac38;\ \frac38,\frac18,\frac38$
(48) $n(\frac12,\frac12,\frac12)\quad x,y,x$

For $(0,\frac12,\frac12)$+ set

(1) $t(0,\frac12,\frac12)$
(2) $2\quad \frac18,\frac18,z$
(3) $2\quad \frac38,y,\frac38$
(4) $2(\frac12,0,0)\quad x,\frac38,\frac18$
(5) $3^{+}(\frac13,\frac13,\frac13)\quad x-\frac13,x-\frac16,x$
(6) $3^{+}\ \bar{x}+\frac12,x+\frac14,\bar{x}$
(7) $3^{+}\ x+\frac14,\bar{x},\bar{x}$
(8) $3^{+}\ \bar{x}+\frac34,\bar{x}+\frac34,x$
(9) $3^{-}(\frac13,\frac13,\frac13)\quad x-\frac16,x+\frac16,x$
(10) $3^{-}\ x+\frac34,\bar{x},\bar{x}$
(11) $3^{-}(\frac13,\frac13,-\frac13)\quad \bar{x}+\frac{7}{12},\bar{x}+\frac{5}{12},x$
(12) $3^{-}\ \bar{x},x+\frac14,\bar{x}$
(13) $2(\frac34,\frac34,0)\quad x,x,\frac14$
(14) $2(\frac14,-\frac14,0)\quad x,\bar{x}+\frac14,0$
(15) $4^{-}(0,0,\frac14)\quad \frac38,\frac18,z$
(16) $4^{+}(0,0,\frac34)\quad -\frac18,\frac18,z$
(17) $4^{-}(\frac34,0,0)\quad x,\frac58,-\frac18$
(18) $2(0,\frac12,\frac12)\quad 0,y-\frac14,y$
(19) $2\quad \frac14,y,\bar{y}$
(20) $4^{+}(\frac14,0,0)\quad x,\frac18,\frac38$
(21) $4^{+}(0,\frac34,0)\quad \frac58,y,-\frac18$
(22) $2(\frac14,0,\frac14)\quad x,\frac14,x$
(23) $4^{-}(0,\frac14,0)\quad -\frac38,y,\frac38$
(24) $2(\frac14,0,-\frac14)\quad \bar{x}+\frac14,0,x$
(25) $\bar{1}\quad 0,\frac14,\frac14$
(26) $d(\frac34,\frac34,0)\quad x,y,0$
(27) $d(\frac14,0,\frac14)\quad x,0,z$
(28) $d(0,\frac14,\frac34)\quad \frac14,y,z$
(29) $\bar{3}^{+}\ x,x+\frac12,x;\ 0,\frac12,0$
(30) $\bar{3}^{+}\ \bar{x}-1,x+\frac34,\bar{x};\ -\frac14,0,\frac34$
(31) $\bar{3}^{+}\ x-\frac34,\bar{x}+\frac32,\bar{x};\ 0,\frac34,-\frac34$
(32) $\bar{3}^{+}\ \bar{x}+\frac14,\bar{x}-\frac14,x;\ \frac14,-\frac14,0$
(33) $\bar{3}^{-}\ x-\frac12,x-\frac12,x;\ 0,0,\frac12$
(34) $\bar{3}^{-}\ x+\frac14,\bar{x}-\frac12,\bar{x};\ 0,-\frac14,\frac14$
(35) $\bar{3}^{-}\ \bar{x}+\frac14,\bar{x}+\frac54,x;\ -\frac14,\frac34,\frac12$
(36) $\bar{3}^{-}\ \bar{x}+\frac32,x-\frac34,\bar{x};\ \frac34,0,-\frac34$
(37) $c\quad x+\frac14,\bar{x},z$
(38) $g(\frac14,\frac14,0)\quad x+\frac14,x,z$
(39) $\bar{4}^{-}\ \frac18,\frac58,z;\ \frac18,\frac58,\frac38$
(40) $\bar{4}^{+}\ \frac38,\frac38,z;\ \frac38,\frac38,\frac18$
(41) $\bar{4}^{-}\ x,-\frac18,\frac38;\ \frac18,-\frac18,\frac38$
(42) $g(0,\frac14,-\frac14)\quad x,y+\frac12,\bar{y}$
(43) $a\quad x,y,y$
(44) $\bar{4}^{+}\ x,\frac58,\frac18;\ \frac38,\frac58,\frac18$
(45) $\bar{4}^{+}\ -\frac18,y,\frac38;\ -\frac18,\frac18,\frac38$
(46) $b\quad \bar{x}+\frac34,y,x$
(47) $\bar{4}^{-}\ \frac18,y,\frac18;\ \frac18,\frac38,\frac18$
(48) $g(\frac14,0,\frac14)\quad x+\frac14,y,x$

For $(\frac12,0,\frac12)$+ set

(1) $t(\frac12,0,\frac12)$
(2) $2\quad \frac38,\frac38,z$
(3) $2(0,\frac12,0)\quad \frac18,y,\frac38$
(4) $2\quad x,\frac18,\frac18$
(5) $3^{+}(\frac13,\frac13,\frac13)\quad x+\frac16,x-\frac16,x$
(6) $3^{+}\ \bar{x},x+\frac14,\bar{x}$
(7) $3^{+}\ x+\frac34,\bar{x},\bar{x}$
(8) $3^{+}\ \bar{x}+\frac14,\bar{x}+\frac34,x$
(9) $3^{-}(\frac13,\frac13,\frac13)\quad x-\frac16,x-\frac13,x$
(10) $3^{-}(-\frac13,\frac13,\frac13)\quad x+\frac{5}{12},\bar{x}+\frac16,\bar{x}$
(11) $3^{-}\ \bar{x}+\frac14,\bar{x}+\frac14,x$
(12) $3^{-}\ \bar{x},x+\frac34,\bar{x}$
(13) $2(\frac14,\frac14,0)\quad x,x,\frac14$
(14) $2(-\frac14,\frac14,0)\quad x,\bar{x}+\frac14,0$
(15) $4^{-}(0,0,\frac14)\quad \frac38,-\frac38,z$
(16) $4^{+}(0,0,\frac34)\quad -\frac18,\frac58,z$
(17) $4^{-}(\frac14,0,0)\quad x,\frac38,\frac18$
(18) $2(0,\frac34,\frac34)\quad \frac14,y,y$
(19) $2(0,\frac14,-\frac14)\quad 0,y+\frac14,\bar{y}$
(20) $4^{+}(\frac34,0,0)\quad x,-\frac18,\frac18$
(21) $4^{+}(0,\frac14,0)\quad \frac38,y,\frac18$
(22) $2(\frac12,0,\frac12)\quad x+\frac14,0,x$
(23) $4^{-}(0,\frac34,0)\quad -\frac18,y,\frac58$
(24) $2\quad \bar{x},\frac14,x$
(25) $\bar{1}\quad \frac14,0,\frac14$
(26) $d(\frac14,\frac14,0)\quad x,y,0$
(27) $d(\frac34,0,\frac14)\quad x,\frac14,z$
(28) $d(0,\frac34,\frac34)\quad 0,y,z$
(29) $\bar{3}^{+}\ x-\frac12,x-\frac12,x;\ 0,0,\frac12$
(30) $\bar{3}^{+}\ \bar{x}-\frac32,x+\frac34,\bar{x};\ -\frac34,0,\frac34$
(31) $\bar{3}^{+}\ x-\frac14,\bar{x}+\frac12,\bar{x};\ 0,\frac14,-\frac14$
(32) $\bar{3}^{+}\ \bar{x}+\frac34,\bar{x}-\frac14,x;\ \frac34,-\frac14,0$
(33) $\bar{3}^{-}\ x+\frac12,x,x;\ \frac12,0,0$
(34) $\bar{3}^{-}\ x+\frac54,\bar{x}-1,\bar{x};\ \frac12,-\frac14,\frac34$
(35) $\bar{3}^{-}\ \bar{x}-\frac34,\bar{x}+\frac34,x;\ -\frac34,\frac34,0$
(36) $\bar{3}^{-}\ \bar{x}+\frac12,x-\frac14,\bar{x};\ \frac14,0,-\frac14$
(37) $c\quad x+\frac34,\bar{x},z$
(38) $g(\frac14,\frac14,0)\quad x-\frac14,x,z$
(39) $\bar{4}^{-}\ \frac18,\frac18,z;\ \frac18,\frac18,\frac38$
(40) $\bar{4}^{+}\ \frac38,-\frac18,z;\ \frac38,-\frac18,\frac18$
(41) $\bar{4}^{-}\ x,\frac18,\frac58;\ \frac38,\frac18,\frac58$
(42) $a\quad x,y+\frac14,\bar{y}$
(43) $g(0,\frac14,\frac14)\quad x,y+\frac14,y$
(44) $\bar{4}^{+}\ x,\frac38,\frac38;\ \frac18,\frac38,\frac38$
(45) $\bar{4}^{+}\ \frac18,y,\frac58;\ \frac18,\frac38,\frac58$
(46) $g(-\frac14,0,\frac14)\quad \bar{x}+\frac12,y,x$
(47) $\bar{4}^{-}\ \frac38,y,-\frac18;\ \frac38,\frac18,-\frac18$
(48) $b\quad x,y,x$

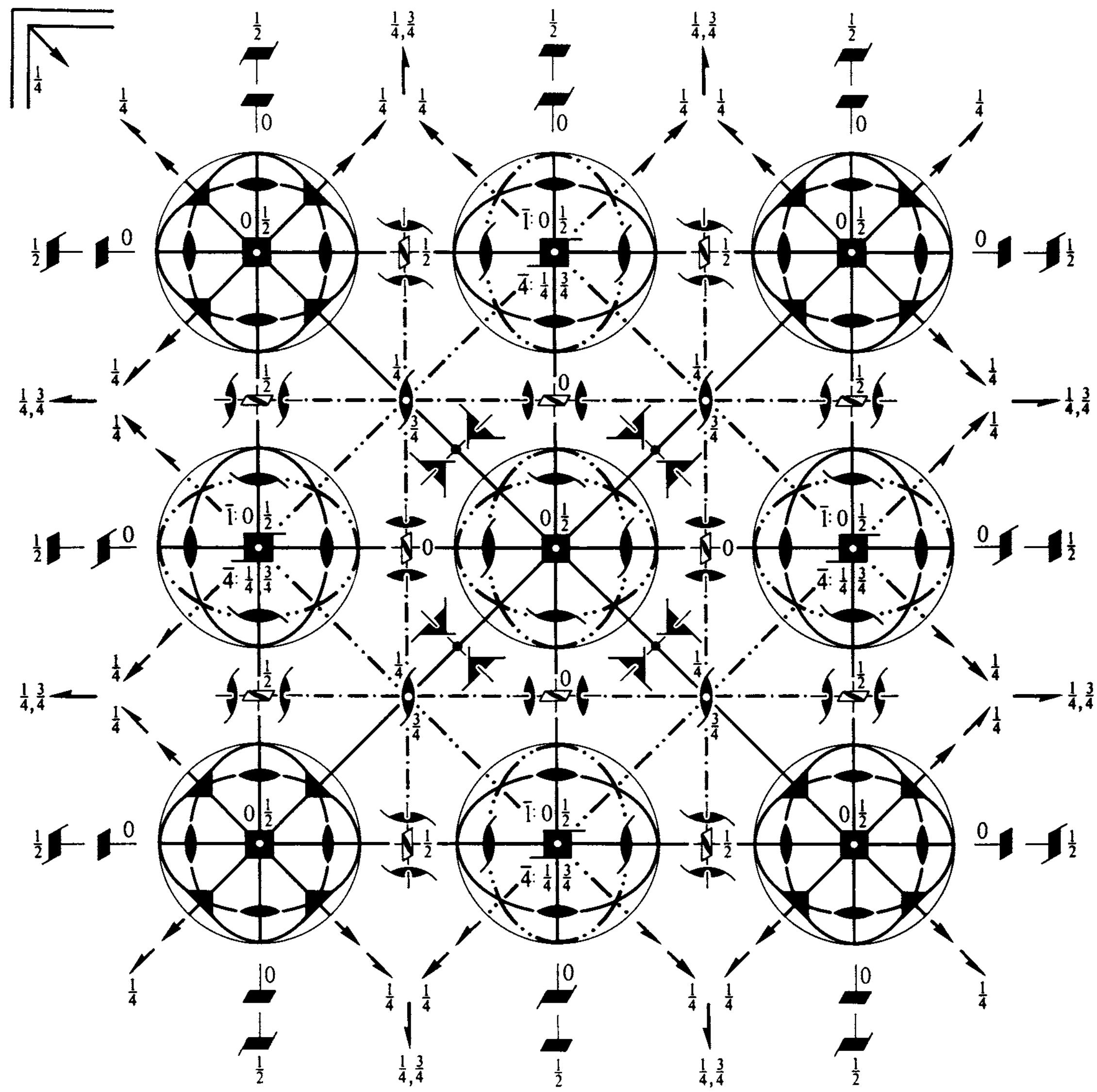
For $(\frac12,\frac12,0)$+ set

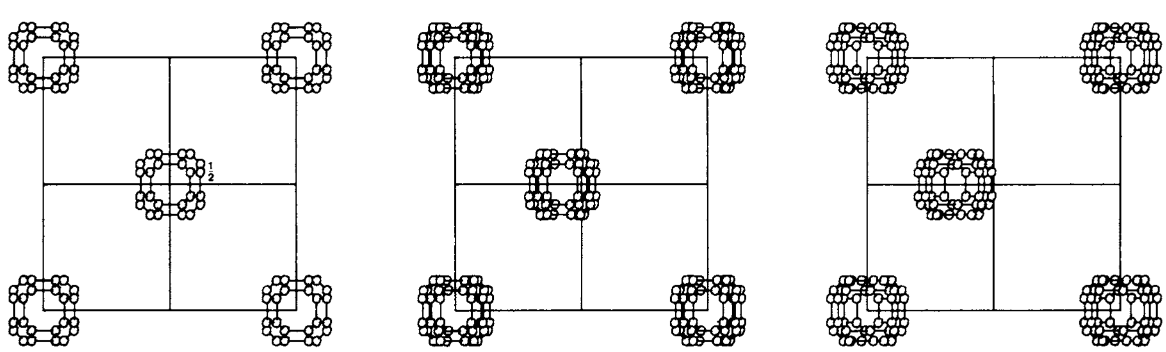
(1) $t(\frac12,\frac12,0)$
(2) $2(0,0,\frac12)\quad \frac38,\frac18,z$
(3) $2\quad \frac18,y,\frac18$
(4) $2\quad x,\frac38,\frac38$
(5) $3^{+}(\frac13,\frac13,\frac13)\quad x+\frac16,x+\frac13,x$
(6) $3^{+}\ \bar{x},x+\frac34,\bar{x}$
(7) $3^{+}\ x+\frac34,\bar{x}-\frac12,\bar{x}$
(8) $3^{+}\ \bar{x}+\frac14,\bar{x}+\frac14,x$
(9) $3^{-}(\frac13,\frac13,\frac13)\quad x+\frac13,x+\frac16,x$
(10) $3^{-}\ x+\frac14,\bar{x},\bar{x}$
(11) $3^{-}\ \bar{x}+\frac34,\bar{x}+\frac34,x$
(12) $3^{-}(\frac13,-\frac13,\frac13)\quad \bar{x}-\frac16,x+\frac{7}{12},\bar{x}$
(13) $2(\frac12,\frac12,0)\quad x,x+\frac14,0$
(14) $2\quad x,\bar{x},\frac14$
(15) $4^{-}(0,0,\frac34)\quad \frac58,-\frac18,z$
(16) $4^{+}(0,0,\frac14)\quad \frac18,\frac38,z$
(17) $4^{-}(\frac14,0,0)\quad x,\frac38,-\frac38$
(18) $2(0,\frac14,\frac14)\quad \frac14,y,y$
(19) $2(0,-\frac14,\frac14)\quad 0,y+\frac14,\bar{y}$
(20) $4^{+}(\frac34,0,0)\quad x,-\frac18,\frac58$
(21) $4^{+}(0,\frac34,0)\quad \frac18,y,-\frac18$
(22) $2(\frac34,0,\frac34)\quad x,\frac14,x$
(23) $4^{-}(0,\frac14,0)\quad \frac18,y,\frac38$
(24) $2(-\frac14,0,\frac14)\quad \bar{x}+\frac14,0,x$
(25) $\bar{1}\quad \frac14,\frac14,0$
(26) $d(\frac14,\frac34,0)\quad x,y,\frac14$
(27) $d(\frac34,0,\frac34)\quad x,0,z$
(28) $d(0,\frac14,\frac14)\quad 0,y,z$
(29) $\bar{3}^{+}\ x+\frac12,x,x;\ \frac12,0,0$
(30) $\bar{3}^{+}\ \bar{x}-\frac12,x+\frac14,\bar{x};\ -\frac14,0,\frac14$
(31) $\bar{3}^{+}\ x-\frac14,\bar{x}+1,\bar{x};\ 0,\frac34,-\frac14$
(32) $\bar{3}^{+}\ \bar{x}+\frac34,\bar{x}-\frac34,x;\ \frac34,-\frac34,0$
(33) $\bar{3}^{-}\ x,x+\frac12,x;\ 0,\frac12,0$
(34) $\bar{3}^{-}\ x+\frac34,\bar{x}-\frac32,\bar{x};\ 0,-\frac34,\frac34$
(35) $\bar{3}^{-}\ \bar{x}-\frac14,\bar{x}+\frac14,x;\ -\frac14,\frac14,0$
(36) $\bar{3}^{-}\ \bar{x}+1,x+\frac14,\bar{x};\ \frac34,\frac12,-\frac14$
(37) $g(\frac14,-\frac14,0)\quad x+\frac12,\bar{x},z$
(38) $c\quad x,x,z$
(39) $\bar{4}^{-}\ -\frac18,\frac38,z;\ -\frac18,\frac38,\frac18$
(40) $\bar{4}^{+}\ \frac58,\frac18,z;\ \frac58,\frac18,\frac38$
(41) $\bar{4}^{-}\ x,\frac18,\frac18;\ \frac38,\frac18,\frac18$
(42) $a\quad x,y+\frac34,\bar{y}$
(43) $g(0,\frac14,\frac14)\quad x,y-\frac14,y$
(44) $\bar{4}^{+}\ x,\frac38,-\frac18;\ \frac18,\frac38,-\frac18$
(45) $\bar{4}^{+}\ \frac38,y,\frac38;\ \frac38,\frac18,\frac38$
(46) $b\quad \bar{x}+\frac14,y,x$
(47) $\bar{4}^{-}\ \frac58,y,\frac18;\ \frac58,\frac38,\frac18$
(48) $g(\frac14,0,\frac14)\quad x-\frac14,y,x$

International Tables for Crystallography (2006). Vol. A, Space group 229, pp. 712–714.

$Im\bar{3}m$ $\quad O_h^9$ $\quad m\bar{3}m$ $\quad$ Cubic

No. 229 $\quad I\ 4/m\ \bar{3}\ 2/m$ $\quad$ Patterson symmetry $Im\bar{3}m$





Origin at centre ($m\bar{3}m$)

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}$; $\quad 0 \le y \le \frac{1}{2}$; $\quad 0 \le z \le \frac{1}{4}$; $\quad y \le x$; $\quad z \le \min(\frac{1}{2} - x, y)$

Vertices $\quad 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$

Symmetry operations

(*given on page* 714)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$						Reflection conditions h,k,l permutable
									General:
96	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			hkl : $h+k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			$0kl$: $k+l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			hhl : $l=2n$
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$			$h00$: $h=2n$
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$			
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$			
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$			
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$			
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$			
			(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$			
			(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$			
			(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x			
									Special: as above, plus
48	k	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x	$z,\bar{x},\bar{x}$	no extra conditions
			$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$	
			$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$x,\bar{x},z$	$\bar{x},x,z$	$x,z,\bar{x}$	$\bar{x},z,x$	
			$\bar{x},\bar{z},\bar{x}$	$x,\bar{z},x$	$z,x,\bar{x}$	$z,\bar{x},x$	$\bar{z},x,x$	$\bar{z},\bar{x},\bar{x}$	
48	j	$m..$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$z,0,y$	$z,0,\bar{y}$	no extra conditions
			$\bar{z},0,y$	$\bar{z},0,\bar{y}$	$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$	
			$y,0,\bar{z}$	$\bar{y},0,\bar{z}$	$y,0,z$	$\bar{y},0,z$	$0,z,\bar{y}$	$0,z,y$	
			$0,\bar{z},\bar{y}$	$0,\bar{z},y$	$z,y,0$	$z,\bar{y},0$	$\bar{z},y,0$	$\bar{z},\bar{y},0$	
48	i	$..2$	$\frac{1}{4},y,\bar{y}+\frac{1}{2}$	$\frac{3}{4},\bar{y},\bar{y}+\frac{1}{2}$	$\frac{3}{4},y,y+\frac{1}{2}$	$\frac{1}{4},\bar{y},y+\frac{1}{2}$			no extra conditions
			$\bar{y}+\frac{1}{2},\frac{1}{4},y$	$\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}$	$y+\frac{1}{2},\frac{3}{4},y$	$y+\frac{1}{2},\frac{1}{4},\bar{y}$			
			$y,\bar{y}+\frac{1}{2},\frac{1}{4}$	$\bar{y},\bar{y}+\frac{1}{2},\frac{3}{4}$	$y,y+\frac{1}{2},\frac{3}{4}$	$\bar{y},y+\frac{1}{2},\frac{1}{4}$			
			$\frac{3}{4},\bar{y},y+\frac{1}{2}$	$\frac{1}{4},y,y+\frac{1}{2}$	$\frac{1}{4},\bar{y},\bar{y}+\frac{1}{2}$	$\frac{3}{4},y,\bar{y}+\frac{1}{2}$			
			$y+\frac{1}{2},\frac{3}{4},\bar{y}$	$y+\frac{1}{2},\frac{1}{4},y$	$\bar{y}+\frac{1}{2},\frac{1}{4},\bar{y}$	$\bar{y}+\frac{1}{2},\frac{3}{4},y$			
			$\bar{y},y+\frac{1}{2},\frac{3}{4}$	$y,y+\frac{1}{2},\frac{1}{4}$	$\bar{y},\bar{y}+\frac{1}{2},\frac{1}{4}$	$y,\bar{y}+\frac{1}{2},\frac{3}{4}$			
24	h	$m.m2$	$0,y,y$	$0,\bar{y},y$	$0,y,\bar{y}$	$0,\bar{y},\bar{y}$	$y,0,y$	$y,0,\bar{y}$	no extra conditions
			$\bar{y},0,y$	$\bar{y},0,\bar{y}$	$y,y,0$	$\bar{y},y,0$	$y,\bar{y},0$	$\bar{y},\bar{y},0$	
24	g	$mm2..$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$0,\frac{1}{2},x$	$0,\frac{1}{2},\bar{x}$	no extra conditions
			$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},0,\bar{x}$	$\frac{1}{2},0,x$	
16	f	$.3m$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			no extra conditions
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$			
12	e	$4m.m$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	no extra conditions
12	d	$\bar{4}m.2$	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},0$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	no extra conditions
8	c	$.\bar{3}m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$			hkl : $k,l=2n$
6	b	$4/mm.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
2	a	$m\bar{3}m$	$0,0,0$						no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\quad\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\quad\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}3m$ (217)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+
	[2] $I432$ (211)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+
	[2] $Im\bar{3}1$ ($Im\bar{3}$, 204)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+
	[3] $I4/m12/m$ ($I4/mmm$, 139)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
	[3] $I4/m12/m$ ($I4/mmm$, 139)	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
	[3] $I4/m12/m$ ($I4/mmm$, 139)	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
	[4] $I1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
	[4] $I1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
	[4] $I1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
	[4] $I1\bar{3}2/m$ ($R\bar{3}m$, 166)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+
IIa	[2] $Pn\bar{3}m$ (224)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pm\bar{3}n$ (223)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pn\bar{3}n$ (222)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; (25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $Im\bar{3}m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (229)

Minimal non-isomorphic supergroups

I none

II [4] $Pm\bar{3}m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (221)

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) 2 $x,x,0$	(14) 2 $x,\bar{x},0$	(15) 4^- $0,0,z$	(16) 4^+ $0,0,z$
(17) 4^- $x,0,0$	(18) 2 $0,y,y$	(19) 2 $0,y,\bar{y}$	(20) 4^+ $x,0,0$
(21) 4^+ $0,y,0$	(22) 2 $x,0,x$	(23) 4^- $0,y,0$	(24) 2 $\bar{x},0,x$
(25) $\bar{1}$ $0,0,0$	(26) m $x,y,0$	(27) m $x,0,z$	(28) m $0,y,z$
(29) $\bar{3}^+$ x,x,x; $0,0,0$	(30) $\bar{3}^+$ $\bar{x},x,\bar{x}$; $0,0,0$	(31) $\bar{3}^+$ $x,\bar{x},\bar{x}$; $0,0,0$	(32) $\bar{3}^+$ $\bar{x},\bar{x},x$; $0,0,0$
(33) $\bar{3}^-$ x,x,x; $0,0,0$	(34) $\bar{3}^-$ $x,\bar{x},\bar{x}$; $0,0,0$	(35) $\bar{3}^-$ $\bar{x},\bar{x},x$; $0,0,0$	(36) $\bar{3}^-$ $\bar{x},x,\bar{x}$; $0,0,0$
(37) m $x,\bar{x},z$	(38) m x,x,z	(39) $\bar{4}^-$ $0,0,z$; $0,0,0$	(40) $\bar{4}^+$ $0,0,z$; $0,0,0$
(41) $\bar{4}^-$ $x,0,0$; $0,0,0$	(42) m $x,y,\bar{y}$	(43) m x,y,y	(44) $\bar{4}^+$ $x,0,0$; $0,0,0$
(45) $\bar{4}^+$ $0,y,0$; $0,0,0$	(46) m $\bar{x},y,x$	(47) $\bar{4}^-$ $0,y,0$; $0,0,0$	(48) m x,y,x

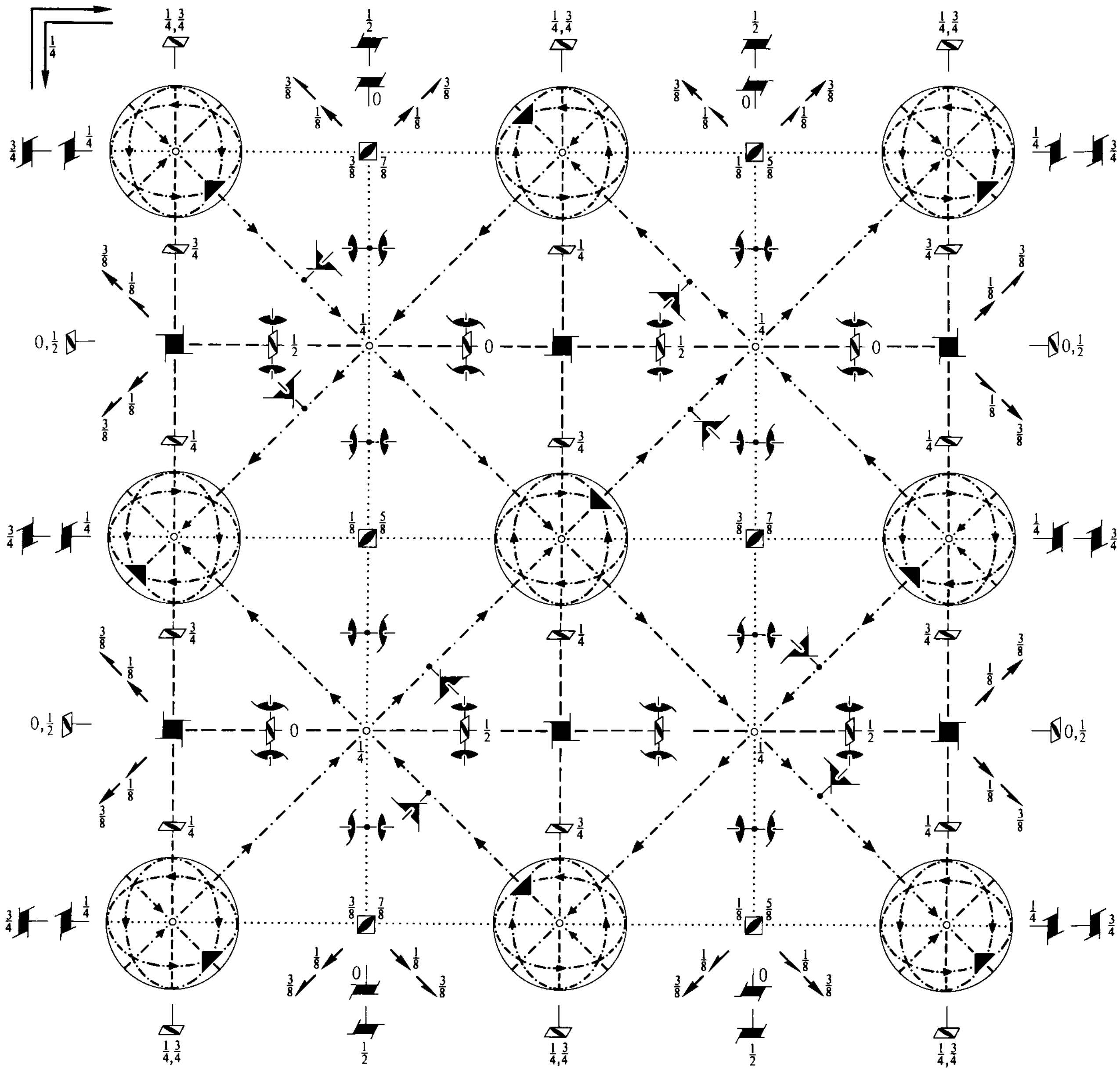
For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+ set

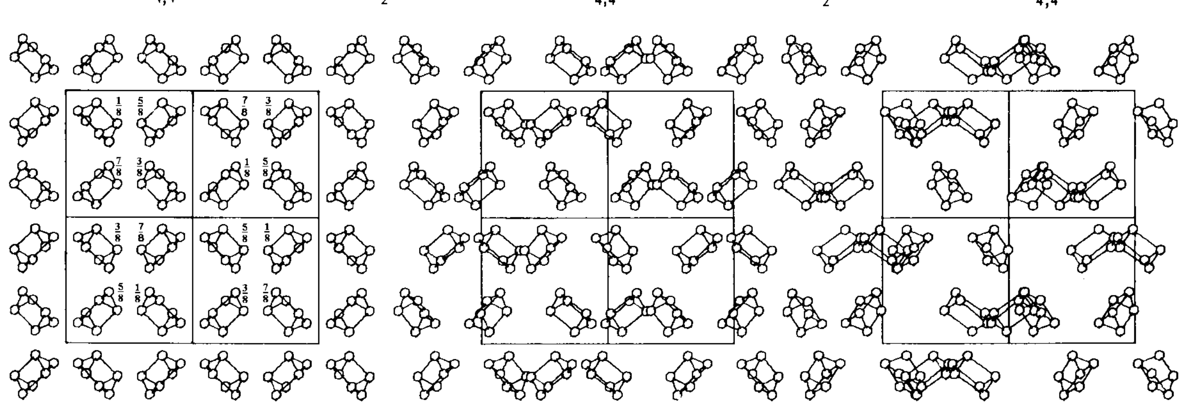
(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}+\frac{1}{3},x+\frac{1}{3},\bar{x}$	(7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{2}{3},\bar{x}-\frac{1}{3},\bar{x}$	(8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{2}{3},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(10) $3^-(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{3},\bar{x}+\frac{1}{3},\bar{x}$	(11) $3^-(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{2}{3},\bar{x}+\frac{1}{3},x$	(12) $3^-(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}-\frac{1}{3},x+\frac{2}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$	(14) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$	(15) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$	(16) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$
(17) $4^-(\frac{1}{2},0,0)$ $x,\frac{1}{2},0$	(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,y$	(19) 2 $\frac{1}{4},y+\frac{1}{2},\bar{y}$	(20) $4^+(\frac{1}{2},0,0)$ $x,0,\frac{1}{2}$
(21) $4^+(0,\frac{1}{2},0)$ $\frac{1}{2},y,0$	(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},x$	(23) $4^-(0,\frac{1}{2},0)$ $0,y,\frac{1}{2}$	(24) 2 $\bar{x}+\frac{1}{2},\frac{1}{4},x$
(25) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(26) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(27) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(28) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$
(29) $\bar{3}^+$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(30) $\bar{3}^+$ $\bar{x}-1,x+1,\bar{x}$; $-\frac{1}{4},\frac{1}{4},\frac{3}{4}$	(31) $\bar{3}^+$ $x,\bar{x}+1,\bar{x}$; $\frac{1}{4},\frac{3}{4},-\frac{1}{4}$	(32) $\bar{3}^+$ $\bar{x}+1,\bar{x},x$; $\frac{3}{4},-\frac{1}{4},\frac{1}{4}$
(33) $\bar{3}^-$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(34) $\bar{3}^-$ $x+1,\bar{x}-1,\bar{x}$; $\frac{1}{4},-\frac{1}{4},\frac{3}{4}$	(35) $\bar{3}^-$ $\bar{x},\bar{x}+1,x$; $-\frac{1}{4},\frac{3}{4},\frac{1}{4}$	(36) $\bar{3}^-$ $\bar{x}+1,x,\bar{x}$; $\frac{3}{4},\frac{1}{4},-\frac{1}{4}$
(37) c $x+\frac{1}{2},\bar{x},z$	(38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z	(39) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$	(40) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$
(41) $\bar{4}^-$ $x,0,\frac{1}{2}$; $\frac{1}{4},0,\frac{1}{2}$	(42) a $x,y+\frac{1}{2},\bar{y}$	(43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y	(44) $\bar{4}^+$ $x,\frac{1}{2},0$; $\frac{1}{4},\frac{1}{2},0$
(45) $\bar{4}^+$ $0,y,\frac{1}{2}$; $0,\frac{1}{4},\frac{1}{2}$	(46) b $\bar{x}+\frac{1}{2},y,x$	(47) $\bar{4}^-$ $\frac{1}{2},y,0$; $\frac{1}{2},\frac{1}{4},0$	(48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x

International Tables for Crystallography (2006). Vol. A, Space group 230, pp. 715–717.

$I\,a\,\bar{3}\,d$ $\quad O_h^{10}$ $\quad m\,\bar{3}\,m$ $\quad$ Cubic

No. 230 $\quad I\ 4_1/a\ \bar{3}\ 2/d$ $\quad$ Patterson symmetry $I\,m\,\bar{3}\,m$





Origin at centre ($\bar{3}$)

Asymmetric unit $\quad -\frac{1}{8} \le x \le \frac{1}{8}; \quad -\frac{1}{8} \le y \le \frac{1}{8}; \quad 0 \le z \le \frac{1}{4}; \quad \max(x,-x,y,-y) \le z$

Vertices $\quad 0,0,0 \quad \frac{1}{8},\frac{1}{8},\frac{1}{8} \quad -\frac{1}{8},\frac{1}{8},\frac{1}{8} \quad -\frac{1}{8},-\frac{1}{8},\frac{1}{8} \quad \frac{1}{8},-\frac{1}{8},\frac{1}{8}$

$\frac{1}{8},\frac{1}{8},\frac{1}{4} \quad -\frac{1}{8},\frac{1}{8},\frac{1}{4} \quad -\frac{1}{8},-\frac{1}{8},\frac{1}{4} \quad \frac{1}{8},-\frac{1}{8},\frac{1}{4}$

Symmetry operations

(*given on page* 715)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac12,\frac12,\frac12)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac12,\frac12,\frac12)+$			h,k,l permutable General:
96	h	1	(1) x,y,z	(2) $\bar{x}+\frac12,\bar{y},z+\frac12$	(3) $\bar{x},y+\frac12,\bar{z}+\frac12$	(4) $x+\frac12,\bar{y}+\frac12,\bar{z}$	hkl : $h+k+l=2n$
			(5) z,x,y	(6) $z+\frac12,\bar{x}+\frac12,\bar{y}$	(7) $\bar{z}+\frac12,\bar{x},y+\frac12$	(8) $\bar{z},x+\frac12,\bar{y}+\frac12$	$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z+\frac12,\bar{x}+\frac12$	(11) $y+\frac12,\bar{z}+\frac12,\bar{x}$	(12) $\bar{y}+\frac12,\bar{z},x+\frac12$	hhl : $2h+l=4n$
			(13) $y+\frac34,x+\frac14,\bar{z}+\frac14$	(14) $\bar{y}+\frac34,\bar{x}+\frac34,\bar{z}+\frac34$	(15) $y+\frac14,\bar{x}+\frac14,z+\frac34$	(16) $\bar{y}+\frac14,x+\frac34,z+\frac14$	$h00$: $h=4n$
			(17) $x+\frac34,z+\frac14,\bar{y}+\frac14$	(18) $\bar{x}+\frac14,z+\frac34,y+\frac14$	(19) $\bar{x}+\frac34,\bar{z}+\frac34,\bar{y}+\frac34$	(20) $x+\frac14,\bar{z}+\frac14,y+\frac34$	
			(21) $z+\frac34,y+\frac14,\bar{x}+\frac14$	(22) $z+\frac14,\bar{y}+\frac14,x+\frac34$	(23) $\bar{z}+\frac14,y+\frac34,x+\frac14$	(24) $\bar{z}+\frac34,\bar{y}+\frac34,\bar{x}+\frac34$	
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac12,y,\bar{z}+\frac12$	(27) $x,\bar{y}+\frac12,z+\frac12$	(28) $\bar{x}+\frac12,y+\frac12,z$	
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z}+\frac12,x+\frac12,y$	(31) $z+\frac12,x,\bar{y}+\frac12$	(32) $z,\bar{x}+\frac12,y+\frac12$	
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z}+\frac12,x+\frac12$	(35) $\bar{y}+\frac12,z+\frac12,x$	(36) $y+\frac12,z,\bar{x}+\frac12$	
			(37) $\bar{y}+\frac14,\bar{x}+\frac34,z+\frac34$	(38) $y+\frac14,x+\frac14,z+\frac14$	(39) $\bar{y}+\frac34,x+\frac34,\bar{z}+\frac14$	(40) $y+\frac34,\bar{x}+\frac14,\bar{z}+\frac34$	
			(41) $\bar{x}+\frac14,\bar{z}+\frac34,y+\frac34$	(42) $x+\frac34,\bar{z}+\frac14,\bar{y}+\frac34$	(43) $x+\frac14,z+\frac14,y+\frac14$	(44) $\bar{x}+\frac34,z+\frac34,\bar{y}+\frac14$	
			(45) $\bar{z}+\frac14,\bar{y}+\frac34,x+\frac34$	(46) $\bar{z}+\frac34,y+\frac34,\bar{x}+\frac14$	(47) $z+\frac34,\bar{y}+\frac14,\bar{x}+\frac34$	(48) $z+\frac14,y+\frac14,x+\frac14$	

Special: as above, plus

							Reflection conditions
48	g	$..2$	$\frac18,y,\bar{y}+\frac14$	$\frac38,\bar{y},\bar{y}+\frac34$	$\frac78,y+\frac12,y+\frac14$	$\frac58,\bar{y}+\frac12,y+\frac34$	hkl : $h=2n+1$ or $h=4n$
			$\bar{y}+\frac14,\frac18,y$	$\bar{y}+\frac34,\frac38,\bar{y}$	$y+\frac14,\frac78,y+\frac12$	$y+\frac34,\frac58,\bar{y}+\frac12$	
			$y,\bar{y}+\frac14,\frac18$	$\bar{y},\bar{y}+\frac34,\frac38$	$y+\frac12,y+\frac14,\frac78$	$\bar{y}+\frac12,y+\frac34,\frac58$	
			$\frac78,\bar{y},y+\frac34$	$\frac58,y,y+\frac14$	$\frac18,\bar{y}+\frac12,\bar{y}+\frac34$	$\frac38,y+\frac12,\bar{y}+\frac14$	
			$y+\frac34,\frac78,\bar{y}$	$y+\frac14,\frac58,y$	$\bar{y}+\frac34,\frac18,\bar{y}+\frac12$	$\bar{y}+\frac14,\frac38,y+\frac12$	
			$\bar{y},y+\frac34,\frac78$	$y,y+\frac14,\frac58$	$\bar{y}+\frac12,\bar{y}+\frac34,\frac18$	$y+\frac12,\bar{y}+\frac14,\frac38$	

									Reflection conditions
48	f	$2..$	$x,0,\frac14$	$\bar{x}+\frac12,0,\frac34$	$\frac14,x,0$	$\frac34,\bar{x}+\frac12,0$	$0,\frac14,x$	$0,\frac34,\bar{x}+\frac12$	hkl : $2h+l=4n$
			$\frac34,x+\frac14,0$	$\frac34,\bar{x}+\frac34,\frac12$	$x+\frac34,\frac12,\frac14$	$\bar{x}+\frac14,0,\frac14$	$0,\frac14,\bar{x}+\frac14$	$\frac12,\frac14,x+\frac34$	
			$\bar{x},0,\frac34$	$x+\frac12,0,\frac14$	$\frac34,\bar{x},0$	$\frac14,x+\frac12,0$	$0,\frac34,\bar{x}$	$0,\frac14,x+\frac12$	
			$\frac14,\bar{x}+\frac34,0$	$\frac14,x+\frac14,\frac12$	$\bar{x}+\frac14,\frac12,\frac34$	$x+\frac34,0,\frac34$	$0,\frac34,x+\frac34$	$\frac12,\frac34,\bar{x}+\frac14$	

							Reflection conditions
32	e	$.3.$	x,x,x	$\bar{x}+\frac12,\bar{x},x+\frac12$	$\bar{x},x+\frac12,\bar{x}+\frac12$	$x+\frac12,\bar{x}+\frac12,\bar{x}$	hkl : $h=2n+1$ or $h+k+l=4n$
			$x+\frac34,x+\frac14,\bar{x}+\frac14$	$\bar{x}+\frac34,\bar{x}+\frac34,\bar{x}+\frac34$	$x+\frac14,\bar{x}+\frac14,x+\frac34$	$\bar{x}+\frac14,x+\frac34,x+\frac14$	
			$\bar{x},\bar{x},\bar{x}$	$x+\frac12,x,\bar{x}+\frac12$	$x,\bar{x}+\frac12,x+\frac12$	$\bar{x}+\frac12,x+\frac12,x$	
			$\bar{x}+\frac14,\bar{x}+\frac34,x+\frac34$	$x+\frac14,x+\frac14,x+\frac14$	$\bar{x}+\frac34,x+\frac34,\bar{x}+\frac14$	$x+\frac34,\bar{x}+\frac14,\bar{x}+\frac34$	

									Reflection conditions
24	d	$\bar{4}..$	$\frac38,0,\frac14$	$\frac18,0,\frac34$	$\frac14,\frac38,0$	$\frac34,\frac18,0$	$0,\frac14,\frac38$	$0,\frac34,\frac18$	hkl : $h,k=2n$, $h+k+l=4n$ or $h,k=2n+1$, $l=4n+2$ or $h=8n$, $k=8n+4$ and $h+k+l=4n+2$ (24 d and 24 c)
			$\frac34,\frac58,0$	$\frac34,\frac38,\frac12$	$\frac18,\frac12,\frac14$	$\frac78,0,\frac14$	$0,\frac14,\frac78$	$\frac12,\frac14,\frac18$	
24	c	2.22	$\frac18,0,\frac14$	$\frac38,0,\frac34$	$\frac14,\frac18,0$	$\frac34,\frac38,0$	$0,\frac14,\frac18$	$0,\frac34,\frac38$	
			$\frac78,0,\frac34$	$\frac58,0,\frac14$	$\frac34,\frac78,0$	$\frac14,\frac58,0$	$0,\frac34,\frac78$	$0,\frac14,\frac58$	

											Reflection conditions
16	b	$.32$	$\frac18,\frac18,\frac18$	$\frac38,\frac78,\frac58$	$\frac78,\frac58,\frac38$	$\frac58,\frac38,\frac78$	$\frac78,\frac78,\frac78$	$\frac58,\frac18,\frac38$	$\frac18,\frac38,\frac58$	$\frac38,\frac58,\frac18$	hkl : $h,k=2n+1$, $l=4n+2$ or $h,k,l=4n$
16	a	$.\bar{3}.$	$0,0,0$	$\frac12,0,\frac12$	$0,\frac12,\frac12$	$\frac12,\frac12,0$	$\frac34,\frac14,\frac14$	$\frac34,\frac34,\frac34$	$\frac14,\frac14,\frac34$	$\frac14,\frac34,\frac14$	hkl : $h,k=2n$, $h+k+l=4n$

(*Continued on page 715*)

(*from page* 717)

Symmetry of special projections

Along [001] $p4mm$	Along [111] $p6mm$	Along [110] $c2mm$
$\mathbf{a}' = \frac12\mathbf{a} \quad \mathbf{b}' = \frac12\mathbf{b}$	$\mathbf{a}' = \frac13(2\mathbf{a}-\mathbf{b}-\mathbf{c}) \quad \mathbf{b}' = \frac13(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$	$\mathbf{a}' = \frac12(-\mathbf{a}+\mathbf{b}) \quad \mathbf{b}' = \frac12\mathbf{c}$
Origin at $\frac14,0,z$	Origin at x,x,x	Origin at $x,x+\frac14,\frac18$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}3d$ (220)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+
	[2] $I4_132$ (214)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+
	[2] $Ia\bar{3}1$ ($Ia\bar{3}$, 206)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+
	[3] $I4_1/a12/d$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
	[3] $I4_1/a12/d$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
	[3] $I4_1/a12/d$ ($I4_1/acd$, 142)	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
	[4] $I1\bar{3}2/d$ ($R\bar{3}c$, 167)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
	[4] $I1\bar{3}2/d$ ($R\bar{3}c$, 167)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
	[4] $I1\bar{3}2/d$ ($R\bar{3}c$, 167)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
	[4] $I1\bar{3}2/d$ ($R\bar{3}c$, 167)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+
IIa	none	
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [27] $Ia\bar{3}d$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (230)

Minimal non-isomorphic supergroups

I none

II [4] $Pm\bar{3}n$ ($\mathbf{a}' = \frac12\mathbf{a}, \mathbf{b}' = \frac12\mathbf{b}, \mathbf{c}' = \frac12\mathbf{c}$) (223)

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) $2(0,0,\frac12)\ \ \frac14,0,z$	(3) $2(0,\frac12,0)\ \ 0,y,\frac14$	(4) $2(\frac12,0,0)\ \ x,\frac14,0$
(5) $3^{+}\ x,x,x$	(6) $3^{+}\ \bar{x}+\frac12,x,\bar{x}$	(7) $3^{+}\ x+\frac12,\bar{x}-\frac12,\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x}+\frac12,x$
(9) $3^{-}\ x,x,x$	(10) $3^{-}(-\frac13,\frac13,\frac13)\ \ x+\frac16,\bar{x}+\frac16,\bar{x}$	(11) $3^{-}(\frac13,\frac13,-\frac13)\ \ \bar{x}+\frac13,\bar{x}+\frac16,x$	(12) $3^{-}(\frac13,-\frac13,\frac13)\ \ \bar{x}-\frac16,x+\frac13,\bar{x}$
(13) $2(\frac12,\frac12,0)\ \ x,x-\frac14,\frac18$	(14) $2\ \ x,\bar{x}+\frac34,\frac38$	(15) $4^{-}(0,0,\frac34)\ \ \frac14,0,z$	(16) $4^{+}(0,0,\frac14)\ \ -\frac14,\frac12,z$
(17) $4^{-}(\frac34,0,0)\ \ x,\frac14,0$	(18) $2(0,\frac12,\frac12)\ \ \frac18,y+\frac14,y$	(19) $2\ \ \frac38,y+\frac34,\bar{y}$	(20) $4^{+}(\frac14,0,0)\ \ x,-\frac14,\frac12$
(21) $4^{+}(0,\frac14,0)\ \ \frac12,y,-\frac14$	(22) $2(\frac12,0,\frac12)\ \ x-\frac14,\frac18,x$	(23) $4^{-}(0,\frac34,0)\ \ 0,y,\frac14$	(24) $2\ \ \bar{x}+\frac34,\frac38,x$
(25) $\bar{1}\ \ 0,0,0$	(26) $a\ \ x,y,\frac14$	(27) $c\ \ x,\frac14,z$	(28) $b\ \ \frac14,y,z$
(29) $\bar{3}^{+}\ x,x,x;\ 0,0,0$	(30) $\bar{3}^{+}\ \bar{x}-\frac12,x+1,\bar{x};\ 0,\frac12,\frac12$	(31) $\bar{3}^{+}\ x+\frac12,\bar{x}+\frac12,\bar{x};\ \frac12,\frac12,0$	(32) $\bar{3}^{+}\ \bar{x}+1,\bar{x}+\frac12,x;\ \frac12,0,\frac12$
(33) $\bar{3}^{-}\ x,x,x;\ 0,0,0$	(34) $\bar{3}^{-}\ x+\frac12,\bar{x}-\frac12,\bar{x};\ 0,0,\frac12$	(35) $\bar{3}^{-}\ \bar{x},\bar{x}+\frac12,x;\ 0,\frac12,0$	(36) $\bar{3}^{-}\ \bar{x}+\frac12,x,\bar{x};\ \frac12,0,0$
(37) $d(-\frac14,\frac14,\frac34)\ \ x+\frac12,\bar{x},z$	(38) $d(\frac14,\frac14,\frac14)\ \ x,x,z$	(39) $\bar{4}^{-}\ 0,\frac34,z;\ 0,\frac34,\frac18$	(40) $\bar{4}^{+}\ \frac12,-\frac14,z;\ \frac12,-\frac14,\frac38$
(41) $\bar{4}^{-}\ x,0,\frac34;\ \frac18,0,\frac34$	(42) $d(\frac34,-\frac14,\frac14)\ \ x,y+\frac12,\bar{y}$	(43) $d(\frac14,\frac14,\frac14)\ \ x,y,y$	(44) $\bar{4}^{+}\ x,\frac12,-\frac14;\ \frac38,\frac12,-\frac14$
(45) $\bar{4}^{+}\ -\frac14,y,\frac12;\ -\frac14,\frac38,\frac12$	(46) $d(\frac14,\frac34,-\frac14)\ \ \bar{x}+\frac12,y,x$	(47) $\bar{4}^{-}\ \frac34,y,0;\ \frac34,\frac18,0$	(48) $d(\frac14,\frac14,\frac14)\ \ x,y,x$

For $(\frac12,\frac12,\frac12)$+ set

(1) $t(\frac12,\frac12,\frac12)$	(2) $2\ \ 0,\frac14,z$	(3) $2\ \ \frac14,y,0$	(4) $2\ \ x,0,\frac14$
(5) $3^{+}(\frac12,\frac12,\frac12)\ \ x,x,x$	(6) $3^{+}(\frac16,-\frac16,\frac16)\ \ \bar{x}-\frac16,x+\frac13,\bar{x}$	(7) $3^{+}(-\frac16,\frac16,\frac16)\ \ x+\frac16,\bar{x}+\frac16,\bar{x}$	(8) $3^{+}(\frac16,\frac16,-\frac16)\ \ \bar{x}+\frac13,\bar{x}+\frac16,x$
(9) $3^{-}(\frac12,\frac12,\frac12)\ \ x,x,x$	(10) $3^{-}(\frac16,-\frac16,-\frac16)\ \ x+\frac16,\bar{x}+\frac16,\bar{x}$	(11) $3^{-}(-\frac16,-\frac16,\frac16)\ \ \bar{x}+\frac13,\bar{x}+\frac16,x$	(12) $3^{-}(-\frac16,\frac16,-\frac16)\ \ \bar{x}-\frac16,x+\frac13,\bar{x}$
(13) $2(\frac12,\frac12,0)\ \ x,x+\frac14,\frac38$	(14) $2\ \ x,\bar{x}+\frac14,\frac18$	(15) $4^{-}(0,0,\frac14)\ \ \frac34,0,z$	(16) $4^{+}(0,0,\frac34)\ \ \frac14,\frac12,z$
(17) $4^{-}(\frac14,0,0)\ \ x,\frac34,0$	(18) $2(0,\frac12,\frac12)\ \ \frac38,y-\frac14,y$	(19) $2\ \ \frac18,y+\frac14,\bar{y}$	(20) $4^{+}(\frac34,0,0)\ \ x,\frac14,\frac12$
(21) $4^{+}(0,\frac34,0)\ \ \frac12,y,\frac14$	(22) $2(\frac12,0,\frac12)\ \ x+\frac14,\frac38,x$	(23) $4^{-}(0,\frac14,0)\ \ 0,y,\frac34$	(24) $2\ \ \bar{x}+\frac14,\frac18,x$
(25) $\bar{1}\ \ \frac14,\frac14,\frac14$	(26) $b\ \ x,y,0$	(27) $a\ \ x,0,z$	(28) $c\ \ 0,y,z$
(29) $\bar{3}^{+}\ x,x,x;\ \frac14,\frac14,\frac14$	(30) $\bar{3}^{+}\ \bar{x}-\frac12,x,\bar{x};\ -\frac14,-\frac14,\frac14$	(31) $\bar{3}^{+}\ x-\frac12,\bar{x}+\frac12,\bar{x};\ -\frac14,\frac14,-\frac14$	(32) $\bar{3}^{+}\ \bar{x},\bar{x}-\frac12,x;\ \frac14,-\frac14,-\frac14$
(33) $\bar{3}^{-}\ x,x,x;\ \frac14,\frac14,\frac14$	(34) $\bar{3}^{-}\ x+\frac12,\bar{x}-\frac12,\bar{x};\ \frac14,-\frac14,\frac14$	(35) $\bar{3}^{-}\ \bar{x},\bar{x}+\frac12,x;\ -\frac14,\frac14,\frac14$	(36) $\bar{3}^{-}\ \bar{x}+\frac12,x,\bar{x};\ \frac14,\frac14,-\frac14$
(37) $d(\frac14,-\frac14,\frac14)\ \ x+\frac12,\bar{x},z$	(38) $d(\frac34,\frac34,\frac34)\ \ x,x,z$	(39) $\bar{4}^{-}\ 0,\frac14,z;\ 0,\frac14,\frac38$	(40) $\bar{4}^{+}\ \frac12,\frac14,z;\ \frac12,\frac14,\frac18$
(41) $\bar{4}^{-}\ x,0,\frac14;\ \frac38,0,\frac14$	(42) $d(\frac14,\frac14,-\frac14)\ \ x,y+\frac12,\bar{y}$	(43) $d(\frac34,\frac34,\frac34)\ \ x,y,y$	(44) $\bar{4}^{+}\ x,\frac12,\frac14;\ \frac18,\frac12,\frac14$
(45) $\bar{4}^{+}\ \frac14,y,\frac12;\ \frac14,\frac18,\frac12$	(46) $d(-\frac14,\frac14,\frac14)\ \ \bar{x}+\frac12,y,x$	(47) $\bar{4}^{-}\ \frac14,y,0;\ \frac14,\frac38,0$	(48) $d(\frac34,\frac34,\frac34)\ \ x,y,x$

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8.1. Basic concepts

BY H. WONDRATSCHEK

8.1.1. Introduction

The aim of this part is to define and explain some of the concepts and terms frequently used in crystallography, and to present some basic knowledge in order to enable the reader to make best use of the space-group tables.

The reader will be assumed to have some familiarity with analytical geometry and linear algebra, including vector and matrix calculus. Even though one can solve a good number of practical crystallographic problems without this knowledge, some mathematical insight is necessary for a more thorough understanding of crystallography. In particular, the application of symmetry theory to problems in crystal chemistry and crystal physics requires a background of group theory and, sometimes, also of representation theory.

The symmetry of crystals is treated in textbooks by different methods and at different levels of complexity. In this part, a mainly algebraic approach is used, but the geometric viewpoint is presented also. The algebraic approach has two advantages: it facilitates computer applications and it permits statements to be formulated in such a way that they are independent of the dimension of the space. This is frequently done in this part.

A great selection of textbooks and monographs is available for the study of crystallography. Only Giacovazzo (2002) and Vainshtein (1994) will be mentioned here.

Surveys of the history of crystallographic symmetry can be found in Burckhardt (1988) and Lima-de-Faria (1990).

In addition to books, many programs exist by which crystallographic computations can be performed. For example, the programs can be used to derive the classes of point groups, space groups, lattices (Bravais lattices) and crystal families; to calculate the subgroups of point groups and space groups, Wyckoff positions, irreducible representations *etc.* The mathematical program packages *GAP* (Groups, Algorithms and Programming), in particular *CrystGap*, and *Carat* (Crystallographic Algorithms and Tables) are examples of powerful tools for the solution of problems of crystallographic symmetry. For *GAP*, see http://www.gap-system.org/; for *Carat*, see http://wwwb.math.rwth-aachen.de/carat/. Other programs are provided by the crystallographic server in Bilbao: http://www.cryst.ehu.es/cryst/.

Essential for the determination of crystal structures are extremely efficient program systems that implicitly make use of crystallographic (and noncrystallographic) symmetries.

In this part, as well as in the space-group tables of this volume, 'classical' crystallographic groups in three, two and one dimensions are described, *i.e.* space groups, plane groups, line groups and their associated point groups. In addition to three-dimensional crystallography, which is the basis for the treatment of crystal structures, crystallography of two- and one-dimensional space is of practical importance. It is encountered in sections and projections of crystal structures, in mosaics and in frieze ornaments.

There are several expansions of 'classical' crystallographic groups (groups of motions) that are not treated in this volume but will or may be included in future volumes of the *IT* series.

(*a*) Generalization of crystallographic groups to spaces of dimension $n > 3$ is the field of n-dimensional crystallography. Some results are available. The crystallographic symmetry operations for spaces of any dimension n have already been derived by Hermann (1949). The crystallographic groups of four-dimensional space are also completely known and have been tabulated by Brown *et al.* (1978) and Schwarzenberger (1980). The present state of the art and results for higher dimensions are described by Opgenorth *et al.* (1998), Plesken & Schulz (2000) and Souvignier (2003). Some of their results are displayed in Table 8.1.1.1.

(*b*) One can deal with groups of motions whose lattices of translations have lower dimension than the spaces on which the groups act. This expansion yields the *subperiodic groups*. In particular, there are frieze groups (groups in a plane with one-dimensional translations), rod groups (groups in space with one-dimensional translations) and layer groups (groups in space with two-dimensional translations). These subperiodic groups are treated in *IT* E (2002) in a similar way to that in which line groups, plane groups and space groups are treated in this volume. Subperiodic groups are strongly related to 'groups of generalized symmetry'.

(*c*) Incommensurate phases, *e.g.* modulated structures or inclusion compounds, as well as quasicrystals, have led to an extension of crystallography beyond periodicity. Such structures are not really periodic in three-dimensional space but their symmetry may be described as that of an n-dimensional periodic structure, *i.e.* by an n-dimensional space group. In practical cases, $n = 4$, 5 or 6 holds. The crystal structure is then an irrational three-dimensional section through the n-dimensional periodic structure. The description by crystallographic groups of higher-dimensional spaces is thus of practical interest, *cf.* Janssen *et al.* (2004), van Smaalen (1995) or Yamamoto (1996).

(*d*) Generalized symmetry. Other generalizations of crystallographic symmetry combine the geometric symmetry operations with changes of properties: black–white groups, colour groups *etc.* They are treated in the classical book by Shubnikov & Koptsik (1974). Janner (2001) has given an overview of further generalizations.

Table 8.1.1.1. *Number of crystallographic classes for dimensions 1 to 6*

The numbers are those of the *affine* equivalence classes. The numbers for the enantiomorphic pairs are given in parentheses preceded by a + sign (Souvignier, 2003).

Dimension of space	Crystal families	Lattice (Bravais) types	(Geometric) crystal classes	Arithmetic crystal classes	Space-group types
1	1	1	2	2	2
2	4	5	10	13	17
3	6	14	32	73	(+11) 219
4	(+6) 23	(+10) 64	(+44) 227	(+70) 710	(+111) 4783
5	32	189	955	6079	222018
6	91	841	7104	(+30) 85311	(+7052) 28927922

8.1.2. Spaces and motions

Crystals are objects in the physical three-dimensional space in which we live. A model for the mathematical treatment of this space is the so-called *point space*, which in crystallography is known as *direct* or *crystal space*. In this space, the structures of finite real crystals are idealized as infinite perfect three-dimensional crystal structures (*cf.* Section 8.1.4). This implies that for crystal structures and their symmetries the surfaces of crystals as well as their defects and imperfections are neglected; for most applications, this is an excellent approximation.

The description of crystal structures and their symmetries is not as simple as it appears at first sight. It is useful to consider not only the above-mentioned point space but also to introduce simultaneously a *vector space* which is closely connected with the point space. Crystallographers are used to working in both spaces: crystal structures are described in point space, whereas face normals, translation vectors, Patterson vectors and reciprocal-lattice vectors are elements of vector spaces.

In order to carry out crystallographic calculations it is necessary to have a *metrics* in point space. Metrical relations, however, are most easily introduced in vector space by defining scalar products between vectors from which the length of a vector and the angle between two vectors are derived. The connection between the vector space $\mathbf{V}^n$ and the point space E^n transfers both the metrics and the dimension of $\mathbf{V}^n$ onto the point space E^n in such a way that distances and angles in point space may be calculated.

The connection between the two spaces is achieved in the following way:

(i) To any two points P and Q of the point space E^n a vector $\overrightarrow{PQ} = \mathbf{r}$ of the vector space $\mathbf{V}^n$ is attached.

(ii) For each point P of E^n and each vector $\mathbf{r}$ of $\mathbf{V}^n$ there is exactly one point Q of E^n for which $\overrightarrow{PQ} = \mathbf{r}$ holds.

(iii) $\overrightarrow{PQ} + \overrightarrow{QR} = \overrightarrow{PR}$.

The distance between two points P and Q in point space is given by the length $|\overrightarrow{PQ}| = (\overrightarrow{PQ}, \overrightarrow{PQ})^{1/2}$ of the attached vector $\overrightarrow{PQ}$ in vector space. In this expression, $(\overrightarrow{PQ}, \overrightarrow{PQ})$ is the scalar product of $\overrightarrow{PQ}$ with itself.

The angle determined by P, Q and R with vertex Q is obtained from

$$\cos(P,Q,R) = \cos(\overrightarrow{QP}, \overrightarrow{QR}) = \frac{(\overrightarrow{QP}, \overrightarrow{QR})}{|\overrightarrow{QP}| \cdot |\overrightarrow{QR}|}.$$

Here, $(\overrightarrow{QP}, \overrightarrow{QR})$ is the scalar product between $\overrightarrow{QP}$ and $\overrightarrow{QR}$. Such a point space is called an n-dimensional *Euclidean space*.

If we select in the point space E^n an arbitrary point O as the *origin*, then to each point X of E^n a unique vector $\overrightarrow{OX}$ of $\mathbf{V}^n$ is assigned, and there is a one-to-one correspondence between the points X of E^n and the vectors $\overrightarrow{OX}$ of $\mathbf{V}^n : X \leftrightarrow \overrightarrow{OX} = \mathbf{x}$.

Referred to a vector basis $\mathbf{a}_1, \ldots, \mathbf{a}_n$ of $\mathbf{V}^n$, each vector $\mathbf{x}$ is uniquely expressed as $\mathbf{x} = x_1\mathbf{a}_1 + \ldots + x_n\mathbf{a}_n$ or, using matrix multiplication,* $\mathbf{x} = (\mathbf{a}_1, \ldots, \mathbf{a}_n)\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$.

Referred to the coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$ of E^n, Fig. 8.1.2.1, each point X is uniquely described by the column of coordinates

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}.$$

Thus, the real numbers x_i are either the *coefficients of the vector* $\mathbf{x}$ of $\mathbf{V}^n$ or the *coordinates of the point* X of E^n.

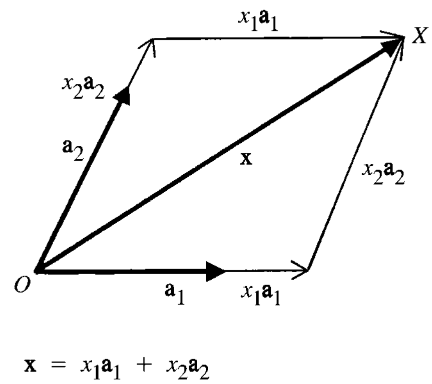

Fig. 8.1.2.1. Representation of the point X with respect to origin O by the vector $\overrightarrow{OX} = \mathbf{x}$. The vector $\mathbf{x}$ is described with respect to the vector basis $\{\mathbf{a}_1, \mathbf{a}_2\}$ of $\mathbf{V}^2$ by the coefficients x_1, x_2. The coordinate system $(O, \mathbf{a}_1, \mathbf{a}_2)$ of the point space E^2 consists of the point O of E^2 and the vector basis $\{\mathbf{a}_1, \mathbf{a}_2\}$ of $\mathbf{V}^2$.

An instruction assigning uniquely to each point X of the point space E^n an 'image' point $\tilde{X}$, whereby all distances are left invariant, is called an *isometry*, an *isometric mapping* or a *motion* M of E^n. Motions are invertible, *i.e.*, for a given motion $\mathsf{M} : X \to \tilde{X}$, the inverse motion $\mathsf{M}^{-1} : \tilde{X} \to X$ exists and is unique.

Referred to a coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$, any motion $X \to \tilde{X}$ may be described in the form

$$\begin{array}{ccccccc} \tilde{x}_1 & = & W_{11}x_1 & + \ldots + & W_{1n}x_n & + & w_1 \\ \vdots & = & \vdots & & \vdots & & \vdots \\ \tilde{x}_n & = & W_{n1}x_1 & + \ldots + & W_{nn}x_n & + & w_n. \end{array}$$

In matrix formulation, this is expressed as

$$\begin{pmatrix} \tilde{x}_1 \\ \vdots \\ \tilde{x}_n \end{pmatrix} = \begin{pmatrix} W_{11} & \ldots & W_{1n} \\ \vdots & & \vdots \\ W_{n1} & \ldots & W_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} + \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix}$$

or, in abbreviated form, as $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$, where $\tilde{\boldsymbol{x}}$, $\boldsymbol{x}$ and $\boldsymbol{w}$ are all $(n \times 1)$ columns and $\boldsymbol{W}$ is an $(n \times n)$ square matrix. One often writes this in even more condensed form as $\tilde{\boldsymbol{x}} = (\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x}$, or $\tilde{\boldsymbol{x}} = (\boldsymbol{W}|\boldsymbol{w})\boldsymbol{x}$; here, $(\boldsymbol{W}|\boldsymbol{w})$ is called the *Seitz symbol*.

A motion consists of a *rotation part* or *linear part* and a *translation part*. If the motion is represented by $(\boldsymbol{W}, \boldsymbol{w})$, the matrix $\boldsymbol{W}$ describes the rotation part of the motion and is called the *matrix part* of $(\boldsymbol{W}, \boldsymbol{w})$. The column $\boldsymbol{w}$ describes the translation part of the motion and is called the *vector part* or *column part* of $(\boldsymbol{W}, \boldsymbol{w})$. For a given motion, the matrix $\boldsymbol{W}$ depends only on the choice of the basis vectors, whereas the column $\boldsymbol{w}$ in general depends on the choice of the basis vectors *and* of the origin O; *cf.* Section 8.3.1.

It is possible to combine the $(n \times 1)$ column and the $(n \times n)$ matrix representing a motion into an $(n+1) \times (n+1)$ square matrix which is called the *augmented matrix*. The system of equations $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$ may then be expressed in the following form:

$$\left(\begin{array}{c} \tilde{x}_1 \\ \vdots \\ \tilde{x}_n \\ \hline 1 \end{array}\right) = \left(\begin{array}{ccc:c} & & & w_1 \\ & \boldsymbol{W} & & \vdots \\ & & & w_n \\ \hline 0 & \ldots & 0 & 1 \end{array}\right) \left(\begin{array}{c} x_1 \\ \vdots \\ x_n \\ \hline 1 \end{array}\right)$$

or, in abbreviated form, by $\tilde{\mathbb{x}} = \mathbb{W}\mathbb{x}$. The augmentation is done in two steps. First, the $(n \times 1)$ column $\boldsymbol{w}$ is attached to the $(n \times n)$ matrix and then the matrix is made square by attaching the $[1 \times (n+1)]$ row $(0 \ldots 0\ 1)$. Similarly, the $(n \times 1)$ columns $\boldsymbol{x}$ and $\tilde{\boldsymbol{x}}$

* For this volume, the following conventions for the writing of vectors and matrices have been adopted:

(i) point coordinates and vector coefficients are written as $(n \times 1)$ column matrices;

(ii) the vectors of the vector basis are written as a $(1 \times n)$ row matrix;

(iii) *all* running indices are written as subscripts.

It should be mentioned that other conventions are also found in the literature, *e.g.* interchange of row and column matrices and simultaneous use of subscripts and superscripts for running indices.

have to be augmented to $[(n+1)\times 1]$ columns $\mathbb{X}$ and $\tilde{\mathbb{X}}$. The motion is now described by the one matrix $\mathbb{W}$ instead of the pair $(\boldsymbol{W}, \boldsymbol{w})$.

If the motion M is described by $\mathbb{W}$, the 'inverse motion' M^{-1} is described by $\mathbb{W}^{-1}$, where $(\boldsymbol{W},\boldsymbol{w})^{-1} = (\boldsymbol{W}^{-1}, -\boldsymbol{W}^{-1}\boldsymbol{w})$. Successive application of two motions, W_1 and W_2, results in another motion W_3:

$$\tilde{X} = \mathsf{W}_1 X \text{ and } \tilde{\tilde{X}} = \mathsf{W}_2\tilde{X} = \mathsf{W}_2\mathsf{W}_1 X = \mathsf{W}_3 X.$$

with $\mathsf{W}_3 = \mathsf{W}_2\mathsf{W}_1$.

This can be described in matrix notation as follows

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{w}_1$$

and

$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{W}_2\tilde{\boldsymbol{x}} + \boldsymbol{w}_2 = \boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2 = \boldsymbol{W}_3\boldsymbol{x} + \boldsymbol{w}_3,$$

with $(\boldsymbol{W}_3, \boldsymbol{w}_3) = (\boldsymbol{W}_2\boldsymbol{W}_1, \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2)$ or

$$\tilde{\mathbb{X}} = \mathbb{W}_1\mathbb{X} \text{ and } \tilde{\tilde{\mathbb{X}}} = \mathbb{W}_2\tilde{\mathbb{X}} = \mathbb{W}_2\mathbb{W}_1\mathbb{X} = \mathbb{W}_3\mathbb{X}$$

with $\mathbb{W}_3 = \mathbb{W}_2\mathbb{W}_1$.

It is a special advantage of the augmented matrices that successive application of motions is described by the product of the corresponding augmented matrices.

A point X is called a *fixed point* of the mapping M if it is invariant under the mapping, *i.e.* $\tilde{X} = X$.

In an n-dimensional Euclidean space E^n, three types of motions can be distinguished:

(1) *Translation.* In this case, $\boldsymbol{W} = \boldsymbol{I}$, where $\boldsymbol{I}$ is the unit matrix; the vector $\mathbf{w} = w_1\mathbf{a}_1 + \ldots + w_n\mathbf{a}_n$ is called the *translation vector.*

(2) *Motions with at least one fixed point.* In E^1, E^2 and E^3, such motions are called proper motions or *rotations* if $\det(\boldsymbol{W}) = +1$ and improper motions if $\det(\boldsymbol{W}) = -1$. Improper motions are called *inversions* if $\boldsymbol{W} = -\boldsymbol{I}$; *reflections* if $\boldsymbol{W}^2 = \boldsymbol{I}$ and $\boldsymbol{W} \neq -\boldsymbol{I}$; and *rotoinversions* in all other cases. The inversion is a rotation for spaces of even dimension, but an (improper) motion of its own kind in spaces of odd dimension. The origin is among the fixed points if $\boldsymbol{w} = \boldsymbol{o}$, where $\boldsymbol{o}$ is the $(n\times 1)$ column consisting entirely of zeros.

(3) *Fixed-point-free motions which are not translations.* In E^3, they are called *screw rotations* if $\det(\boldsymbol{W}) = +1$ and *glide reflections* if $\det(\boldsymbol{W}) = -1$. In E^2, only glide reflections occur. No such motions occur in E^1.

In Fig. 8.1.2.2, the relations between the different types of motions in E^3 are illustrated. The diagram contains all kinds of motions except the identity mapping I which leaves the whole space invariant and which is described by $\mathbb{W} = \mathbb{I}$. Thus, it is simultaneously a special rotation (with rotation angle 0) and a special translation (with translation vector $\mathbf{o}$).

So far, motions M in point space E^n have been considered. Motions give rise to mappings of the corresponding vector space $\mathbf{V}^n$ onto itself. If M maps the points P_1 and Q_1 of E^n onto P_2 and Q_2, the vector $\overrightarrow{P_1Q_1}$ is mapped onto the vector $\overrightarrow{P_2Q_2}$. If the motion in E^n is described by $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$, the vectors $\mathbf{v}$ of $\mathbf{V}^n$ are mapped according to $\tilde{\mathbf{v}} = \boldsymbol{W}\mathbf{v}$. In other words, of the linear and translation parts of the motion of E^n, only the linear part remains in the corresponding mapping of $\mathbf{V}^n$ (*linear mapping*). This difference between the mappings in the two spaces is particularly obvious for translations. For a translation T with translation vector $\mathbf{t} \neq \mathbf{o}$, no fixed point exists in E^n, *i.e.* no point of E^n is mapped onto itself by T. In $\mathbf{V}^n$, however, any vector $\mathbf{v}$ is mapped onto itself since the corresponding linear mapping is the identity mapping.

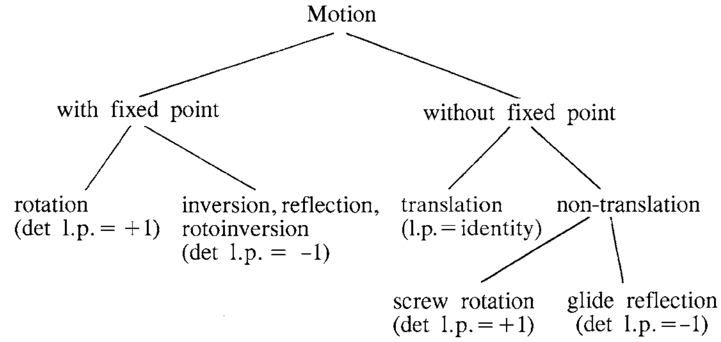

Fig. 8.1.2.2. Relations between the different kinds of motions in E^3; det l.p. = determinant of the linear part. The identity mapping does not fit into this scheme properly and hence has been omitted.

8.1.3. Symmetry operations and symmetry groups

Definition: A *symmetry operation* of a given object in point space E^n is a motion of E^n which maps this object (point, set of points, crystal pattern *etc.*) onto itself.

Remark: Any motion may be a symmetry operation, because for any motion one can construct an object which is mapped onto itself by this motion.

For the set of *all* symmetry operations of a given object, the following relations hold:

(*a*) successive application of two symmetry operations of an object results in a third symmetry operation of that object;

(*b*) the inverse of a symmetry operation is also a symmetry operation;

(*c*) there exists an 'identity operation' I which leaves each point of the space fixed: $X \rightarrow X$. This operation I is described (in any coordinate system) by $(\boldsymbol{W},\boldsymbol{w}) = (\boldsymbol{I},\boldsymbol{o})$ or by $\mathbb{W} = \mathbb{I}$ and it is a symmetry operation of any object.

(*d*) The 'associative law' $(\mathsf{W}_3\mathsf{W}_2)\mathsf{W}_1 = \mathsf{W}_3(\mathsf{W}_2\mathsf{W}_1)$ is valid.

One can show, however, that in general the 'commutative law' $\mathsf{W}_2\mathsf{W}_1 = \mathsf{W}_1\mathsf{W}_2$ is not obeyed for symmetry operations.

The properties (*a*) to (*d*) are the group axioms. Thus, the set of all symmetry operations of an object forms a group, *the symmetry group of the object* or its *symmetry.* The mathematical theorems of *group theory*, therefore, may be applied to the symmetries of objects.

So far, only rather general objects have been considered. Crystallographers, however, are particularly interested in the symmetries of crystals. In order to introduce the concept of crystallographic symmetry operations, crystal structures, crystal patterns and lattices have to be taken into consideration. This will be done in the following section.

8.1.4. Crystal patterns, vector lattices and point lattices

Crystals are finite real objects in physical space which may be idealized by infinite three-dimensional periodic 'crystal structures' in point space. Three-dimensional periodicity means that there are translations among the symmetry operations of the object with the translation vectors spanning a three-dimensional space. Extending this concept of crystal structure to more general periodic objects and to n-dimensional space, one obtains the following definition:

Definition: An object in n-dimensional point space E^n is called an n-dimensional *crystallographic pattern* or, for short, *crystal pattern* if among its symmetry operations

(i) there are n translations, the translation vectors $\mathbf{t}_1, \ldots, \mathbf{t}_n$ of which are linearly independent,

(ii) all translation vectors, except the zero vector $\mathbf{o}$, have a length of at least $d > 0$.

Condition (i) guarantees the n-dimensional periodicity and thus excludes subperiodic symmetries like layer groups, rod groups and frieze groups. Condition (ii) takes into account the finite size of atoms in actual crystals.

Successive application of two translations of a crystal pattern results in another translation, the translation vector of which is the (vector) sum of the original translation vectors. Consequently, in addition to the n linearly independent translation vectors $\mathbf{t}_1, \ldots, \mathbf{t}_n$, all (infinitely many) vectors $\mathbf{t} = u_1\mathbf{t}_1 + \ldots + u_n\mathbf{t}_n$ ($u_1, \ldots, u_n$ arbitrary integers) are translation vectors of the pattern. Thus, infinitely many translations belong to each crystal pattern. The periodicity of crystal patterns is represented by their lattices. It is useful to distinguish two kinds of lattices: vector lattices and point lattices. This distinction corresponds to that between vector space and point space, discussed above. The vector lattice is treated first.

Definition: The (infinite) set of *all* translation vectors of a crystal pattern is called the lattice of translation vectors or the *vector lattice* $\mathbf{L}$ of this crystal pattern.

In principle, any set of n linearly independent vectors may be used as a basis of the vector space $\mathbf{V}^n$. Most of these sets, however, result in a rather complicated description of a given vector lattice. The following theorem shows that among the (infinitely many) possible bases of the vector space $\mathbf{V}^n$ special bases always exist, referred to which the survey of a given vector lattice becomes particularly simple.

Definitions: (1) A basis of n vectors $\mathbf{a}_1, \ldots, \mathbf{a}_n$ of $\mathbf{V}^n$ is called a *crystallographic basis* of the n-dimensional vector lattice $\mathbf{L}$ if *every* integral linear combination $\mathbf{t} = u_1\mathbf{a}_1 + \ldots + u_n\mathbf{a}_n$ is a lattice vector of $\mathbf{L}$. (2) A basis is called a primitive crystallographic basis of $\mathbf{L}$ or, for short, a *primitive basis* if it is a crystallographic basis and if, furthermore, *every* lattice vector $\mathbf{t}$ of $\mathbf{L}$ may be obtained as an *integral* linear combination of the basis vectors.

The distinction between these two kinds of bases can be expressed as follows. Referred to a crystallographic basis, the coefficients of each lattice vector must be either integral or rational. Referred to a primitive crystallographic basis, only integral coefficients occur. It should be noted that nonprimitive crystallographic bases are used conventionally for the description of 'centred lattices', whereas reduced bases are always primitive; see Chapter 9.2.

Example

The basis used conventionally for the description of the 'cubic body-centred lattice' is a crystallographic basis because the basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ are lattice vectors. It is not a primitive basis because lattice vectors with non-integral but rational coefficients exist, *e.g.* the vector $\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b} + \frac{1}{2}\mathbf{c}$. The bases $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c})$, $\mathbf{b}' = \frac{1}{2}(\mathbf{a} - \mathbf{b} + \mathbf{c})$, $\mathbf{c}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - \mathbf{c})$ or $\mathbf{a}'' = \mathbf{a}$, $\mathbf{b}'' = \mathbf{b}$, $\mathbf{c}'' = \frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ are primitive bases. In the first of these bases, the vector $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ is given by $\mathbf{a}' + \mathbf{b}' + \mathbf{c}'$, in the second basis by $\mathbf{c}''$, both with integral coefficients only.

Fundamental theorem on vector lattices: For every vector lattice $\mathbf{L}$ primitive bases exist.

It can be shown that (in dimensions $n > 1$) the number of primitive bases for each vector lattice is infinite. There exists, however, a procedure called 'basis reduction' (*cf.* Chapter 9.2), which uniquely selects one primitive basis from this infinite set, thus permitting unambiguous description and comparison of vector lattices. Although such a reduced primitive basis always *can* be selected, in many cases conventional coordinate systems are chosen with nonprimitive rather than primitive crystallographic bases. The reasons are given in Section 8.3.1. The term 'primitive' is used not only for bases of lattices but also with respect to the lattices themselves, as in the crystallographic literature a *vector lattice* is frequently called *primitive* if its *conventional basis is primitive.*

With the help of the vector lattices defined above, the concept of point lattices will be introduced.

Definition: Given an arbitrary point X_0 in point space and a vector lattice $\mathbf{L}$ consisting of vectors $\mathbf{t}_j$, the set of all points X_j with $\overrightarrow{X_0X_j} = \mathbf{t}_j$ is called the *point lattice* belonging to X_0 and $\mathbf{L}$.

A point lattice can be visualized as the set of end-points of all vectors of $\mathbf{L}$, where $\mathbf{L}$ is attached to an arbitrary point X_0 of point space. Because each point X of point space could be chosen as the point X_0, an infinite set of point lattices belongs to each vector lattice. Frequently, the point X_0 is chosen as the origin of the coordinate system of the point space.

An important aspect of a lattice is its *unit cell*.

Definition: If $\mathbf{a}_1, \ldots, \mathbf{a}_n$ is a crystallographic basis of a vector lattice $\mathbf{L}$, the set of all vectors $x_1\mathbf{a}_1 + \ldots + x_n\mathbf{a}_n$ with $0 \leq x_i < 1$ is called a *unit cell of the vector lattice.*

The concept of a 'unit cell' is not only applied to vector lattices in vector space but also more often to crystal structures or crystal patterns in point space. Here the coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$ and the origin X_0 of the unit cell have to be chosen. In most cases $X_0 = O$ is taken, but in general we have the following definition:

Definition: Given a crystallographic coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$ of a crystal pattern and a point X_0 with coordinates x_{0i}, a *unit cell of the crystal pattern* is the set of all points X with coordinates x_i such that the equation $0 \leq x_i - x_{0i} < 1$ $(i = 1, \ldots, n)$ holds.

Obviously, the term 'unit cell' may be transferred to real crystals. As the volume of the unit cell and the volumes of atoms are both finite, only a *finite* number N of atoms can occur in a unit cell of a crystal. A crystal structure, therefore, may be described in two ways:

(*a*) One starts with an arbitrary unit cell and builds up the whole crystal structure by infinite repetition of this unit cell. The crystal structure thus consists of an infinite number of finite 'building blocks', each building block being a unit cell.

(*b*) One starts with a point X_1 representing the centre of an atom. To this point belong an infinite number of translationally equivalent points X_j, *i.e.* points for which the vectors $\overrightarrow{X_1X_j}$ are lattice vectors. In this way, from each of the points X_i $(i = 1, \ldots, N)$ within the unit cell a point lattice of translationally equivalent points is obtained. The crystal structure is then described by a finite number of interpenetrating infinite point lattices.

In most cases, one is not interested in the orientation of the vector lattice or the point lattices of a crystal structure in space, but only in the shape and size of a unit cell. From this point of view, a three-dimensional lattice is fully described by the lengths a, b and c of the basis vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ and by the three interaxial angles α, β and γ. These data are called the *lattice parameters*, *cell parameters* or *lattice constants* of both the vector lattice and the associated point lattices of the crystal structure.

8.1.5. Crystallographic symmetry operations

Crystallographic symmetry operations are special motions.

Definition: A motion is called a *crystallographic symmetry operation* if a crystal pattern exists for which it is a symmetry operation.

We consider a crystal pattern with its vector lattice **L** referred to a primitive basis. Then, by definition, each vector of **L** has integral coefficients. The linear part of a symmetry operation maps **L** onto itself: $\mathbf{L} \to \boldsymbol{W}\mathbf{L} = \mathbf{L}$. Since the coefficients of all vectors of **L** are integers, the matrix $\boldsymbol{W}$ is an integral matrix, *i.e.* its coefficients are integers. Thus, the trace of $\boldsymbol{W}$, $\mathrm{tr}(\boldsymbol{W}) = \boldsymbol{W}_{11} + \ldots + \boldsymbol{W}_{nn}$, is also an integer. In $\mathbf{V}^3$, by reference to an appropriate orthonormal (not necessarily crystallographic) basis, one obtains another condition for the trace, $\mathrm{tr}(\boldsymbol{W}) = \pm(1 + 2\cos\varphi)$, where φ is the angle of rotation or rotoinversion. From these two conditions, it follows that φ can only be 0, 60, 90, 120, 180° *etc.*, and hence the familiar restriction to one-, two-, three-, four- and sixfold rotations and rotoinversions results.* These results imply for dimensions 2 and 3 that the matrix $\boldsymbol{W}$ satisfies the condition $(\boldsymbol{W})^k = \boldsymbol{I}$, with $k = 1, 2, 3,$ 4 or 6.† Consequently, for the operation ($\boldsymbol{W}$, $\boldsymbol{w}$) in point space the relation

$$(\boldsymbol{W}, \boldsymbol{w})^k = [\boldsymbol{I}, (\boldsymbol{W}^{k-1} + \boldsymbol{W}^{k-2} + \ldots + \boldsymbol{W} + \boldsymbol{I})\boldsymbol{w}] = (\boldsymbol{I}, \boldsymbol{t})$$

holds.

For the motion described by ($\boldsymbol{W}$, $\boldsymbol{w}$), this implies that a k-fold application results in a translation T (with translation vector **t**) of the crystal pattern. The (fractional) translation $(1/k)\mathsf{T}$ is called the *intrinsic translation part* (*screw or glide part*) of the symmetry operation. Whereas the 'translation part' of a motion depends on the choice of the origin, the 'intrinsic translation part' of a motion is uniquely determined. The intrinsic translation vector $(1/k)\mathbf{t}$ is the shortest translation vector of the motion for any choice of the origin.

If $\boldsymbol{t} = \boldsymbol{o}$, the symmetry operation has at least one fixed point and is a rotation, inversion, reflection or rotoinversion. If $\boldsymbol{t} \neq \boldsymbol{o}$, the term $(1/k)\mathbf{t}$ is called the *glide vector* (for a reflection) or the *screw vector* (for a rotation) of the symmetry operation. Both types of operations, glide reflections and screw rotations, have no fixed point.

For the geometric visualization of symmetry, the concept of *symmetry elements* is useful.‡ The symmetry element of a symmetry operation is the set of its fixed points, together with a characterization of the motion. For symmetry operations without fixed points (screw rotations or glide reflections), the fixed points of the corresponding rotations or reflections, described by $(\boldsymbol{W}, \boldsymbol{w}')$ with $\boldsymbol{w}' = \boldsymbol{w} - (1/k)\boldsymbol{t}$, are taken. Thus, in E^2, symmetry elements are N-fold rotation points (N = 2, 3, 4 or 6), mirror lines and glide lines. In E^3, symmetry elements are rotation axes, screw axes, inversion centres, mirror planes and glide planes. A peculiar situation exists for rotoinversions (except $\bar{1}$ and $\bar{2} \equiv m$). The symmetry element of such a rotoinversion consists of two components, a point and an axis. The point is the *inversion point* of the rotoinversion, and the *axis* of the rotoinversion is that of the corresponding rotation.

The determination of both the nature of a symmetry operation and the location of its symmetry element from the coordinate triplets, listed under *Positions* in the space-group tables, is described in Section 11.2.1 of Chapter 11.2.

8.1.6. Space groups and point groups

As mentioned in Section 8.1.3, the set of all symmetry operations of an object forms a group, the symmetry group of that object.

Definition: The symmetry group of a three-dimensional crystal pattern is called its *space group*. In E^2, the symmetry group of a (two-dimensional) crystal pattern is called its *plane group*. In E^1, the symmetry group of a (one-dimensional) crystal pattern is called its *line group*. To each crystal pattern belongs an infinite set of translations T_j which are symmetry operations of that pattern. The set of all T_j forms a group known as the *translation subgroup* $\mathcal{T}$ of the space group $\mathcal{G}$ of the crystal pattern. Since the commutative law $\mathsf{T}_j\mathsf{T}_k = \mathsf{T}_k\mathsf{T}_j$ holds for any two translations, $\mathcal{T}$ is an Abelian group.

With the aid of the translation subgroup $\mathcal{T}$, an insight into the architecture of the space group $\mathcal{G}$ can be gained.

Referred to a coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$, the space group $\mathcal{G}$ is described by the set $\{(\boldsymbol{W}, \boldsymbol{w})\}$ of matrices $\boldsymbol{W}$ and columns $\boldsymbol{w}$. The group $\mathcal{T}$ is represented by the set of elements $(\boldsymbol{I}, \boldsymbol{t}_j)$, where $\boldsymbol{t}_j$ are the columns of coefficients of the translation vectors $\mathbf{t}_j$ of the lattice **L**. Let ($\boldsymbol{W}$, $\boldsymbol{w}$) describe an arbitrary symmetry operation W of $\mathcal{G}$. Then, all products $(\boldsymbol{I}, \boldsymbol{t}_j)(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{W}, \boldsymbol{w} + \boldsymbol{t}_j)$ for the different j have the same matrix part $\boldsymbol{W}$. Conversely, every symmetry operation W of the space group with the same matrix part $\boldsymbol{W}$ is represented in the set $\{(\boldsymbol{W}, \boldsymbol{w} + \boldsymbol{t}_j)\}$. The corresponding set of symmetry operations can be denoted by $\mathcal{T}\mathsf{W}$. Such a set is called a *right coset of* $\mathcal{G}$ *with respect to* $\mathcal{T}$, because the element W is the right factor in the products $\mathcal{T}\mathsf{W}$. Consequently, the space group $\mathcal{G}$ may be decomposed into the right cosets $\mathcal{T}, \mathcal{T}\mathsf{W}_2, \mathcal{T}\mathsf{W}_3, \ldots, \mathcal{T}\mathsf{W}_i$, where the symmetry operations of the same column have the same matrix part $\boldsymbol{W}$, and the symmetry operations W_j differ by their matrix parts $\boldsymbol{W}_j$. This *coset decomposition of* $\mathcal{G}$ *with respect to* $\mathcal{T}$ may be displayed by the array

$$\begin{array}{lllll}
\mathsf{I} \equiv \mathsf{W}_1 & \mathsf{W}_2 & \mathsf{W}_3 & \ldots & \mathsf{W}_i \\
\mathsf{T}_1 & \mathsf{T}_1\mathsf{W}_2 & \mathsf{T}_1\mathsf{W}_3 & \ldots & \mathsf{T}_1\mathsf{W}_i \\
\mathsf{T}_2 & \mathsf{T}_2\mathsf{W}_2 & \mathsf{T}_2\mathsf{W}_3 & \ldots & \mathsf{T}_2\mathsf{W}_i \\
\mathsf{T}_3 & \mathsf{T}_3\mathsf{W}_2 & \mathsf{T}_3\mathsf{W}_3 & \ldots & \mathsf{T}_3\mathsf{W}_i \\
\vdots & \vdots & \vdots & & \vdots
\end{array}$$

Here, $\mathsf{W}_1 = \mathsf{I}$ is the identity operation and the elements of $\mathcal{T}$ form the first column, those of $\mathcal{T}\mathsf{W}_2$ the second column *etc.* As each column may be represented by the common matrix part $\boldsymbol{W}$ of its symmetry operations, the number i of columns, *i.e.* the number of cosets, is at the same time the number of *different* matrices $\boldsymbol{W}$ of the symmetry operations of $\mathcal{G}$. This number i is always finite, and is the order of the point group belonging to $\mathcal{G}$, as explained below. Any element of a coset $\mathcal{T}\mathsf{W}_j$ may be chosen as the representative element of that coset and listed at the top of its column. Choice of a different representative element merely results in a different order of the elements of a coset, but the coset does not change its content.§

Analogously, a coset $\mathsf{W}\mathcal{T}$ is called a *left coset* of $\mathcal{G}$ with respect to $\mathcal{T}$, and $\mathcal{G}$ can be decomposed into the left cosets $\mathcal{T}, \mathsf{W}_2\mathcal{T}, \mathsf{W}_3\mathcal{T}, \ldots, \mathsf{W}_i\mathcal{T}$. This left coset decomposition of a space group is always possible with the same $\mathsf{W}_1, \mathsf{W}_2, \ldots, \mathsf{W}_i$ as in the right coset decomposition. Moreover, both decompositions result in the same cosets, except for the order of the elements in each coset. A subgroup of a group with these properties is called a *normal subgroup* of the group; *cf.* Ledermann (1976). Thus, the translation subgroup $\mathcal{T}$ is a normal subgroup of the space group $\mathcal{G}$.

The decomposition of a space group into cosets is the basis of the description of the space groups in these *Tables.* The symmetry

* The reflection $m \equiv \bar{2}$ is contained among the rotoinversions. The same restriction is valid for the rotation angle φ in two-dimensional space, where $\mathrm{tr}(\boldsymbol{W}) = 2\cos\varphi$ if $\det(\boldsymbol{W}) = +1$. If $\det(\boldsymbol{W}) = -1$, $\mathrm{tr}(\boldsymbol{W}) = 0$ always holds and the operation is a reflection m.

† A method of deriving the possible orders of $\boldsymbol{W}$ in spaces of arbitrary dimension has been described by Hermann (1949).

‡ For a rigorous definition of the term *symmetry element*, see de Wolff *et al.* (1989, 1992) and Flack *et al.* (2000).

§ A coset decomposition of a group $\mathcal{G}$ is possible with respect to every subgroup $\mathcal{H}$ of $\mathcal{G}$; *cf.* Ledermann (1976). The number of cosets is called the *index* $[i]$ of $\mathcal{H}$ in $\mathcal{G}$. The integer $[i]$ may be finite, as for the coset decomposition of a space group $\mathcal{G}$ with respect to the (infinite) translation group $\mathcal{T}$ or infinite, as for the coset decomposition of a space group $\mathcal{G}$ with respect to a (finite) site-symmetry group $\mathcal{S}$; *cf.* Section 8.3.2. If $\mathcal{G}$ is a finite group, a theorem of Lagrange states that the order of $\mathcal{G}$ is the product of the order of $\mathcal{H}$ and the index of $\mathcal{H}$ in $\mathcal{G}$.

operations of the space group are referred to a 'conventional' coordinate system (*cf.* Section 8.3.1) and described by $(n+1) \times (n+1)$ matrices. In the space-group tables as *general position* (*cf.* Section 8.3.2) for each column, a representative is listed whose coefficients w_j obey the condition $0 \le w_j < 1$. The matrix is not listed completely, however, but is given in a short-hand notation. In the expression $W_{j1}x_1 + \ldots + W_{jn}x_n + w_j$, all vanishing terms and all $W_{jk} = 1$ are omitted, *e.g.*

$$\left.\begin{array}{l} 1x + 0y + 0z + \frac{1}{2} \\ 0x + 1y + 0z + 0 \\ 0x + 0y - 1z + \frac{1}{2} \end{array}\right\}$$

is replaced by $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$. The first entry of the general position is always the identity mapping, listed as x, y, z. It represents all translations of the space group too.

As groups, some space groups are more complicated than others. Most easy to survey are the 'symmorphic' space groups which may be defined as follows:

Definition: A space group is called *symmorphic* if the coset representatives W_j can be chosen in such a way that they leave one common point fixed.

In this case, the representative symmetry operations W_j of a symmorphic space group form a (finite) group. If the fixed point is chosen as the origin of the coordinate system, the column parts $\boldsymbol{w}_j$ of the representative symmetry operations W_j obey the equations $\boldsymbol{w}_j = \boldsymbol{o}$. Thus, for a symmorphic space group the representative symmetry operations may always be described by the special matrix–column pairs $(\boldsymbol{W}_j, \boldsymbol{o})$.

Symmorphic space groups may be easily identified by their Hermann–Mauguin symbols because these do not contain any glide or screw operation. For example, the monoclinic space groups with the symbols $P2$, $C2$, Pm, Cm, $P2/m$ and $C2/m$ are symmorphic, whereas those with the symbols $P2_1$, Pc, Cc, $P2_1/m, P2/c, P2_1/c$ and $C2/c$ are not.

Unlike most textbooks of crystallography, in this section point groups are treated after space groups because the space group of a crystal pattern, and thus of a crystal structure, determines its point group uniquely.

The external shape (morphology) of a macroscopic crystal is formed by its faces. In order to eliminate the influence of growth conditions, the set of crystal faces is replaced by the set of face normals, *i.e.* by a set of vectors. Thus, the symmetry group of the macroscopic crystal is the symmetry group of the *vector set of face normals.* It is not the group of motions in point space, therefore, that determines the symmetry of the macroscopic crystal, but the corresponding group of linear mappings of vector space; *cf.* Section 8.1.2. This group of linear mappings is called the *point group of the crystal.* Since to each macroscopic crystal a crystal structure corresponds and, furthermore, to each crystal structure a space group, the point group of the crystal defined above is also the point group of the crystal structure and the point group of its space group.

To connect more formally the concept of point groups with that of space groups in n-dimensional space, we consider the coset decomposition of a space group $\mathcal{G}$ with respect to the normal subgroup $\mathcal{T}$, as displayed above. We represent the right coset decomposition by $\mathcal{T}, \mathcal{T}\mathsf{W}_2, \ldots, \mathcal{T}\mathsf{W}_i$ and the corresponding left coset decomposition by $\mathcal{T}, \mathsf{W}_2\mathcal{T}, \ldots, \mathsf{W}_i\mathcal{T}$. If $\mathcal{G}$ is referred to a coordinate system, the symmetry operations of $\mathcal{G}$ are described by matrices $\boldsymbol{W}$ and columns $\boldsymbol{w}$. As a result of the one-to-one correspondence between the i cosets $\mathcal{T}\mathsf{W}_j = \mathsf{W}_j\mathcal{T}$ and the i matrices $\boldsymbol{W}_j$, the cosets may alternatively be represented by the matrices $\boldsymbol{W}_j$. These matrices form a group of (finite) order i, and they describe linear mappings of the vector space $\mathbf{V}^n$ connected with E^n; *cf.* Section 8.1.2. This group (of order i) of linear mappings is the *point group $\mathcal{P}$ of the space group $\mathcal{G}$*, introduced above.

The difference between symmetry in point space and that in vector space may be exemplified again by means of some monoclinic space groups. Referred to conventional coordinate systems, space groups Pm, Pc, Cm and Cc have the same (3×3) matrices $\boldsymbol{W}_j$ of their symmetry operations. Thus, the point groups of all these space groups are of the same type m. The space groups themselves, however, show a rather different behaviour. In Pm and Cm reflections occur, whereas in Pc and Cc only glide reflections are present.

Remark: The usage of the term 'point group' in connection with space groups is rather unfortunate as the *point group of a space group* is *not* a group of motions of *point space* but a group acting on *vector space.* As a consequence, the point group of a space group may contain operations which do not occur in the space group at all. This is apparent from the example of monoclinic space groups above. Nevertheless, the term 'point group of a space group' is used here for historical reasons. A more adequate term would be 'vector point group' of a space group or a crystal. It must be mentioned that the term 'point group' is also used for the 'site-symmetry group', defined in Section 8.3.2. Site-symmetry groups are groups acting on point space.

It is of historic interest that the 32 types of three-dimensional crystallographic point groups were determined more than 50 years before the 230 (or 219) types of space group were known. The physical methods of the 19th century, *e.g.* the determination of the symmetry of the external shape or of tensor properties of a crystal, were essentially methods of determining the point group, not the space group of the crystal.

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8.2. Classifications of space groups, point groups and lattices

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8.2.1. Introduction

One of the main tasks of theoretical crystallography is to sort the infinite number of conceivable crystal patterns into a finite number of classes, where the members of each class have certain properties in common. In such a classification, each crystal pattern is assigned only to one class. The elements of a class are called equivalent, the classes being equivalence classes in the mathematical sense of the word. Sometimes the word 'type' is used instead of 'class'.

An important principle in the classification of crystals and crystal patterns is symmetry, in particular the space group of a crystal pattern. The different classifications of space groups discussed here are displayed in Fig. 8.2.1.1.

Classification of crystals according to symmetry implies three steps. First, criteria for the symmetry classes have to be defined. The second step consists of the derivation and complete listing of the possible symmetry classes. The third step is the actual assignment of the existing crystals to these symmetry classes. In this chapter, only the first step is dealt with. The space-group tables of this volume are the result of the second step. The third step is beyond the scope of this volume.

8.2.2. Space-group types

The finest commonly used classification of three-dimensional space groups, *i.e.* the one resulting in the highest number of classes, is the *classification into the* 230 *(crystallographic) space-group types.** The word 'type' is preferred here to the word 'class', since in crystallography 'class' is already used in the sense of 'crystal class', *cf.* Sections 8.2.3 and 8.2.4. The classification of space groups into space-group types reveals the common symmetry properties of all space groups belonging to one type. Such common properties of the space groups can be considered as 'properties of the space-group types'.

The practising crystallographer usually assumes the 230 space-group types to be known and to be described in this volume by representative data such as figures and tables. To the experimentally determined space group of a particular crystal structure, *e.g.* of pyrite FeS_2, the corresponding space-group type No. 205 ($Pa\bar{3} \equiv T_h^6$) of *International Tables* is assigned. Two space groups, *e.g.* those of FeS_2 and CO_2, belong to the same space-group type if their symmetries correspond to the same entry in *International Tables.*

The rigorous definition of the classification of space groups into space-group types can be given in a more geometric or a more algebraic way. Here matrix algebra will be followed, by which primarily the classification into the 219 so-called *affine space-group types* is obtained.† For this classification, each space group is referred to a primitive basis and an origin. In this case, the matrices $\boldsymbol{W}_j$ of the symmetry operations consist of integral coefficients and $\det(\boldsymbol{W}_j) = \pm 1$ holds. Two space groups $\mathcal{G}$ and $\mathcal{G}'$ are then represented by their $(n+1)\times(n+1)$ matrix groups $\{\mathbb{W}\}$ and $\{\mathbb{W}'\}$. These two matrix groups are now compared.

Definition: The space groups $\mathcal{G}$ and $\mathcal{G}'$ belong to the same *space-group type* if, for each primitive basis and each origin of $\mathcal{G}$, a primitive basis and an origin of $\mathcal{G}'$ can be found so that the matrix groups $\{\mathbb{W}\}$ and $\{\mathbb{W}'\}$ are identical. In terms of matrices, this can be expressed by the following definition:

Definition: The space groups $\mathcal{G}$ and $\mathcal{G}'$ *belong to the same space-group type* if an $(n+1)\times(n+1)$ matrix $\mathbb{P}$ exists, for which the matrix part $\boldsymbol{P}$ is an integral matrix with $\det(\boldsymbol{P}) = \pm 1$ and the column part $\boldsymbol{p}$ consists of real numbers, such that

$$\{\mathbb{W}'\} = \mathbb{P}^{-1}\{\mathbb{W}\}\mathbb{P} \qquad (8.2.2.1)$$

holds. The matrix part $\boldsymbol{P}$ of $\mathbb{P}$ describes the transition from the primitive basis of $\mathcal{G}$ to the primitive basis of $\mathcal{G}'$. The column part $\boldsymbol{p}$ of $\mathbb{P}$ expresses the (possibly) different origin choices for the descriptions of $\mathcal{G}$ and $\mathcal{G}'$.

Equation (8.2.2.1) is an equivalence relation for space groups. The corresponding classes are called *affine space-group types*. By this definition, one obtains 17 plane-group types for E^2 and 219 space-group types for E^3, see Fig. 8.2.1.1. Listed in the space-group

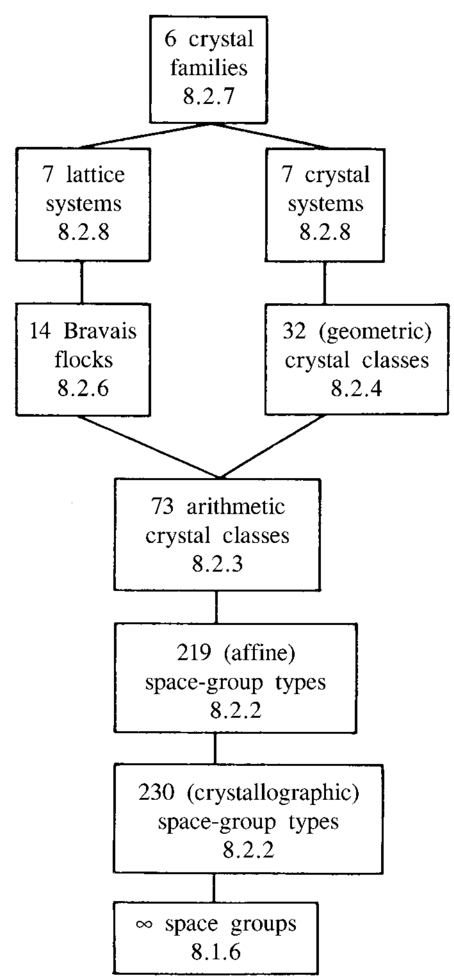

Fig. 8.2.1.1. Classifications of space groups. In each box, the number of classes, *e.g.* 32, and the section in which the corresponding term is defined, *e.g.* 8.2.4, are stated.

* These space-group types are often denoted by the word 'space group' when speaking of the 17 'plane groups' or of the 219 or 230 'space groups'. In a number of cases, the use of the same word 'space group' with two different meanings ('space group' and 'space-group type' which is an infinite set of space groups) is of no further consequence. In some cases, however, it obscures important relations. For example, it is impossible to appreciate the concept of isomorphic subgroups of a space group if one does not strictly distinguish between space groups and space-group types: *cf.* Section 8.3.3 and Part 13.

† According to the 'Theorem of Bieberbach', in all dimensions the classification into affine space-group types results in the same types as the classification into *isomorphism types of space groups*. Thus, the affine equivalence of different space groups can also be recognized by purely group-theoretical means: *cf.* Ascher & Janner (1965, 1968/69).

tables are 17 plane-group types for E^2 and 230 space-group types for E^3. Obviously, the equivalence definition of the space-group tables differs somewhat from the one used above. In practical crystallography, one wants to distinguish between right- and left-handed screws and does not want to change from a right-handed to a left-handed coordinate system. In order to avoid such transformations, the matrix $\boldsymbol{P}$ of equation (8.2.2.1) is restricted by the additional condition $\det(\boldsymbol{P}) = +1$. Using matrices $\mathbb{P}$ with $\det(\boldsymbol{P}) = +1$ only, 11 space-group types of E^3 split into pairs, which are the so-called pairs of *enantiomorphic space-group types*. The Hermann–Mauguin and Schoenflies symbols (in parentheses) of the pairs of enantiomorphic space-group types are $P4_1$–$P4_3$ (C_4^2–C_4^4), $P4_122$–$P4_322$ (D_4^3–D_4^7), $P4_12_12$–$P4_32_12$ (D_4^4–D_4^8), $P3_1$–$P3_2$ (C_3^2–C_3^3), $P3_121$–$P3_221$ (D_3^4–D_3^6), $P3_112$–$P3_212$ (D_3^3–D_3^5), $P6_1$–$P6_5$ (C_6^2–C_6^3), $P6_2$–$P6_4$ (C_6^4–C_6^5), $P6_122$–$P6_522$ (D_6^2–D_6^3), $P6_222$–$P6_422$ (D_6^4–D_6^5) and $P4_132$–$P4_332$ (O^7–O^6). In order to distinguish between the two definitions of space-group types, the first is called the classification into the 219 *affine space-group types* and the second the classification into the 230 *crystallographic* or *positive affine* or *proper affine space-group types*, see Fig. 8.2.1.1. Both classifications are useful.

In Section 8.1.6, symmorphic space groups were defined. It can be shown (with either definition of space-group type) that all space groups of a space-group type are symmorphic if one of these space groups is symmorphic. Therefore, it is also possible to speak of types of symmorphic and non-symmorphic space groups. In E^3, symmorphic space groups do not occur in enantiomorphic pairs. This does happen, however, in E^4.

The so-called space-group symbols are really symbols of 'crystallographic space-group types'. There are several different kinds of symbols (for details see Part 12). The *numbers* denoting the crystallographic space-group types and the *Schoenflies symbols* are unambiguous but contain little information. The *Hermann–Mauguin symbols* depend on the choice of the coordinate system but they are much more informative than the other notations.

8.2.3. Arithmetic crystal classes

As space groups not only of the same type but also of different types have symmetry properties in common, coarser classifications can be devised which are classifications of both space-group types and individual space groups. The following classifications are of this kind. Again each space group is referred to a *primitive* basis and an origin.

Definition: All those space groups belong to the same *arithmetic crystal class* for which the matrix parts are identical if suitable primitive bases are chosen, irrespective of their column parts.

Algebraically, this definition may be expressed as follows. Equation (8.2.2.1) of Section 8.2.2 relating space groups of the same type may be written more explicitly as follows:

$$\{(\boldsymbol{W}', \boldsymbol{w}')\} = \{[\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P}, \boldsymbol{P}^{-1}(\boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p})]\}, \qquad (8.2.3.1)$$

the matrix part of which is

$$\{\boldsymbol{W}'\} = \{\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P}\}. \qquad (8.2.3.2)$$

Space groups of different types belong to the same arithmetic crystal class if equation (8.2.3.2), but not equation (8.2.2.1) or equation (8.2.3.1), is fulfilled, *e.g.* space groups of types $P2$ and $P2_1$. This gives rise to the following definition:

Definition: Two space groups belong to the same *arithmetic crystal class* of space groups if there is an *integral* matrix $\boldsymbol{P}$ with $\det(\boldsymbol{P}) = \pm 1$ such that

$$\{\boldsymbol{W}'\} = \{\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P}\} \qquad (8.2.3.2)$$

holds.

By definition, both space groups and space-group types may be classified into arithmetic crystal classes. It is apparent from equation (8.2.3.2) that 'arithmetic equivalence' refers only to the matrix parts and not to the column parts of the symmetry operations. Among the space-group types of each arithmetic crystal class there is exactly one for which the column parts vanish for a suitable choice of the origin. This is the symmorphic space-group type, *cf.* Sections 8.1.6 and 8.2.2. The nomenclature for arithmetic crystal classes makes use of this relation: The lattice letter and the point-group part of the Hermann–Mauguin symbol for the symmorphic space-group type are interchanged to designate the arithmetic crystal class, *cf.* de Wolff *et al.* (1985). This symbolism enables one to recognize easily the arithmetic crystal class to which a space group belongs: One replaces in the Hermann–Mauguin symbol of the space group all screw rotations and glide reflections by the corresponding rotations and reflections and interchanges then the lattice letter and the point-group part.

Examples

The space groups with Hermann–Mauguin symbols $P2/m$, $P2_1/m$, $P2/c$ and $P2_1/c$ belong to the arithmetic crystal class $2/mP$, whereas $C2/m$ and $C2/c$ belong to the different arithmetic crystal class $2/mC$. The space groups with symbols $P31m$ and $P31c$ form the arithmetic crystal class $31mP$; those with symbols $P3m1$ and $P3c1$ form the different arithmetic crystal class $3m1P$. A further arithmetic crystal class, $3mR$, is composed of the space groups $R3m$ and $R3c$.

Remark: In order to belong to the same arithmetic crystal class, space groups must belong to the same geometric crystal class, *cf.* Section 8.2.4 and to the same Bravais flock; *cf.* Section 8.2.6. These two conditions, however, are only necessary but not sufficient.

There are 13 arithmetic crystal classes of plane groups in E^2 and 73 arithmetic crystal classes of space groups in E^3, see Fig. 8.2.1.1. Arithmetic crystal classes are rarely used in practical crystallography, even though they play some role in structural crystallography because the 'permissible origins' (see Giacovazzo, 2002) are the same for all space groups of one arithmetic crystal class. The classification of space-group types into arithmetic crystal classes, however, is of great algebraic consequence. In fact, the arithmetic crystal classes are the basis for the further classifications of space groups.

In E^3, enantiomorphic pairs of space groups always belong to the same arithmetic crystal class. Enantiomorphism of arithmetic crystal classes can be defined analogously to enantiomorphism of space groups. It does not occur in E^2 and E^3, but appears in spaces of higher dimensions, *e.g.* in E^4; *cf.* Brown *et al.* (1978).

In addition to space groups, equation (8.2.3.2) also classifies the set of all finite integral-matrix groups. Thus, one can speak of *arithmetic crystal classes of finite integral-matrix groups.* It is remarkable, however, that this classification of the matrix groups does *not* imply a classification of the corresponding point groups. Although *every* finite integral-matrix group represents the point group of some space group, referred to a primitive coordinate basis, there are *no* arithmetic crystal classes of point groups. For example, space-group types $P2$ and $C2$ both have point groups of the same type, 2, but referred to primitive bases their (3×3) matrix groups are not arithmetically equivalent, *i.e.* there is no integral matrix $\boldsymbol{P}$ with $\det(\boldsymbol{P}) = \pm 1$, such that equation (8.2.3.2) holds.

The arithmetic crystal classes of finite integral-matrix groups are the basis for the classification of lattices into Bravais types of lattices: see Section 8.2.5. Even though the consideration of finite integral-matrix groups in connection with space groups is not common in practical crystallography, these matrix groups play a very important role in the classifications discussed in subsequent sections. Finite integral-matrix groups have the advantage of being particularly suitable for computer calculations.

8.2.4. Geometric crystal classes

The widely used term 'crystal class' corresponds to the 'geometric crystal class' described in this section, and must be distinguished from the 'arithmetic' crystal class, introduced in Section 8.2.3. Geometric crystal classes classify the space groups *and* their point groups, *i.e.* the symmetry groups of the external shape of macroscopic crystals. Classification by morphological symmetry was done long before space groups were known. In Section 8.1.6, the reasons are stated why the two seemingly different classifications agree, namely that of space groups according to their matrix groups $\{\boldsymbol{W}\}$, and that of macroscopic crystals according to the 'point groups' of their sets of face normals.

To define geometric crystal classes, we again compare the matrix parts of the space groups.

Definition: All space groups belong to the same *geometric crystal class* for which the matrix parts are identical if suitable bases are chosen, irrespective of their column parts.

In contrast to the definition of arithmetic crystal classes, nonprimitive bases are admitted. To express this definition in matrix terms, we refer to equation (8.2.3.2) of the previous section.

Definition: Two space groups belong to the same *geometric crystal class* or *crystal class* if there is a *real* matrix $\boldsymbol{P}$ such that

$$\{\boldsymbol{W}'\} = \{\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P}\} \qquad (8.2.4.1)$$

holds.

In contrast to arithmetic crystal classes where $\boldsymbol{P}$ is a *unimodular integral* matrix, for geometric crystal classes only a *real* matrix $\boldsymbol{P}$ is required. Thus, the restriction $\det(\boldsymbol{P}) = \pm 1$ is no longer necessary, $\det(\boldsymbol{P})$ may have any value except zero.

Example

Referred to appropriate primitive bases, the matrix parts of mirror and glide reflections in space groups *Pm* and *Cm* are

$$\boldsymbol{W}_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \boldsymbol{W}_2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

respectively. There is no integral matrix $\boldsymbol{P}$ with $\det(\boldsymbol{P}) = \pm 1$ for which equation (8.2.3.2) holds because $\det(\boldsymbol{P}) = 2(P_{11}P_{22}P_{33} - P_{31}P_{22}P_{13})$.

Thus, *Pm* and *Cm* are members of different arithmetic crystal classes. The matrix

$$\boldsymbol{P} = \begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ with } \det(\boldsymbol{P}) = 2,$$

however, does solve equation (8.2.4.1) and, therefore, *Pm* and *Cm* are members of the same geometric crystal class, as are *Pc* and *Cc*.

Clearly, space groups of the same arithmetic crystal class always obey condition (8.2.4.1). Thus, the geometric crystal classes form a classification not only of space groups and space-group types but also of arithmetic crystal classes. There are ten geometric crystal classes in E^2 and 32 geometric crystal classes in E^3; see Fig. 8.2.1.1. As $\{(\boldsymbol{W})\}$ is a matrix representation of the point group of a space group, the definition may be restated as follows:

Definition: Two space groups $\mathcal{G}$ and $\mathcal{G}'$ belong to the same geometric crystal class if the matrix representations $\{\boldsymbol{W}\}$ and $\{\boldsymbol{W}'\}$ of their point groups are equivalent, *i.e.* if there is a real matrix $\boldsymbol{P}$ such that equation (8.2.4.1) holds.

This definition may also be used to classify point groups, *via* their matrix groups, into *geometric crystal classes of point groups*. Moreover, the geometric crystal classes provide a classification of the finite groups of integral matrices. Again, matrix groups of the same arithmetic crystal class always belong to the same geometric crystal class.

Enantiomorphism of geometric crystal classes may occur in dimensions greater than three, as it does for arithmetic crystal classes.

8.2.5. Bravais classes of matrices and Bravais types of lattices (*lattice types*)

Every space group $\mathcal{G}$ has a vector lattice $\mathbf{L}$ of translation vectors. The elements of the point group $\mathcal{P}$ of $\mathcal{G}$ are symmetry operations of $\mathbf{L}$. The lattice $\mathbf{L}$ of $\mathcal{G}$, however, may have additional symmetry in comparison with $\mathcal{P}$.

The symmetry of a vector lattice $\mathbf{L}$ is its point group according to the following definition:

Definition: The group $\mathcal{D}$ of *all* linear mappings which map a vector lattice $\mathbf{L}$ onto itself is called the *point group* or the *point symmetry of the lattice* $\mathbf{L}$. Those geometric crystal classes to which point symmetries of lattices belong are called *holohedries*.

The inversion $\mathbf{x} \to -\mathbf{x}$ is always a symmetry operation of $\mathbf{L}$, even if $\mathcal{G}$ does not contain inversions. If, for instance, $\mathcal{G}$ belongs to space-group type $P6_3mc$, its point group $\mathcal{P}$ is $6mm$ but the point symmetry $\mathcal{D}$ of $\mathbf{L}$ is $6/mmm$. Thus, the point group $\mathcal{D}$ of the lattice $\mathbf{L}$ is of higher order than the point group $\mathcal{P}$ of $\mathcal{G}$.

Other symmetry operations of $\mathbf{L}$ may also have no counterpart in $\mathcal{G}$. Space groups of type $P6_3/m$, for instance, have inversions but no reflections across 'vertical' mirror planes. The point symmetry of their lattices again is $6/mmm$, *i.e.* in this case too there are more elements in the point group $\mathcal{D}$ of $\mathbf{L}$ than in the point group $\mathcal{P}$ of $\mathcal{G}$.

For purposes of classification, lattices $\mathbf{L}$ will now be considered independently of their space groups $\mathcal{G}$. Associated with each vector lattice $\mathbf{L}$ is a finite group $\mathcal{L}$ of $(n \times n)$ integral matrices which describes the point group $\mathcal{D}$ of $\mathbf{L}$ with respect to some primitive basis of $\mathbf{L}$. This matrix group $\mathcal{L}$ is a member of an arithmetic crystal class; *cf.* Section 8.2.3. Thus, there are some arithmetic crystal classes with matrix groups $\mathcal{L}$ of lattices, *e.g.* the arithmetic crystal class $6/mmmP$. Other arithmetic crystal classes, however, are not associated with lattices, like $6/mP$ or $6mmP$. One can distinguish these two cases with the following definition:

Definition: An arithmetic crystal class with matrix groups $\mathcal{L}$ of lattices is called a Bravais arithmetic crystal class or a *Bravais class*.

By this definition, each lattice is associated with a Bravais class. On the other hand, each matrix group of a Bravais class represents the point group of a lattice referred to an appropriate primitive basis. Closer inspection shows that there are five Bravais classes of E^2 and 14 of E^3. With the use of Bravais classes, lattices may be classified using the following definition:

Definition: All those vector lattices belong to the same *Bravais type or lattice type of vector lattices*, for which the matrix groups belong to the same Bravais class.

Thus, five Bravais types of lattices exist in E^2, and 14 in E^3. This classification can be transferred from vector lattices $\mathbf{L}$ to point lattices L. To each point lattice L a vector lattice $\mathbf{L}$ is uniquely assigned. Thus, one can define Bravais types of point lattices *via* the Bravais types of vector lattices by the definition:

Definition: All those point lattices belong to the same *Bravais type of point lattices* for which the vector lattices belong to the same Bravais type of (vector) lattices.

Usually the Bravais types are called 'the five' or 'the 14 Bravais lattices' of E^2 or E^3. It must be emphasized, however, that 'Bravais lattices' are not individual lattices but types (or classes) of all lattices with certain common properties. Geometrically, these common properties are expressed by the 'centring type' and the well known relations between the lattice parameters, provided the lattices are referred to conventional bases, *cf.* Chapters 2.1 and 9.1. In these chapters a nomenclature of Bravais types is presented.

8.2.6. Bravais flocks of space groups

Another plausible classification of space groups and space-group types, as well as of arithmetic crystal classes, is based on the lattice of the space group. One is tempted to use the definition: 'Two space groups are members of the same class if their lattices belong to the same Bravais type'. There is, however, a difficulty which will become apparent by an example.

It was shown in Section 8.2.5 with the two examples of space groups $P6_3mc$ and $P6_3/m$ that the lattice $\mathbf{L}$ of the space group $\mathcal{G}$ may *systematically* have higher symmetry than the point group $\mathcal{P}$ of $\mathcal{G}$. The lattice $\mathbf{L}$, however, may also *accidentally* have higher symmetry than $\mathcal{P}$ because the lattice parameters may have special metrical values.

Example

For a monoclinic crystal structure at some temperature T_1, the monoclinic angle β may be equal to 91°, whereas, for the same monoclinic crystal structure at some other temperature T_2, $\beta = 90°$ may hold. In this case, the lattice $\mathbf{L}$ at temperature T_2, if considered to be detached from the crystal structure and its space group, has orthorhombic symmetry, because all the symmetry operations of an orthorhombic lattice map $\mathbf{L}$ onto itself. The lattice $\mathbf{L}$ at other temperatures, however, has always monoclinic symmetry.

This is of importance for the practising crystallographer, because quite often difficulties arise in the interpretation of X-ray powder diagrams if no single crystals are available. In some cases, changes of temperature or pressure may enable one to determine the true symmetry of the substance. The example shows, however, that the lattices of different space groups of the same space-group type *may* have different symmetries. The possibility of accidental lattice symmetry prevents the direct use of lattice types for a rigorous classification of space-group types.

Such a classification is possible, however, *via* the point group $\mathcal{P}$ of the space group $\mathcal{G}$ and its matrix groups. Referred to a primitive basis, the point group $\mathcal{P}$ of $\mathcal{G}$ is represented by a finite group of integral $(n \times n)$ matrices which belongs to some arithmetic crystal class. This matrix group can be uniquely assigned to a Bravais class: It either belongs already to a Bravais class, *e.g.* for space groups $Pmna$ and $C2/c$, or it may be uniquely connected to a Bravais class by the following two conditions:

(i) The matrix group of $\mathcal{P}$ is a subgroup of a matrix group of the Bravais class.

(ii) The order of the matrix group of the Bravais class is the smallest possible one compatible with condition (i).

Example

A space group of type $I4_1$ belongs to the arithmetic crystal class $4I$. The Bravais classes fulfilling condition (i) are $4/mmmI$ and $m\bar{3}mI$. With condition (ii), the Bravais class $m\bar{3}mI$ is excluded. Thus, the space group $I4_1$ is uniquely assigned to the Bravais class $4/mmmI$. Even though, with accidental lattice parameters $a = b = c = 5$ Å, the symmetry of the lattice alone is higher, namely $Im\bar{3}m$, this does not change the Bravais class of $I4_1$.

This assignment leads to the definition:

Definition: Space groups that are assigned to the same Bravais class belong to the same *Bravais flock of space groups.*

By this definition, the space group $I4_1$ mentioned above belongs to the Bravais flock of $4/mmmI$, despite the fact that the Bravais class of the lattice may be $m\bar{3}mI$ as a result of accidental symmetry.

Obviously, to each Bravais class a Bravais flock corresponds. Thus, there exist five Bravais flocks of plane groups and 14 Bravais flocks of space groups, see Fig. 8.2.1.1, and the Bravais flocks may be denoted by the symbols of the corresponding Bravais classes; *cf.* Section 8.2.5.

Though Bravais flocks themselves are of little practical importance, they are necessary for the definition of crystal families and lattice systems, as described in Sections 8.2.7 and 8.2.8.

8.2.7. Crystal families

Another classification of space groups, which is a classification of geometric crystal classes and Bravais flocks as well, is that into crystal families.

Definition: A *crystal family** is the smallest set of space groups containing, for any of its members, all space groups of the Bravais flock and all space groups of the geometric crystal class to which this member belongs.

Example

The space-group types $R3$ and $P6_1$ belong to the same crystal family because both $R3$ and $P3$ belong to the geometric crystal class 3, whereas both $P3$ and $P6_1$ are members of the same Bravais flock $6/mmmP$. In this example, $P3$ serves as a link between $R3$ and $P6_1$.

There are four crystal families in E^2 (oblique *m,* rectangular *o,* square *t* and hexagonal *h*) and six crystal families in E^3 [triclinic (anorthic) *a,* monoclinic *m,* orthorhombic *o,* tetragonal *t,* hexagonal *h* and cubic *c*]; see Fig. 8.2.1.1.

The classification into crystal families is a rather universal crystallographic concept as it applies to many crystallographic objects: space groups, space-group types, arithmetic and geometric crystal classes of space groups, point groups (morphology of crystals), lattices and Bravais types of lattices.

Remark: In most cases of E^2 and E^3, the lattices of a given crystal family of lattices have the same point symmetry (for the symbols, see Table 2.1.2.1): rectangular *op* and *oc* in E^2; monoclinic *mP* and *mS,* orthorhombic *oP*, *oS*, *oF* and *oI*, tetragonal *tP* and *tI*, cubic *cP*, *cF* and *cI* in E^3. Only to the hexagonal crystal family in E^3 do lattices with two different point symmetries belong: the hexagonal lattice type *hP* with point symmetry $6/mmm$ and the rhombohedral

* The classes defined here have been called 'crystal families' by Neubüser *et al.* (1971). For the same concept the term 'crystal system' has been used, particularly in American and Russian textbooks. In these *Tables,* however, 'crystal system' designates a different classification, described in Section 8.2.8. To avoid confusion, the term 'crystal family' is used here.

Table 8.2.8.1. *Distribution of trigonal and hexagonal space groups into crystal systems and lattice systems*

The hexagonal lattice system is also the hexagonal Bravais flock, the rhombohedral lattice system is the rhombohedral Bravais flock.

		Hexagonal lattice system	Rhombohedral lattice system
Crystal system	Crystal class	Hexagonal Bravais flock	Rhombohedral Bravais flock
Hexagonal	$6/mmm$	$P6/mmm$, $P6/mcc$, $P6_3/mcm$, $P6_3/mmc$	
	$\bar{6}2m$	$P\bar{6}m2$, $P\bar{6}c2$, $P\bar{6}2m$, $P\bar{6}2c$	
	$6mm$	$P6mm$, $P6cc$, $P6_3cm$, $P6_3mc$	
	622	$P622$, $P6_122$, …, $P6_322$	
	$6/m$	$P6/m$, $P6_3/m$	
	$\bar{6}$	$P\bar{6}$	
	6	$P6$, $P6_1$, $P6_5$, $P6_2$, $P6_4$, $P6_3$	
Trigonal	$\bar{3}m$	$P\bar{3}1m$, $P\bar{3}1c$, $P\bar{3}m1$, $P\bar{3}c1$	$R\bar{3}m$, $R\bar{3}c$
	$3m$	$P3m1$, $P31m$, $P3c1$, $P31c$	$R3m$, $R3c$
	32	$P312$, $P321$, $P3_112$, $P3_121$, $P3_212$, $P3_221$	$R32$
	$\bar{3}$	$P\bar{3}$	$R\bar{3}$
	3	$P3$, $P3_1$, $P3_2$	$R3$

lattice type *hR* with point symmetry $\bar{3}m$. In E^4 and higher dimensions, such cases are much more abundant.

Usually, the same type of coordinate system, the so-called 'conventional coordinate system', is used for all space groups of a crystal family, for instance 'hexagonal axes' for both hexagonal and rhombohedral lattices; *cf.* Chapters 2.1, 2.2 and 9.1. Other coordinate systems, however, may be used when convenient. To avoid confusion, the use of unconventional coordinate systems should be stated explicitly.

8.2.8. Crystal systems and lattice systems*

At least three different classifications of space groups, crystallographic point groups and lattice types have been called 'crystal systems' in crystallographic literature. Only one of them classifies space groups, crystallographic point groups *and* lattice types. It has been introduced in the preceding section under the name 'crystal families'. The two remaining classifications are called here 'crystal systems' and 'lattice systems', and are considered in this section. Crystal systems classify space groups and crystallographic point groups but *not* lattice types. Lattice systems classify space groups and lattice types but *not* crystallographic point groups.

The '*crystal-class systems*' or '*crystal systems*' are used in these *Tables*. In E^2 and E^3, the crystal systems provide the same classification as the crystal families, with the exception of the hexagonal crystal family in E^3. Here, the hexagonal family is subdivided into the *trigonal* and the *hexagonal* crystal system. Each of these crystal systems consists of complete geometric crystal classes of space groups. The space groups of the five trigonal crystal classes 3, $\bar{3}$, 32, $3m$ and $\bar{3}m$ belong to either the hexagonal or the rhombohedral Bravais flock, and both Bravais flocks are represented in each of these crystal classes. The space groups of the seven hexagonal crystal classes 6, $\bar{6}$, $6/m$, 622, $6mm$, $\bar{6}2m$ and $6/mmm$, however, belong only to the hexagonal Bravais flock.

These observations will be used to define crystal systems by the concept of intersection. A geometric crystal class and a Bravais flock of space groups are said to *intersect* if there is at least one space group common to both. Accordingly, the rhombohedral Bravais flock intersects all trigonal crystal classes but none of the hexagonal crystal classes. The hexagonal Bravais flock, on the other hand, intersects all trigonal *and* hexagonal crystal classes, see Table 8.2.8.1.

Using the concept of intersection, one obtains the definition:

Definition: A crystal-class system or a *crystal system* contains complete geometric crystal classes of space groups. All those geometric crystal classes belong to the same crystal system which intersect exactly the same set of Bravais flocks.

There are four crystal systems in E^2 and seven in E^3. The classification into crystal systems applies to space groups, space-group types, arithmetic crystal classes and geometric crystal classes, see Fig. 8.2.1.1. Moreover, *via* their geometric crystal classes, the crystallographic point groups are classified by 'crystal systems of point groups'. Historically, point groups were the first to be classified by crystal systems. Bravais flocks of space groups and Bravais types of lattices are not classified, as members of both can occur in more than one crystal system. For example, $P3$ and $P6_1$ belong to the same hexagonal Bravais flock but to different crystal systems, $P3$ to the trigonal, $P6_1$ to the hexagonal crystal system. Thus, a crystal system of space groups does not necessarily contain complete Bravais flocks (it does so, however, in E^2 and in all crystal systems of E^3, except for the trigonal and hexagonal systems).

The use of crystal systems has some practical advantages.

(i) Classical crystal physics considers physical properties of anisotropic continua. The symmetry of these properties as well as the symmetry of the external shape of a crystal are determined by point groups. Thus, crystal systems provide a classification for both tensor properties and morphology of crystals.

(ii) The 11 'Laue classes' determine both the symmetry of X-ray photographs (if Friedel's rule is valid) and the symmetry of the physical properties that are described by polar tensors of even rank and axial tensors of odd rank. Crystal systems classify Laue classes.

(iii) The correspondence between trigonal, tetragonal and hexagonal crystal classes becomes visible, as displayed in Table 10.1.1.2.

Whereas crystal systems classify geometric crystal classes and point groups, lattice systems classify Bravais flocks and Bravais types of lattices. Lattice systems may be defined in two ways. The first definition is analogous to that of crystal systems and uses once again the concept of intersection, introduced above.

Definition: A *lattice system* of space groups contains complete Bravais flocks. All those Bravais flocks which intersect exactly the same set of geometric crystal classes belong to the same lattice system, *cf.* footnote to heading of this section.

There are four lattice systems in E^2 and seven lattice systems in E^3. In E^2 and E^3, the classification into lattice systems is the same as that into crystal families and crystal systems except for the hexagonal crystal family of E^3. The space groups of the hexagonal Bravais flock (lattice letter *P*) belong to the twelve geometric crystal classes from 3 to $6/mmm$, whereas the space groups of the rhombohedral Bravais flock (lattice letter *R*) only belong to the five geometric crystal classes 3, $\bar{3}$, 32, $3m$ and $\bar{3}m$. Thus, these two Bravais flocks form the hexagonal and the rhombohedral lattice systems with 45 and 7 types of space groups, respectively.

The lattice systems provide a classification of space groups, see Fig. 8.2.1.1. Geometric crystal classes are not classified, as they can

* 'Lattice systems' were called 'Bravais systems' in editions 1 to 4 of this volume. The name has been changed because in practice 'Bravais systems' may be confused with 'Bravais types' or 'Bravais lattices'.

occur in more than one lattice system. For example, space groups $P3_1$ and $R3$, both of crystal class 3, belong to the hexagonal and rhombohedral lattice systems, respectively.

The above definition of lattice systems corresponds closely to the definition of crystal systems. There exists, however, another definition of lattice systems which emphasizes the geometric aspect more. For this it should be remembered that each Bravais flock is related to the point symmetry of a lattice type *via* its Bravais class; *cf.* Sections 8.2.5 and 8.2.6. It can be shown that Bravais flocks intersect the same set of crystal classes if their Bravais classes belong to the same (holohedral) geometric crystal class. Therefore, one can use the definition:

Definition: A *lattice system* of space groups contains complete Bravais flocks. All those Bravais flocks belong to the same lattice system for which the Bravais classes belong to the same (holohedral) geometric crystal class.

According to this second definition, it is sufficient to compare only the Bravais classes instead of all space groups of different Bravais flocks. The comparison of Bravais classes can be replaced by the comparison of their holohedries; *cf.* Section 8.2.5. This gives rise to a special advantage of lattice systems, the possibility of classifying lattices and lattice types. (Such a classification is not possible using crystal systems.) All those lattices belong to the same *lattice system of lattices* for which the lattice point groups belong to the same holohedry. As lattices of the same lattice type always belong to the same holohedry, lattice systems also classify lattice types.

The adherence of a space group of the hexagonal crystal family to the trigonal or hexagonal crystal system and the rhombohedral or hexagonal lattice system is easily recognized by means of its Hermann–Mauguin symbol. The Hermann–Mauguin symbols of the trigonal crystal system display a '3' or '$\bar{3}$', those of the hexagonal crystal system a '6' or '$\bar{6}$'. On the other hand, the rhombohedral lattice system displays lattice letter '*R*' and the hexagonal one '*P*' in the Hermann–Mauguin symbols of their space groups.

It should be mentioned that the lattice system of the lattice of a space group may be different from the lattice system of the space group itself. This always happens if the lattice symmetry is accidentally higher than is required by the space group, *e.g.* for a monoclinic space group with an orthorhombic lattice, *i.e.* $\beta = 90°$, or a tetragonal space group with cubic metrics, *i.e.* $c/a = 1$. These accidental lattice symmetries are special cases of *metrical pseudo-symmetries*. Owing to the anisotropy of the thermal expansion or the contraction under pressure, for special values of temperature and pressure singular lattice parameters may represent higher lattice symmetries than correspond to the symmetry of the crystal structure. The same may happen, and be much more pronounced, in continuous series of solid solutions owing to the change of cell dimensions with composition. Note that this phenomenon does not represent a new phase and a phase transition is not involved. Therefore, accidental lattice symmetries cannot be the basis for a classification in practice, *e.g.* for crystal structures or phase transitions. In contrast, *structural* pseudo-symmetries of crystals often lead to (displacive) phase transitions resulting in a new phase with higher structural *and* lattice symmetry.

In spite of its name, the classification of space groups into 'lattice systems of space groups' does *not* depend on the accidental symmetry of the translation lattice of a space group.

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8.3. Special topics on space groups

BY H. WONDRATSCHEK

8.3.1. Coordinate systems in crystallography

The matrices $\boldsymbol{W}$ and the columns $\boldsymbol{w}$ of crystallographic symmetry operations W depend on the choice of the coordinate system. A suitable choice is essential if $\boldsymbol{W}$ and $\boldsymbol{w}$ are to be obtained in a convenient form.

Example

In a space group $I4mm$, the matrix part of a clockwise fourfold rotation around the c axis is described by the $\boldsymbol{W}$ matrix

$$4^{-}\ 00z: \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

if referred to the *conventional* crystallographic basis **a**, **b**, **c**. Correspondingly, the matrix

$$m\ 0yz: \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

represents a reflection in a plane parallel to **b** and **c**. These matrices are easy to handle and their geometrical significance is evident. Referred to the *primitive* basis $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$, defined by $\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\mathbf{b}' = \frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\mathbf{c}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$, the matrices representing the same symmetry operations would be

$$4^{-}: \begin{pmatrix} 1 & 0 & -1 \\ 1 & 0 & 0 \\ 1 & -1 & 0 \end{pmatrix}; \quad m: \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & -1 \\ 1 & -1 & 0 \end{pmatrix}.$$

These matrices are more complicated to work with, and their geometrical significance is less obvious.

The conventional coordinate systems obey rules concerning the vector bases and the origins.

(i) In all cases, the *conventional* coordinate bases are chosen such that the matrices $\boldsymbol{W}$ only consist of the integers 0, +1 and −1, that they are reduced as much as possible, and that they are of simplest form, *i.e.* contain six or at least five zeros for three dimensions and two or at least one zeros for two dimensions. This fact can be expressed in geometric terms by stating that 'symmetry directions (*Blickrichtungen*) are chosen as coordinate axes' (axes of rotation, screw rotation or rotoinversion, normals of reflection or glide planes); *cf.* Section 2.2.4 and Chapter 9.1. Shortest translation vectors compatible with these conditions are chosen as basis vectors. In many cases, the conventional vector basis is not a primitive but rather a nonprimitive crystallographic basis, *i.e.* there are lattice vectors with fractional coefficients. The centring type of the conventional cell and thus the lattice type can be recognized from the first letter of the Hermann–Mauguin symbol.

Example

The letter P for E^3 (or p for E^2), taken from 'primitive', indicates that a primitive basis is being used conventionally for describing the crystal structure and its symmetry operations. In this case, the vector lattice **L** consists of all vectors $\mathbf{u} = u_1\mathbf{a}_1 + \ldots + u_n\mathbf{a}_n$ with integral coefficients u_i, but contains no other vectors. If the Hermann–Mauguin symbol starts with a 'C' in E^3 or with a 'c' in E^2, in addition to all such vectors **u** all vectors $\mathbf{u} + \frac{1}{2}(\mathbf{a}+\mathbf{b})$ also belong to **L**. The letters A, B, I, F and R are used for the conventional bases of the other types of lattices, *cf.* Section 1.2.1.

In a number of cases, the symmetry of the space group determines the conventional vector basis uniquely; in other cases, metrical criteria, *e.g.* the length of basis vectors, may be used to define a conventional vector basis.

(ii) The choice of the *conventional origin* in the space-group tables of this volume has been dealt with by Burzlaff & Zimmermann (1980). In general, the origin is a point of highest site symmetry, *i.e.* as many symmetry operations W_j as possible leave the origin fixed, and thus have $\boldsymbol{w}_j = \boldsymbol{o}$. Special reasons may justify exceptions from this rule, for example for space groups $I2_12_12_1 \equiv D_2^9$ (No. 24), $P4_332 \equiv O^6$ (No. 212), $P4_132 \equiv O^7$ (No. 213), $I4_132 \equiv O^8$ (No. 214) and $I\bar{4}3d \equiv T_d^6$ (No. 220); *cf.* Section 2.2.7. If in a centrosymmetric space group a centre of inversion is not a point of highest site symmetry, the space group is described twice, first with the origin in a point of highest site symmetry, and second with the origin in a centre of inversion, *e.g.* at 222 and at $\bar{1}$ for space group $Pnnn \equiv D_{2h}^2$ (No. 48); *cf.* Section 2.2.1.* For space groups with low site symmetries, the origin is chosen so as to minimize the number of nonzero coefficients of the w_j, *e.g.* on a twofold screw axis for space group $P2_1 \equiv C_2^2$ (No. 4).

A change of the coordinate system, *i.e.* referring the crystal pattern and its symmetry operations W to a new coordinate system, results in new coordinates $\mathbb{X}'$ and new matrices $\mathbb{W}'$; *cf.* Section 5.1.3.

8.3.2. (Wyckoff) positions, site symmetries and crystallographic orbits

The concept of *positions* and their *site symmetries* is fundamental for the determination and description of crystal structures. Let, for instance, $P\bar{1}$ be the space group of a crystal structure with tetrahedral AX_4 and triangular BY_3 groups. Then the atoms A and B cannot be located at centres of inversion, as the symmetry of tetrahedra and triangles is incompatible with site symmetry $\bar{1}$. If the space group is $P2/m$, again the points with site symmetry $2/m$ cannot be the loci of A or B, but points with site symmetries 2, m or 1 can.

The relations between 'site symmetry' and 'positions' can be formulated in a rather general way.

Definition: The set of all symmetry operations of a space group $\mathcal{G}$ that leave a point X invariant forms a finite group, the *site-symmetry group* $\mathcal{S}(X)$ of X with respect to $\mathcal{G}$.†

With regard to the symmetry operations of a space group $\mathcal{G}$, two kinds of points are to be distinguished. A point X is called a *point of general position* with respect to a space group $\mathcal{G}$ if there is no symmetry operation of $\mathcal{G}$ (apart from the identity operation) that leaves X fixed, *i.e.* if $\mathcal{S}(X) = \mathcal{I}$. A point X is called a *point of special position* with respect to a space group $\mathcal{G}$ if there is at least one other symmetry operation of $\mathcal{G}$, in addition to the identity operation, that leaves X fixed, *i.e.* if $\mathcal{S}(X) > \mathcal{I}$.

The subdivision of the set of all points into two classes, those of general and those of special position with respect to a space group

* Also space group $P4_2/ncm \equiv D_{4h}^{16}$ (No. 138) is listed with two origins. The first origin is chosen at a point with site symmetry $\bar{4}$ as in Hermann (1935). The site symmetries $(2/m)$ of the centres of inversion have the same order 4.

† Instead of 'site-symmetry group', the term 'point group' is frequently used for the local symmetry in a crystal structure or for the symmetry of a molecule. In order to avoid confusion, in this chapter the term 'point group' is exclusively used for the symmetry of the external shape and of the physical properties of the macroscopic crystal, *i.e.* for a symmetry in vector space.

$\mathcal{G}$, constitutes only a very coarse classification. A finer classification is obtained as follows.

Definition: A *Wyckoff position* $\mathsf{W}_{\mathcal{G}}$ (for short, position; in German, *Punktlage*) consists of all points X for which the site-symmetry groups $\mathcal{S}(X)$ are conjugate subgroups* of $\mathcal{G}$.

For practical purposes, each Wyckoff position of a space group is labelled by a letter which is called the *Wyckoff letter* (*Wyckoff notation* in earlier editions of these *Tables*). Wyckoff positions *without* variable *parameters* (*e.g.* $0,0,0; 0,0,\frac{1}{2};\ldots$) and *with* variable *parameters* (*e.g.* $x,y,z; x,0,\frac{1}{4};\ldots$) have to be distinguished.

The number of different Wyckoff positions of each space group is finite, the maximal numbers being nine for plane groups (realized in *p*2*mm*) and 27 for space groups (realized in *Pmmm*).

A finer classification of the points of E^n with respect to $\mathcal{G}$, which always results in an infinite number of classes, is the subdivision of all points into sets of symmetrically equivalent points. In the following, these sets will be called crystallographic orbits according to the following definition.

Definition: The set of all points that are symmetrically equivalent to a point X with respect to a space group $\mathcal{G}$ is called the *crystallographic orbit* of X with respect to $\mathcal{G}$.

Example

Described in a conventional coordinate system, the crystallographic orbit of a point X of general position with respect to a plane group *p*2 consists of the points x,y; $\bar{x},\bar{y}$; $x+1,y$; $\bar{x}+1,\bar{y}$; $x, y+1$; $\bar{x}, \bar{y}+1$; $x-1, y$; $\bar{x}-1, \bar{y}$; $x, y-1$; $\bar{x}, \bar{y}-1$; $x+1, y+1$; ... *etc.*

Crystallographic orbits are infinite sets of points due to the infinite number of translations in each space group. Any one of its points may represent the whole crystallographic orbit, *i.e.* may be the generating point X of a crystallographic orbit.†

Because the site-symmetry groups of different points of the same crystallographic orbit are conjugate subgroups of $\mathcal{G}$, a crystallographic orbit consists either of points of general position or of points of special position only. Therefore, one can speak of 'crystallographic orbits of general position' or *general crystallographic orbits* and of 'crystallographic orbits of special position' or *special crystallographic orbits* with respect to $\mathcal{G}$. Because all points of a crystallographic orbit belong to the same Wyckoff position of $\mathcal{G}$, one also can speak of *Wyckoff positions of crystallographic orbits.*‡

The points of each *general crystallographic orbit* of a space group $\mathcal{G}$ are in a one-to-one correspondence with the symmetry operations of $\mathcal{G}$. Starting with the generating point X (to which the identity operation corresponds), to each point $\tilde{X}$ of the crystallographic orbit belongs exactly one symmetry operation W of $\mathcal{G}$ such that $\tilde{X}$ is the image of X under W. This one-to-one correspondence is the reason why the 'coordinates' listed for the general position in the space-group tables may be interpreted in two different ways, either as the coordinates of the image points of X under $\mathcal{G}$ or as a short-hand notation for the pairs $(\boldsymbol{W}, \boldsymbol{w})$ of the symmetry operations W of $\mathcal{G}$; *cf.* Sections 8.1.6 and 11.1.1. Such a one-to-one correspondence does not exist for the *special crystallographic orbits*, where each point corresponds to a complete coset of a left coset decomposition of $\mathcal{G}$ with respect to the site-symmetry group $\mathcal{S}(X)$ of X. Thus, the data listed for the special positions are to be understood only as the coordinates of the image points of X under $\mathcal{G}$.

Space groups with no special crystallographic orbits are called *fixed-point-free space groups.* The following types of fixed-point-free space groups occur: *p*1 and *pg* in E^2; $P1 \equiv C_1^1$ (No. 1), $P2_1 \equiv C_2^2$ (No. 4), $Pc \equiv C_s^2$ (No. 7), $Cc \equiv C_s^4$ (No. 9), $P2_12_12_1 \equiv D_2^4$ (No. 19), $Pca2_1 \equiv C_{2v}^5$ (No. 29), $Pna2_1 \equiv C_{2v}^9$ (No. 33), $P4_1 \equiv C_4^2$ (No. 76), $P4_3 \equiv C_4^4$ (No. 78), $P3_1 \equiv C_3^2$ (No. 144), $P3_2 \equiv C_3^3$ (No. 145), $P6_1 \equiv C_6^2$ (No. 169) and $P6_5 \equiv C_6^3$ (No. 170) in E^3.

Though the classification of the points of space E^n into Wyckoff positions $\mathsf{W}_{\mathcal{G}}$ of a space group $\mathcal{G}$ is unique, the labelling of the Wyckoff positions by Wyckoff letters (Wyckoff notation) is not.

Example

In a space group $P\bar{1}$ there are eight classes of centres of inversion $\bar{1}$, represented in the space-group tables by $0,0,0$; $0,0,\frac{1}{2}$; $0,\frac{1}{2},0;\ldots;\frac{1}{2},\frac{1}{2},\frac{1}{2}$. The site-symmetry groups $\{\mathsf{I},\bar{1}\}$ *within* each class are 'symmetrically equivalent', *i.e.* they are conjugate subgroups of $P\bar{1}$. The groups $\{\mathsf{I},\bar{1}\}$ of *different* classes, however, are *not* 'symmetrically equivalent' with respect to $P\bar{1}$. Each class is labelled by one of the Wyckoff letters $a, b, \ldots, h$. This letter depends on the choice of origin and on the choice of coordinate axes. Cyclic permutation of the labels of the basis vectors **a**, **b**, **c**, for instance, induces a cyclic permutation of Wyckoff positions *b*–*c*–*d* and *e*–*f*–*g*; origin shift from 0, 0, 0 to the point $\frac{1}{2},0,0$ results in an exchange of Wyckoff letters in the pairs *a*–*d*, *b*–*f*, *c*–*e* and *g*–*h*. Even if the coordinate axes are determined by some extra condition, *e.g.* $a \le b \le c$, there exist no rules for fixing the origin in $P\bar{1}$ when describing a crystal structure. The eight classes of centres of inversion of $P\bar{1}$ are well established but none of them is inherently distinguished from the others.

The example shows that the different Wyckoff positions of a space group $\mathcal{G}$ may permute under an isomorphic mapping of $\mathcal{G}$ onto itself, *i.e.* under an automorphism of $\mathcal{G}$. Accordingly, it is useful to collect into one set all those Wyckoff positions of a space group $\mathcal{G}$ that may be permuted by automorphisms of $\mathcal{G}$. These sets are called 'Wyckoff sets'. The Wyckoff letters belonging to the different Wyckoff positions of the same Wyckoff set are listed by Koch & Fischer (1975); changes in Wyckoff letters caused by changes of the coordinate system have been listed by Boyle & Lawrenson (1973, 1978).

To introduce 'Wyckoff sets' more formally, it is advantageous to use the concept of normalizers; *cf.* Ledermann (1976). The *affine normalizer* $\mathcal{N}$§ of a space group $\mathcal{G}$ in the group $\mathcal{A}$ of all affine mappings is the set of those affine mappings which map $\mathcal{G}$ onto itself. The space group $\mathcal{G}$ is a normal subgroup of $\mathcal{N}$, $\mathcal{N}$ itself is a subgroup of $\mathcal{A}$. The mappings of $\mathcal{N}$ which are not symmetry operations of $\mathcal{G}$ may transfer one Wyckoff position of $\mathcal{G}$ onto another Wyckoff position.

Definition: Let $\mathcal{N}$ be the normalizer of a space group $\mathcal{G}$ in the group of all affine mappings. A *Wyckoff set* with respect to $\mathcal{G}$ consists of all points X for which the site-symmetry groups are conjugate subgroups of $\mathcal{N}$.

The difference between Wyckoff positions and Wyckoff sets of $\mathcal{G}$ may be explained as follows. Any Wyckoff position of $\mathcal{G}$ is transformed onto itself by all elements of $\mathcal{G}$, but not necessarily by the elements of the (larger) group $\mathcal{N}$. Any Wyckoff set, however, is

* For the term 'conjugate subgroups', see Section 8.3.6.

† For the crystallographic orbits different names have been used by different authors: *regelmässiges Punktsystem*, Sohncke (1879) and Schoenflies (1891); *regular system of points,* Fedorov (1891); *Punktkonfiguration*, Fischer & Koch (1974); *orbit*, Wondratschek (1976); *point configuration*, Fischer & Koch (1978) and Part 14 of this volume; *crystallographic orbit,* Matsumoto & Wondratschek (1979) and Wondratschek (1980).

‡ Fischer & Koch (1974) use the name *Punktlage.*

§ Section 8.3.6 and Part 15 deal with normalizers of space groups in more detail.

transformed onto itself even by those elements of $\mathcal{N}$ which are not contained in $\mathcal{G}$.

Remark: A Wyckoff set of $\mathcal{G}$ is a set of points. Obviously, with each point X it contains all points of the crystallographic orbit of X and all points of the Wyckoff position of X. Accordingly, one can speak not only of 'Wyckoff sets of points', but also of 'Wyckoff sets of crystallographic orbits' and 'Wyckoff sets of Wyckoff positions' of $\mathcal{G}$. Wyckoff sets of crystallographic orbits have been used in the definition of lattice complexes (*Gitterkomplexe*), under the name *Konfigurationslage,* by Fischer & Koch (1974); *cf.* Part 14.

The concepts 'crystallographic orbit', 'Wyckoff position' and 'Wyckoff set' have so far been defined for individual space groups only. It is no problem, but is of little practical interest, to transfer the concept of 'crystallographic orbit' to space-group types. It would be, on the other hand, of great interest to transfer 'Wyckoff positions' from individual space groups to space-group types. As mentioned above, however, such a step is not unique. For this reason, the concept of 'Wyckoff set' has been introduced to replace 'Wyckoff positions'. Different space groups of the same space-group type have corresponding Wyckoff sets, and one can define 'types of Wyckoff sets' (consisting of individual Wyckoff sets) in the same way that 'types of space groups' (consisting of individual space groups) were defined in Section 8.2.2.

Definition: Let the space groups $\mathcal{G}$ and $\mathcal{G}'$ belong to the same space-group type. The Wyckoff sets K of $\mathcal{G}$ and K' of $\mathcal{G}'$ belong to the same *type of Wyckoff sets* if the affine mappings which transform $\mathcal{G}$ onto $\mathcal{G}'$ also transform K onto K'.

Types of Wyckoff sets have been used by Fischer & Koch (1974), under the name *Klasse von Konfigurationslagen*, when defining lattice complexes. There are 1128 types of Wyckoff sets of the 219 (affine) space-group types and 51 types of Wyckoff sets of the 17 plane-group types [Koch & Fischer (1975) and Chapter 14.1].

8.3.3. Subgroups and supergroups of space groups

Relations between crystal structures imply relations between their space groups, which can often be expressed by group–subgroup relations. These group–subgroup relations may be recognized from relations between the lattices and between the point groups of the crystal structures.

Example

The crystal structures of silicon, Si, and sphalerite, ZnS, belong to space-group types $Fd\bar{3}m \equiv O_h^7$ (No. 227) and $F\bar{4}3m \equiv T_d^2$ (No. 216) with lattice constants $a_{\rm Si} = 5.43$ and $a_{\rm ZnS} = 5.41$ Å. The structure of sphalerite is obtained from that of silicon by replacing alternately half of the Si atoms by Zn and half by S, and by adjusting the lattice constant. The strong connection between the two crystal structures is reflected in the relation between their space groups: the space group of sphalerite is a subgroup (of index 2) of that of silicon (ignoring the small difference in lattice constants).

Data on sub- and supergroups of the space groups are useful for the discussion of structural relations and phase transitions. It must be kept in mind, however, that group–subgroup relations only describe symmetry relations. It is important, therefore, to ascertain that the consequential relations between the atomic coordinates of the particles of the crystal structures also hold, before a structural relation can be deduced from a symmetry relation.

Examples

NaCl and CaF_2 belong to the same space-group type $Fm\bar{3}m \equiv O_h^5$ (No. 225) and have lattice constants $a = 5.64$ and $a = 5.46$ Å, respectively. The ions, however, occupy unrelated positions and so the symmetry relation does not express a structural relation. Pyrite, FeS_2, and solid carbon dioxide, CO_2, belong to the same space-group type $Pa\bar{3} \equiv T_h^6$ (No. 205). They have lattice constants $a = 5.42$ and $a = 5.55$ Å, respectively, and the particles occupy analogous Wyckoff positions. Nevertheless, the structures of these compounds are not related because the positional parameters $x = 0.386$ of S in FeS_2 and $x = 0.11$ of O in CO_2 differ so much that the coordinations of corresponding atoms are dissimilar.

To formulate group–subgroup relations some definitions are necessary:

Definitions: A set $\{\mathsf{H}_i\}$ of symmetry operations H_i of a space group $\mathcal{G}$ is called a *subgroup* $\mathcal{H}$ of $\mathcal{G}$ if $\{\mathsf{H}_i\}$ obeys the group conditions, *i.e.* is a symmetry group. The subgroup $\mathcal{H}$ is called a *proper subgroup* of $\mathcal{G}$ if there are symmetry operations of $\mathcal{G}$ not contained in $\mathcal{H}$. A subgroup $\mathcal{H}$ of a space group $\mathcal{G}$ is called a *maximal subgroup* of $\mathcal{G}$ if there is no proper subgroup $\mathcal{M}$ of $\mathcal{G}$ such that $\mathcal{H}$ is a proper subgroup of $\mathcal{M}$, *i.e.* $\mathcal{G} > \mathcal{M} > \mathcal{H}$.

Examples: Maximal subgroups $\mathcal{H}$ of a space group $P1$ with lattice vectors **a**, **b**, **c** are, among others, subgroups $P1$ for which $\mathbf{a}'' = p\mathbf{a}$, $\mathbf{b}'' = \mathbf{b}$, $\mathbf{c}'' = \mathbf{c}$, p prime. If p is not a prime number, *e.g.* $p = q \cdot r$, the subgroup $\mathcal{H}$ is not maximal, because a proper subgroup $\mathcal{M}$ exists with $\mathbf{a}' = q\mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$. $\mathcal{M}$ again has $\mathcal{H}$ as a proper subgroup with $\mathbf{a}'' = r\mathbf{a}'$, $\mathbf{b}'' = \mathbf{b}'$, $\mathbf{c}'' = \mathbf{c}'$.

$P2_1/c$ has maximal subgroups $P2_1$, Pc and $P\bar{1}$ with the same unit cell, whereas $P1$ is obviously not a maximal subgroup of $P2_1/c$.

A three-dimensional space group may have subgroups with no translations (site-symmetry groups; *cf.* Section 8.3.2), with one- or two-dimensional lattices of translations (line groups, frieze groups, rod groups, plane groups and layer groups), or with a three-dimensional lattice of translations (space groups). The number of subgroups of a space group is always infinite.

In this section, only those subgroups of a space group will be considered which are also space groups. This includes all maximal subgroups because a maximal subgroup of a space group is itself a space group. To simplify the discussion, we suppose the set of all *maximal* subgroups of every space group to be known. In this case, *any* subgroup $\mathcal{H}$ of a given space group $\mathcal{G}$ may be obtained *via* a chain of maximal subgroups $\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_{r-1}, \mathcal{H}_r = \mathcal{H}$ such that $\mathcal{G} = \mathcal{H}_0 > \mathcal{H}_1 > \mathcal{H}_2 > \ldots > \mathcal{H}_{r-1} > \mathcal{H}_r = \mathcal{H}$ where $\mathcal{H}_j$ is a maximal subgroup of $\mathcal{H}_{j-1}$ of index $[i_j]$, with $j = 1, \ldots, r$; for the term 'index' see below and Section 8.1.6. There may be many such chains between $\mathcal{G}$ and $\mathcal{H}$. On the other hand, all subgroups of $\mathcal{G}$ of a given index $[i]$ are obtained if all chains are constructed for which $[i_1] * [i_2] * \ldots * [i_r] = [i]$ holds.

For example, $P2/c > P2 > P1$, $P2/c > P\bar{1} > P1$, $P2/c > Pc > P1$ are all possible chains of maximal subgroups for $P2/c$ if the original translations are retained completely. The seven subgroups of index [4] with the same translations as the original space group $P6_3/mcm$ are obtained *via* the 21 different chains of Fig. 8.3.3.1.

Not only the number of all subgroups but even the number of all maximal subgroups of a given space group is infinite. This infinite number, however, only occurs for a certain kind of subgroup and can be reduced as described below. It is thus useful to consider the different kinds of subgroups of a space group in a way introduced by Hermann (1929).

It should be kept in mind that all group–subgroup relations considered here are relations between individual space groups but they are valid for all space groups of a space-group type, as the following example shows. A particular space group $P2$ has a subgroup $P1$ which is obtained from $P2$ by retaining all translations

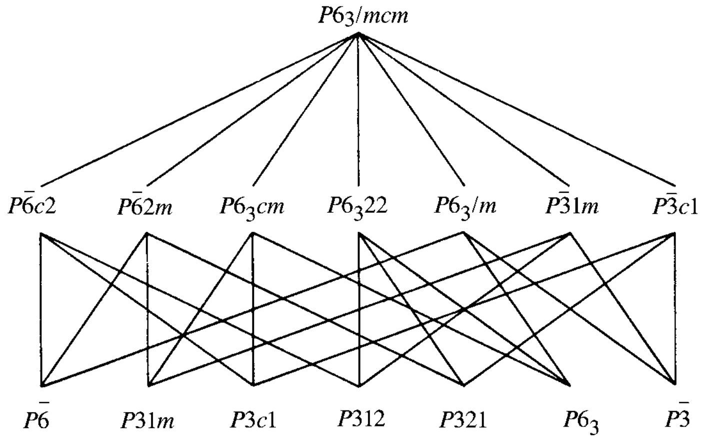

Fig. 8.3.3.1. Space group $P6_3/mcm$ with t subgroups of index [2] and [4]. All 21 possible subgroup chains are displayed by lines.

but eliminating all rotations and combinations of rotations with translations. For every space group of space-group type $P2$ such a subgroup $P1$ exists. Thus the relationship exists, in an extended sense, for the two space-group types involved. One can, therefore, list these relationships by means of the symbols of the space-group types.

For every subgroup $\mathcal{H}$ of a space group $\mathcal{G}$, a 'right coset decomposition' of $\mathcal{G}$ relative to $\mathcal{H}$ can be defined as

$$\mathcal{G} = \mathcal{H} + \mathcal{H}\mathsf{G}_2 + \ldots + \mathcal{H}\mathsf{G}_i.$$

The elements $\mathsf{G}_2, \ldots, \mathsf{G}_i$ of $\mathcal{G}$ are such that G_j is contained only in the coset $\mathcal{H}\mathsf{G}_j$. The integer $[i]$, *i.e.* the number of cosets, is called the index of $\mathcal{H}$ in $\mathcal{G}$; *cf.* Section 8.1.6, footnote §.

The index $[i]$ of a subgroup has a geometric significance. It determines the 'dilution' of symmetry operations of $\mathcal{H}$ compared with those of $\mathcal{G}$. This dilution can occur in essentially three different ways:

(i) by reducing the order of the point group, *i.e.* by eliminating all symmetry operations of some kind. The example $P2 \rightarrow P1$ mentioned above is of this type.

(ii) by loss of translations, *i.e.* by 'thinning out' the lattice of translations. For the space group $P121$ mentioned above this may happen in different ways:

(*a*) by suppressing all translations of the kind $(2u+1)\mathbf{a} + v\mathbf{b} + w\mathbf{c}$, u, v, w integral (new basis $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$), and, hence, by eliminating half of the twofold axes, or

(*b*1) by $\mathbf{b}' = 2\mathbf{b}$, *i.e.* by thinning out the translations parallel to the twofold axes, or

(*b*2) again by $\mathbf{b}' = 2\mathbf{b}$ but replacing the twofold rotation axes by twofold screw axes.

(iii) by combination of (i) and (ii), *e.g.* by reducing the order of the point group *and* by thinning out the lattice of translations.

Subgroups of the first kind (i) are called *translationengleiche* or *t* subgroups* because the set $\mathcal{T}$ of all (pure) translations is retained. In case (ii), the point group $\mathcal{P}$ and thus the crystal class of the space group is unchanged. These subgroups are called *klassengleiche* or *k* subgroups. In the general case (iii), both the translation subgroup $\mathcal{T}$ of $\mathcal{G}$ and the point group $\mathcal{P}$ are changed; the subgroup has lost translations *and* belongs to a crystal class of lower order.

* Hermann (1929) used the term *zellengleich* but this term caused misunderstandings because it was sometimes understood to refer to the conventional unit cell. Not the conservation of the conventional unit cell but rather the retention of *all* translations of the space group is the essential feature of *t* subgroups.

Obviously the third kind (iii) of subgroups is more difficult to survey than kinds (i) and (ii). Fortunately, a theorem of Hermann states that the maximal subgroups of a space group $\mathcal{G}$ are of type (i) or (ii).

Theorem of Hermann (1929). A maximal subgroup of a space group $\mathcal{G}$ is either a t subgroup or a k subgroup of $\mathcal{G}$.

According to this theorem, subgroups of kind (iii) can never occur among the maximal subgroups. They can, however, be derived by a stepwise process of linking maximal subgroups of types (i) and (ii), as has been shown by the chains discussed above.

8.3.3.1. *Translationengleiche or t subgroups of a space group*

The 'point group' $\mathcal{P}$ of a given space group $\mathcal{G}$ is a finite group. Hence, the number of subgroups and consequently the number of maximal subgroups of $\mathcal{P}$ is finite. There exist, therefore, only a finite number of maximal t subgroups of $\mathcal{G}$. *All* maximal t subgroups of every space group $\mathcal{G}$ are listed in the space-group tables of this volume; *cf.* Section 2.2.15. The possible t subgroups were first listed by Hermann (1935); corrections have been reported by Ascher *et al.* (1969).

8.3.3.2. *Klassengleiche or k subgroups of a space group*

Every space group $\mathcal{G}$ has an infinite number of maximal k subgroups. For dimensions 1, 2 and 3, however, it can be shown that the number of maximal k subgroups is finite, if subgroups belonging to the same affine space-group type as $\mathcal{G}$ are excluded. The number of maximal subgroups of $\mathcal{G}$ belonging to the same affine space-group type as $\mathcal{G}$ is always infinite. These subgroups are called *maximal isomorphic subgroups*. In Part 13 isomorphic subgroups are treated in detail. In the space-group tables, only data on the isomorphic subgroups of lowest index are listed. The way in which the isomorphic and non-isomorphic k subgroups are listed in the space-group tables is described in Section 2.2.15.

Remark: Enantiomorphic space groups have an infinite number of maximal isomorphic subgroups of the same type *and* an infinite number of maximal isomorphic subgroups of the enantiomorphic type.

Example

All k subgroups $\mathcal{G}'$ of a given space group $\mathcal{G} \equiv P3_1$, with basis vectors $\mathbf{a}' = \mathbf{a}, \mathbf{b}' = \mathbf{b}, \mathbf{c}' = p\mathbf{c}, p$ being any prime number except 3, are maximal isomorphic subgroups. They belong to space-group type $P3_1$ if $p = 3r + 1, r$ any integer. They belong to the enantiomorphic space-group type $P3_2$ if $p = 3r + 2$.

Even though in the space-group tables some kinds of maximal subgroups are listed completely whereas others are listed only partly, it must be emphasized that in principle there is no difference in importance between t, non-isomorphic k and isomorphic k subgroups. Roughly speaking, a group–subgroup relation is 'strong' if the index $[i]$ of the subgroup is low. All maximal t and maximal non-isomorphic k subgroups have indices less than four in E^2 and five in E^3, index four already being rather exceptional. Maximal isomorphic k subgroups of arbitrarily high index exist for every space group.

8.3.3.3. *Supergroups*

Sometimes a space group $\mathcal{H}$ is known and the possible space groups $\mathcal{G}$, of which $\mathcal{H}$ is a subgroup, are of interest.

Definition: A space group $\mathcal{R}$ is called a *minimal supergroup* of a space group $\mathcal{G}$ if $\mathcal{G}$ is a maximal subgroup of $\mathcal{R}$.

Examples

In Fig. 8.3.3.1, the space group $P6_3/mcm$ is a minimal supergroup of $P\bar{6}c2, \ldots, P\bar{3}c1$; $P\bar{6}c2$ is a minimal supergroup of $P\bar{6}, P3c1$ and $P312$; *etc.*

If $\mathcal{G}$ is a maximal t subgroup of $\mathcal{R}$ then $\mathcal{R}$ is a minimal t supergroup of $\mathcal{G}$. If $\mathcal{G}$ is a maximal k subgroup of $\mathcal{R}$ then $\mathcal{R}$ is a minimal k supergroup of $\mathcal{G}$. Finally, if $\mathcal{G}$ is a maximal isomorphic subgroup of $\mathcal{R}$, then $\mathcal{R}$ is a minimal isomorphic supergroup of $\mathcal{G}$. Data on minimal t and minimal non-isomorphic k supergroups are listed in the space-group tables; *cf.* Section 2.2.15. Data on minimal isomorphic supergroups are not listed because they can be derived easily from the corresponding subgroup relations.

The complete data on maximal subgroups of plane and space groups are listed in Volume A1 of *International Tables for Crystallography* (2004). For each space group, all maximal subgroups of index [2], [3] and [4] are listed individually. The infinitely many maximal isomorphic subgroups are listed as members of a few (infinite) series. The main parameter in these series is the index p, p^2 or p^3, where p runs through the infinite number of primes.

8.3.4. Sequence of space-group types

The sequence of space-group entries in the space-group tables follows that introduced by Schoenflies (1891) and is thus established historically. Within each geometric crystal class, Schoenflies has numbered the space-group types in an obscure way. As early as 1919, Niggli (1919) considered this Schoenflies sequence to be unsatisfactory and suggested that another sequence might be more appropriate. Fedorov (1891) used a different sequence in order to distinguish between symmorphic, hemisymmorphic and asymmorphic space groups.

The basis of the Schoenflies symbols and thus of the Schoenflies listing is the geometric crystal class. For the present *Tables*, a sequence might have been preferred in which, in addition, space-group types belonging to the same arithmetic crystal class were grouped together. It was decided, however, that the long-established sequence in the earlier editions of *International Tables* should not be changed.

In Table 8.3.4.1, those geometric crystal classes are listed in which the Schoenflies sequence separates space groups belonging to the same arithmetic crystal class. The space groups are rearranged in such a way that space groups of the same arithmetic crystal class are grouped together. The arithmetic crystal classes are separated by broken lines, the geometric crystal classes by full lines. In all cases not listed in Table 8.3.4.1, the Schoenflies sequence, as used in these *Tables,* does not break up arithmetic crystal classes. Nevertheless, some rearrangement would be desirable in other arithmetic crystal classes too. For example, the symmorphic space group should always be the first entry of each arithmetic crystal class.

8.3.5. Space-group generators

In group theory, a *set of generators of a group* is a set of group elements such that each group element may be obtained as an ordered product of the generators. For space groups of one, two and three dimensions, generators may always be chosen and ordered in such a way that each symmetry operation W can be written as the product of powers of h generators G_j $(j = 1, 2, \ldots, h)$. Thus,

$$\mathsf{W} = \mathsf{G}_h^{k_h} * \mathsf{G}_{h-1}^{k_{h-1}} * \ldots * \mathsf{G}_3^{k_3} * \mathsf{G}_2^{k_2} * \mathsf{G}_1,$$

where the powers k_j are positive or negative integers (including zero).

Description of a group by means of generators has the advantage of compactness. For instance, the 48 symmetry operations in point

Table 8.3.4.1. *Listing of space-group types according to their geometric and arithmetic crystal classes*

No.	Hermann–Mauguin symbol	Schoenflies symbol	Geometric crystal class
10	$P2/m$	C_{2h}^1	$2/m$
11	$P2_1/m$	C_{2h}^2	
13	$P2/c$	C_{2h}^4	
14	$P2_1/c$	C_{2h}^5	
12	$C2/m$	C_{2h}^3	
15	$C2/c$	C_{2h}^6	
149	$P312$	D_3^1	32
151	$P3_112$	D_3^3	
153	$P3_212$	D_3^5	
150	$P321$	D_3^2	
152	$P3_121$	D_3^4	
154	$P3_221$	D_3^6	
155	$R32$	D_3^7	
156	$P3m1$	C_{3v}^1	$3m$
158	$P3c1$	C_{3v}^3	
157	$P31m$	C_{3v}^2	
159	$P31c$	C_{3v}^4	
160	$R3m$	C_{3v}^5	
161	$R3c$	C_{3v}^6	
195	$P23$	T^1	23
198	$P2_13$	T^4	
196	$F23$	T^2	
197	$I23$	T^3	
199	$I2_13$	T^5	
200	$Pm\bar{3}$	T_h^1	$m\bar{3}$
201	$Pn\bar{3}$	T_h^2	
205	$Pa\bar{3}$	T_h^6	
202	$Fm\bar{3}$	T_h^3	
203	$Fd\bar{3}$	T_h^4	
204	$Im\bar{3}$	T_h^5	
206	$Ia\bar{3}$	T_h^7	
207	$P432$	O^1	432
208	$P4_232$	O^2	
213	$P4_132$	O^7	
212	$P4_332$	O^6	
209	$F432$	O^3	
210	$F4_132$	O^4	
211	$I432$	O^5	
214	$I4_132$	O^8	
215	$P\bar{4}3m$	T_d^1	$\bar{4}3m$
218	$P\bar{4}3n$	T_d^4	
216	$F\bar{4}3m$	T_d^2	
219	$F\bar{4}3c$	T_d^5	
217	$I\bar{4}3m$	T_d^3	
220	$I\bar{4}3d$	T_d^6	

Table 8.3.5.1. *Sequence of generators for the crystal classes*

The *space-group* generators differ from those listed here by their glide or screw components. The generator 1 is omitted, except for crystal class 1. The subscript of a symbol denotes the characteristic direction of that operation, where necessary. The subscripts z, y, 110, $1\bar{1}0$, $10\bar{1}$ and 111 refer to the directions [001], [010], [110], [$1\bar{1}0$], [$10\bar{1}$] and [111], respectively. For mirror reflections *m,* the 'direction of *m*' refers to the normal to the mirror plane. The subscripts may be likewise interpreted as Miller indices of that plane.

Hermann–Mauguin symbol of crystal class	Generators G_i (sequence left to right)
1	1
$\bar{1}$	$\bar{1}$
2	2
m	m
$2/m$	$2, \bar{1}$
222	$2_z, 2_y$
$mm2$	$2_z, m_y$
mmm	$2_z, 2_y, \bar{1}$
4	$2_z, 4$
$\bar{4}$	$2_z, \bar{4}$
$4/m$	$2_z, 4, \bar{1}$
422	$2_z, 4, 2_y$
$4mm$	$2_z, 4, m_y$
$\bar{4}2m$	$2_z, \bar{4}, 2_y$
$\bar{4}m2$	$2_z, \bar{4}, m_y$
$4/mmm$	$2_z, 4, 2_y, \bar{1}$
3	3
$\bar{3}$	$3, \bar{1}$
321	$3, 2_{110}$
(rhombohedral coordinates	$3_{111}, 2_{10\bar{1}}$)
312	$3, 2_{1\bar{1}0}$
$3m1$	$3, m_{110}$
(rhombohedral coordinates	$3_{111}, m_{10\bar{1}}$)
$31m$	$3, m_{1\bar{1}0}$
$\bar{3}m1$	$3, 2_{110}, \bar{1}$
(rhombohedral coordinates	$3_{111}, 2_{10\bar{1}}, \bar{1}$)
$\bar{3}1m$	$3, 2_{1\bar{1}0}, \bar{1}$
6	$3, 2_z$
$\bar{6}$	$3, m_z$
$6/m$	$3, 2_z, \bar{1}$
622	$3, 2_z, 2_{110}$
$6mm$	$3, 2_z, m_{110}$
$\bar{6}m2$	$3, m_z, m_{110}$
$\bar{6}2m$	$3, m_z, 2_{110}$
$6/mmm$	$3, 2_z, 2_{110}, \bar{1}$
23	$2_z, 2_y, 3_{111}$
$m\bar{3}$	$2_z, 2_y, 3_{111}, \bar{1}$
432	$2_z, 2_y, 3_{111}, 2_{110}$
$\bar{4}3m$	$2_z, 2_y, 3_{111}, m_{1\bar{1}0}$
$m\bar{3}m$	$2_z, 2_y, 3_{111}, 2_{110}, \bar{1}$

group $m\bar{3}m$ can be described by two generators. Different choices of generators are possible. For the present *Tables*, generators and generating procedures have been chosen such as to make the entries in the blocks *General position* (*cf.* Section 2.2.11) and *Symmetry operations* (*cf.* Section 2.2.9) as transparent as possible. Space groups of the same crystal class are generated in the same way (for sequence chosen, see Table 8.3.5.1), and the aim has been to accentuate important subgroups of space groups as much as possible. Accordingly, a process of generation in the form of a 'composition series' has been adopted, see Ledermann (1976). The generator G_1 is defined as the identity operation, represented by (1) x, y, z. G_2, G_3 and G_4 are the translations with translation vectors **a**, **b** and **c**, respectively. Thus, the coefficients k_2, k_3 and k_4 may have any integral value. If centring translations exist, they are generated by translations G_5 (and G_6 in the case of an F lattice) with translation vectors **d** (and **e**). For a C lattice, for example, **d** is given by $\mathbf{d} = \frac{1}{2}(\mathbf{a} + \mathbf{b})$. The exponents k_5 (and k_6) are restricted to the following values:

Lattice letter A, B, C, I: $k_5 = 0$ or 1.
Lattice letter R (hexagonal axes): $k_5 = 0$, 1 or 2.
Lattice letter F: $k_5 = 0$ or 1; $k_6 = 0$ or 1.

As a consequence, any translation T of $\mathcal{G}$ with translation vector

$$\mathbf{t} = k_2\mathbf{a} + k_3\mathbf{b} + k_4\mathbf{c}(+k_5\mathbf{d} + k_6\mathbf{e})$$

can be obtained as a product

$$\mathsf{T} = (\mathsf{G}_6)^{k_6} * (\mathsf{G}_5)^{k_5} * \mathsf{G}_4^{k_4} * \mathsf{G}_3^{k_3} * \mathsf{G}_2^{k_2} * \mathsf{G}_1,$$

where $k_2, \ldots, k_6$ are integers determined by T. G_6 and G_5 are enclosed between parentheses because they are effective only in centred lattices.

The remaining generators generate those symmetry operations that are not translations. They are chosen in such a way that only terms G_j or G_j^2 occur. For further specific rules, see below.

The process of generating the entries of the space-group tables may be demonstrated by the example of Table 8.3.5.2, where $\mathcal{G}_j$ denotes the group generated by $\mathsf{G}_1, \mathsf{G}_2, \ldots, \mathsf{G}_j$. For $j \geq 5$, the next generator G_{j+1} has always been taken as soon as $\mathsf{G}_j^{k_j} \in \mathcal{G}_{j-1}$, because in this case no new symmetry operation would be generated by $\mathsf{G}_j^{k_j}$. The generating process is terminated when there is no further generator. In the present example, G_7 completes the generation: $\mathcal{G}_7 \equiv P6_122$.

8.3.5.1. *Selected order for non-translational generators*

For the non-translational generators, the following sequence has been adopted:

(*a*) In all centrosymmetric space groups, an inversion (if possible at the origin O) has been selected as the last generator.

(*b*) Rotations precede symmetry operations of the second kind. In crystal classes $\bar{4}2m$–$\bar{4}m2$ and $\bar{6}2m$–$\bar{6}m2$, as an exception, $\bar{4}$ and $\bar{6}$ are generated first in order to take into account the conventional choice of origin in the fixed points of $\bar{4}$ and $\bar{6}$.

(*c*) The non-translational generators of space groups with C, A, B, F, I or R symbols are those of the corresponding space group with a P symbol, if possible. For instance, the generators of $I2_12_12_1$ are those of $P2_12_12_1$ and the generators of *Ibca* are those of *Pbca,* apart from the centring translations.

Exceptions: $I4cm$ and $I4/mcm$ are generated *via* $P4cc$ and $P4/mcc$, because $P4cm$ and $P4/mcm$ do not exist. In space groups with d glides (except $I\bar{4}2d$) and also in $I4_1/a$, the corresponding rotation subgroup has been generated first. The generators of this subgroup are the same as those of the corresponding space group with a lattice symbol P.

Example
$F4_1/d\bar{3}2/m : P4_132 \rightarrow F4_132 \rightarrow F4_1/d\bar{3}2/m.$

(*d*) In some cases, rule (*c*) could not be followed without breaking rule (*a*), *e.g.* in *Cmme.* In such cases, the generators are chosen to correspond to the Hermann–Mauguin symbol as far as possible. For instance, the generators (apart from centring) of *Cmme* and *Imma* are

Table 8.3.5.2. *Example of a space-group generation $\mathcal{G}$: $P6_122 \equiv D_6^2$ (No. 178)*

	Coordinates	Symmetry operations
G_1	(1) x, y, z;	Identity I
G_2	$t(100)$	These are the generating translations.
G_3	$t(010)$	$\mathcal{G}_4$ is the group $\mathcal{T}$ of all translations
G_4	$t(001)$	of $P6_122$
G_5	(2) $\bar{y}, x-y, z+\frac{1}{3}$;	Threefold screw rotation
G_5^2	(3) $\bar{x}+y, \bar{x}, z+\frac{2}{3}$;	Threefold screw rotation
$\mathsf{G}_5^3 = t(001)$:	Now the space group $\mathcal{G}_5 \equiv P3_1$ has been generated	
G_6	(4) $\bar{x}, \bar{y}, z+\frac{1}{2}$;	Twofold screw rotation
$\mathsf{G}_6 * \mathsf{G}_5$	(5) $y, \bar{x}+y, z+\frac{5}{6}$;	Sixfold screw rotation
$\mathsf{G}_6 * \mathsf{G}_5^2$	$x-y, x, z+\frac{7}{6} \sim$ (6) $x-y, x, z+\frac{1}{6}$;	Sixfold screw rotation
$\mathsf{G}_6^2 = t(001)$:	Now the space group $\mathcal{G}_6 \equiv P6_1$ has been generated	
G_7	(7) $y, x, \bar{z}+\frac{1}{3}$;	Twofold rotation, direction of axis [110]
$\mathsf{G}_7 * \mathsf{G}_5$	(8) $x-y, \bar{y}, \bar{z}$;	Twofold rotation, axis [100]
$\mathsf{G}_7 * \mathsf{G}_5^2$	$\bar{x}, \bar{x}+y, \bar{z}-\frac{1}{3} \sim$ (9) $\bar{x}, \bar{x}+y, \bar{z}+\frac{2}{3}$;	Twofold rotation, axis [010]
$\mathsf{G}_7 * \mathsf{G}_6$	$\bar{y}, \bar{x}, \bar{z}-\frac{1}{6} \sim$ (10) $\bar{y}, \bar{x}, \bar{z}+\frac{5}{6}$;	Twofold rotation, axis $[\bar{1}10]$
$\mathsf{G}_7 * \mathsf{G}_6 * \mathsf{G}_5$	$\bar{x}+y, y, \bar{z}-\frac{1}{2} \sim$ (11) $\bar{x}+y, y, \bar{z}+\frac{1}{2}$;	Twofold rotation, axis [120]
$\mathsf{G}_7 * \mathsf{G}_6 * \mathsf{G}_5^2$	$x, x-y, \bar{z}-\frac{5}{6} \sim$ (12) $x, x-y, \bar{z}+\frac{1}{6}$;	Twofold rotation, axis [210]
$\mathsf{G}_7^2 = \mathsf{I}$	$\mathcal{G}_7 \sim P6_122$	

those of *Pmmb,* which is a non-standard setting of *Pmma.* (Combination of the generators of *Pmma* with the *C*- or *I*-centring translation results in non-standard settings of *Cmme* and *Imma.*)

For the space groups with lattice symbol *P*, the generation procedure has given the same triplets (except for their sequence) as in *IT* (1952). In non-*P* space groups, the triplets listed sometimes differ from those of *IT* (1952) by a centring translation.

8.3.6. Normalizers of space groups

The concept of normalizers, well known to mathematicians since the nineteenth century, is finding more and more applications in crystallography. Normalizers play an important role in the general theory of space groups of *n*-dimensional space. By the so-called Zassenhaus algorithm, one can determine the space-group types of *n*-dimensional space, provided the arithmetic crystal classes and for each arithmetic crystal class a representative integral $(n \times n)$-matrix group are known. The crucial step is then to determine for these matrix groups their normalizers in GL(*n*, *Z*). This was done for $n = 4$ by Brown *et al.* (1978) in the derivation of the 4894 space-group types. Now, the program package *Carat* solves this problem and was used, among others, for the enumeration of the 28 927 922 affine space-group types for six-dimensional space, see Table 8.1.1.1.

Crystallographers have been applying normalizers in their *practical* work for some time without realizing this fact, and only in the last decades have they become aware of the importance of normalizers. Normalizers first seem to have been derived visually, see Hirshfeld (1968). A derivation of the normalizers of the space groups using matrix methods is found in a paper by Boisen *et al.* (1990).

For the practical application of normalizers in crystallographic problems, see Part 15, which also contains detailed lists of normalizers of the point groups and space groups, as well as of space groups with special metrics. In this section, a short elementary introduction to normalizers will be presented.

In Section 8.1.6, the elements of a space group $\mathcal{G}$ have been divided into classes with respect to the subgroup $\mathcal{T}$ of all translations of $\mathcal{G}$; these classes have been called *cosets.* 'Coset decomposition' can be performed for any pair 'group $\mathcal{G}$ and subgroup $\mathcal{H}$'. The subgroup $\mathcal{H}$ is called *normal* if the decomposition of $\mathcal{G}$ into right and left cosets results in the same cosets.

The decomposition of the elements of a group $\mathcal{G}$ into 'conjugacy classes' is equally important in crystallography. These classes are defined as follows:

Definition: The elements A and B of a group $\mathcal{G}$ are said to be *conjugate in* $\mathcal{G}$, if there exists an element $\mathsf{G} \in \mathcal{G}$ such that $\mathsf{B} = \mathsf{G}^{-1}\mathsf{A}\mathsf{G}$.

Example

The symmetry group 4*mm* of a square consists of the symmetry operations 1, 2, 4, 4^{-1}, m_x, m_y, m_d and $m_{d'}$, see Fig. 8.3.6.1. Vertex 1 is left invariant by 1 and $m_{d'}$, vertex 2 by 1 and m_d. The operations m_d and $m_{d'}$ are conjugate, because $m_{d'} = 4^{-1}m_d4$ holds, as are m_x and m_y ($m_y = 4^{-1}m_x4$), or 4 and 4^{-1} ($4^{-1} = m_x^{-1}4m_x$). The operations 1 and 2 have no conjugates.

As proved in mathematical textbooks, *e.g.* Ledermann (1976), conjugacy indeed subdivides a group into classes of elements. The unit element 1 always forms a conjugacy class for itself, as does any element that commutes with every other element of the group. For finite groups, the number of elements in a conjugacy class is a factor of the group order. In infinite groups, such as space groups, conjugacy classes may contain an infinite number of elements.

Conjugacy can be transferred from elements to groups. Let $\mathcal{H}$ be a subgroup of $\mathcal{G}$. Then another subgroup $\mathcal{H}'$ of $\mathcal{G}$ is said to be *conjugate to* $\mathcal{H}$ in $\mathcal{G}$, if there exists an element $\mathsf{G} \in \mathcal{G}$, such that $\mathcal{H}' = \mathsf{G}^{-1}\mathcal{H}\mathsf{G}$. In this way, the set of all subgroups $\mathcal{H}_i$ of a group $\mathcal{G}$ is divided into *classes of conjugate subgroups* or *conjugacy classes of subgroups.* Conjugacy classes may contain different numbers of subgroups but, for finite groups, the number of subgroups in each class is always a factor of the order of the group. Conjugacy classes which contain only one subgroup are of special interest; they are called *normal subgroups.* There are always two trivial normal subgroups of a group $\mathcal{G}$: the group $\mathcal{G}$ itself and the group $\mathcal{I}$ consisting of the unit element 1 only. For space groups, the group $\mathcal{T}$ of all translations of the group always forms a normal subgroup of $\mathcal{G}$.

In the above-mentioned example of the square, the subgroups $\{1, m_x\}$ and $\{1, m_y\}$ as well as $\{1, m_d\}$ and $\{1, m_{d'}\}$ each form conjugate pairs, whereas the subgroups $\{1, 2, 4, 4^{-1}\}$, $\{1, 2, m_x, m_y\}$, $\{1, 2, m_d, m_{d'}\}$ and $\{1, 2\}$ are normal subgroups.

The characterization of normal subgroups, $\mathcal{H}$ must obey the condition $\mathcal{H} = \mathsf{G}^{-1}\mathcal{H}\mathsf{G}$ for all elements $\mathsf{G} \in \mathcal{G}$, is identical with the one used in Section 8.1.6. This relation can also be expressed as

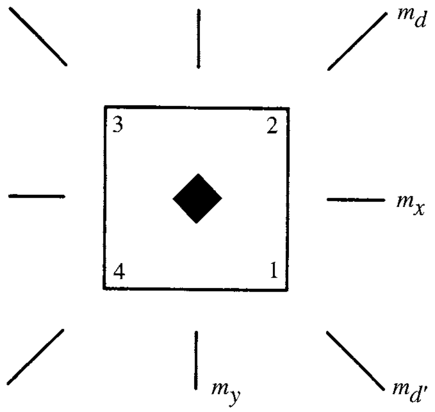

Fig. 8.3.6.1. Square with 'symmetry elements' m_x, m_y, m_d, $m_{d'}$ (mirror lines) and ◆ (fourfold rotation point). The vertices are numbered 1, 2, 3 and 4.

$\mathsf{G}\mathcal{H} = \mathcal{H}\mathsf{G}$ which means that the right and left cosets coincide. Thus each subgroup $\mathcal{H}$ of index [2] is normal, because there is only one coset in addition to $\mathcal{H}$ itself which is then necessarily the right as well as the left coset.

If $\mathcal{H}$ is not a normal subgroup of $\mathcal{G}$, then $\mathcal{H} = \mathsf{G}^{-1}\mathcal{H}\mathsf{G}$ cannot hold for all $\mathsf{G} \in \mathcal{G}$, because there is at least one subgroup $\mathcal{H}'$ of $\mathcal{G}$ which is conjugate to $\mathcal{H}$. This situation leads to the introduction of the normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ of a subgroup $\mathcal{H}$ of $\mathcal{G}$.

Definition: The set of all elements $\mathsf{G} \in \mathcal{G}$, for which $\mathsf{G}^{-1}\mathcal{H}\mathsf{G} = \mathcal{H}$ holds, is called the *normalizer* $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ of $\mathcal{H}$ in $\mathcal{G}$.

The normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ is always a group and thus a subgroup of $\mathcal{G}$ which obeys the relation $\mathcal{G} \geq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \trianglerighteq \mathcal{H}$. The symbol $\trianglerighteq$ means that $\mathcal{H}$ is a *normal* subgroup of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$. The subgroup $\mathcal{H}$ is normal in $\mathcal{G}$ if its normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \mathcal{G}$ coincides with $\mathcal{G}$. Otherwise, other subgroups conjugate to $\mathcal{H}$ exist. To determine the number of conjugate subgroups of $\mathcal{H}$, one decomposes $\mathcal{G}$ into cosets relative to $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$. The elements of each such coset transform $\mathcal{H}$ into a conjugate subgroup $\mathcal{H}'$, such that the number of conjugates (including $\mathcal{H}$ itself) equals the index of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ in $\mathcal{G}$.

Examples

(1) The normalizer $\mathcal{N}_{4mm}(\{1, m_d\})$ of the subgroup $\{1, m_d\}$, see Fig. 8.3.6.1, consists of the elements $\{1, 2, m_d, m_{d'}\}$; its index in the full group $4mm$ of the square is [2]. Therefore, there are two conjugate subgroups $\{1, m_d\}$ and $\{1, m_{d'}\}$. All operations of the normalizer map the group $\{1, m_d\}$ onto itself and thus describe the 'symmetry in $4mm$ of this symmetry group'.

(2) Under space-group type $Fm\bar{3}m$ (No. 225), four subgroups of type $Pm\bar{3}m$ (No. 221) of index [4] are listed; four subgroups of type $Pn\bar{3}m$ (No. 224) are similarly listed. Are these subgroups conjugate in the original space group? Clearly, a space group of type $Pm\bar{3}m$ cannot be conjugate to one of the different type $Pn\bar{3}m$ because there exists no affine mapping transforming one into the other. On the other hand, one verifies that the four subgroups of type $Pm\bar{3}m$ are conjugate relative to $Fm\bar{3}m$: the transforming elements are the (centring) translations 000, $\frac{1}{2}\frac{1}{2}0$, $\frac{1}{2}0\frac{1}{2}$, $0\frac{1}{2}\frac{1}{2}$. Similarly, the four subgroups of type $Pn\bar{3}m$ are conjugate in $Fm\bar{3}m$ by the same (centring) translations. The normalizers $\mathcal{N}_{Fm\bar{3}m}(Pm\bar{3}m)$ and $\mathcal{N}_{Fm\bar{3}m}(Pn\bar{3}m)$ are the subgroups themselves; their indices in $Fm\bar{3}m$ are [4], *i.e.* the numbers of conjugates are four.

Obviously, it would be impractical to list the normalizer for each type of group–subgroup pair. There are, however, some normalizers of outstanding importance from which, moreover, the normalizers determining the usual conjugacy relations can be obtained easily. Since space groups are groups of motions and space-group types are affine equivalence classes of space groups, *cf.* Sections 8.1.6 and 8.2.2, the groups $\mathcal{E}$ of *all* motions and $\mathcal{A}$ of *all* affine mappings are groups of special significance for any space group. The normalizers of a space group relative to these two groups are considered now. Part 15 contains lists of these normalizers with detailed comments.

The normalizer of a space group $\mathcal{G}$ in the group $\mathcal{A}$ of all affine mappings is called the *affine normalizer* $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ of the space group $\mathcal{G}$. The affine normalizers of space groups of the same space-group type are affinely equivalent. One thus can speak of the 'type of normalizers of a space-group type'. In many cases, these normalizers are either space groups or isomorphic to space groups, but they may also be other groups due to arbitrarily small translations (for polar space groups) and/or due to noncrystallographic point groups (for triclinic and monoclinic space groups).

Affine normalizers are of more theoretical interest. For example, they determine the occurrence of enantiomorphism of space groups, *cf.* Section 8.2.2. A space-group type splits into a pair of enantiomorphic space-group types, if and only if its normalizers are contained in $\mathcal{A}^+$, the group of all affine mappings with positive determinant.

The normalizer of a space group $\mathcal{G}$ in the group $\mathcal{E}$ of all motions (Euclidean group) is called the *Euclidean normalizer* $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ of the space group $\mathcal{G}$. For all trigonal, tetragonal, hexagonal and cubic space groups, $\mathcal{N}_{\mathcal{E}} = \mathcal{N}_{\mathcal{A}}$ holds. In these cases, as well as in any context in which statements are valid for both normalizers, the abbreviated form $\mathcal{N}$ is frequently used.

The group $\mathcal{T}(\mathcal{N})$ of all translations of $\mathcal{N}$ is the same for both normalizers, $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$, because any translation is a motion. It can be calculated easily: To be an element of $\mathcal{T}(\mathcal{N})$, the translation $(\boldsymbol{I}, \boldsymbol{t})$ has to satisfy the equation $(\boldsymbol{I}, \boldsymbol{t})^{-1}(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{I}, \boldsymbol{t}) = (\boldsymbol{W}', \boldsymbol{w}') \in \mathcal{G}$ for any operation $(\boldsymbol{W}, \boldsymbol{w})$ of $\mathcal{G}$. This results in $(\boldsymbol{W}, \boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{t}) = (\boldsymbol{W}', \boldsymbol{w}')$ or $\boldsymbol{W}' = \boldsymbol{W}$ and $\boldsymbol{w}' = \boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{t}$. From this $(\boldsymbol{W} - \boldsymbol{I})\boldsymbol{t} \in \mathcal{T}(\mathcal{G})$ follows, *i.e.* $(\boldsymbol{W} - \boldsymbol{I})\boldsymbol{t}$ must be a lattice translation of $\mathcal{G}$. To determine $\mathcal{T}(\mathcal{N})$, it is sufficient to apply this equation to the $\boldsymbol{W}_i$ of the generators of $\mathcal{G}$.

The conditions for the groups $\mathcal{T}(\mathcal{N})$ are the same for all space groups of the same arithmetic crystal class, because those space groups are generated by symmetry operations with the same matrix parts, and their lattices belong to the same centring type, if referred to conventional coordinate systems. The other elements of the normalizer are not obtained as easily.

In contrast to $\mathcal{N}_{\mathcal{A}}$, the type of $\mathcal{N}_{\mathcal{E}}$ is not a property of the space-group type, as the following example shows. The Euclidean normalizer of a space group $P222$ is an orthorhombic space group $Pmmm$ if $a \neq b \neq c \neq a$. It is a tetragonal space group if accidentally $a = b$ (or $b = c$ or $c = a$), and it is even cubic if accidentally $a = b = c$. The listings in Part 15 also contain the normalizers for the case of lattices with accidental symmetries.

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9.1. Bases, lattices, Bravais lattices and other classifications

By H. Burzlaff and H. Zimmermann

9.1.1. Description and transformation of bases

In three dimensions, a coordinate system is defined by an origin and a basis consisting of three non-coplanar vectors. The lengths a, b, c of the basis vectors **a**, **b**, **c** and the intervector angles $\alpha = \angle(\mathbf{b}, \mathbf{c})$, $\beta = \angle(\mathbf{c}, \mathbf{a})$, $\gamma = \angle(\mathbf{a}, \mathbf{b})$ are called the *metric parameters*. In n dimensions, the lengths are designated a_i and the angles α_{ik}, where $1 \leq i < k \leq n$.

Another description of the basis consists of the scalar products of all pairs of basis vectors. The set of these scalar products obeys the rules of covariant tensors of the second rank (see Section 5.1.3). The scalar products may be written in the form of a (3×3) matrix

$$(\mathbf{a}_i \cdot \mathbf{a}_k) = (g_{ik}) = \mathbf{G}; \quad i, k = 1, 2, 3,$$

which is called the *matrix of the metric coefficients* or the *metric tensor*.

The change from one basis to another is described by a transformation matrix $\boldsymbol{P}$. The transformation of the old basis (**a**, **b**, **c**) to the new basis $(\mathbf{a}', \mathbf{b}', \mathbf{c}')$ is given by

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \cdot \boldsymbol{P}.$$

The relation

$$\mathbf{G}' = \boldsymbol{P}^t \cdot \mathbf{G} \cdot \boldsymbol{P} \qquad (9.1.1.1)$$

holds for the metric tensors $\mathbf{G}$ and $\mathbf{G}'$.

9.1.2. Lattices

A three-dimensional lattice can be visualized best as an infinite periodic array of points, which are the termini of the vectors

$$\mathbf{l}_{uvw} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}, \quad u, v, w \text{ all integers.}$$

The parallelepiped determined by the basis vectors **a**, **b**, **c** is called a (primitive) *unit cell* of the lattice (*cf.* Section 8.1.4), **a**, **b** and **c** are a primitive *basis of the lattice*. The number of possible lattice bases is infinite.

For the investigation of the properties of lattices, appropriate bases are required. In order to select suitable bases (see below), transformations may be necessary (Section 5.1.3). Of the several properties of lattices, only symmetry and some topological aspects are considered in this chapter. Some further properties of lattices are given in Chapter 9.3.

9.1.3. Topological properties of lattices

The treatment of the topological properties is restricted here to the consideration of the neighbourhood of a lattice point. For this purpose, the *domain of influence* (*Wirkungsbereich*, Dirichlet domain, Voronoi domain, Wigner–Seitz cell) (Delaunay, 1933) is introduced. The domain of a particular lattice point consists of all points in space that are closer to this lattice point than to any other lattice point or at most equidistant to it. To construct the domain, the selected lattice point is connected to all other lattice points. The set of planes perpendicular to these connecting lines and passing through their midpoints contains the boundary planes of the domain of influence, which is thus a convex polyhedron. (Niggli and Delaunay used the term 'domain of influence' for the interior of the convex polyhedron only.) Without the use of metrical properties, Minkowski (1897) proved that the maximal number of boundary planes resulting from this construction is equal to $2(2^n - 1)$, where n is the dimension of the space. The minimal number of boundary planes is $2n$. Each face of the polyhedron represents a lattice vector. Thus, the topological, metrical and symmetry properties of infinite lattices can be discussed with the aid of a finite polyhedron, namely the domain of influence (*cf.* Burzlaff & Zimmermann, 1977).

9.1.4. Special bases for lattices

Different procedures are in use to select specific bases of lattices. The reduction procedures employ metrical properties to develop a sequence of basis transformations which lead to a *reduced basis* and *reduced cell* (see Chapter 9.3).

Table 9.1.4.1. *Lattice point-group symmetries*

Two dimensions				
Lattice point group	2	$2mm$	$4mm$	$6mm$
Crystal family*	m	o	t	h
	*m*onoclinic (oblique)	*o*rthorhombic (rectangular)	*t*etragonal (square)	*h*exagonal

Three dimensions							
Lattice point group	$C_i \equiv \bar{1}$	$C_{2h} \equiv 2/m$	$D_{2h} \equiv mmm$	$D_{4h} \equiv 4/mmm$	$D_{3d} \equiv \bar{3}m$	$D_{6h} \equiv 6/mmm$	$O_h \equiv m\bar{3}m$
Crystal family*	a	m	o	t	h		c
	*a*northic (triclinic)	*m*onoclinic	*o*rthorhombic	*t*etragonal	*h*exagonal		*c*ubic

* The symbols for crystal families were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985).

Another possibility is to make use of the symmetry properties of lattices. This procedure, with the aid of standardization rules, leads to the *conventional crystallographic basis* and *cell*. In addition to translational symmetry, a lattice possesses point-group symmetry. No crystal can have higher point-group symmetry than the point group of its lattice, which is called *holohedry*. The seven point groups of lattices in three dimensions and the four in two dimensions form the basis for the classification of lattices (Table 9.1.4.1). It may be shown by an algebraic approach (Burckhardt, 1966) or a topological one (Delaunay, 1933) that the arrangement of the symmetry elements with respect to the lattice vectors is not arbitrary but well determined. Taking as basis vectors lattice vectors along important symmetry directions and choosing the origin in a lattice point simplifies the description of the lattice symmetry operations (*cf.* Chapter 12.1). Note that such a basis is not necessarily a (primitive) basis of the lattice (see below). The choice of a basis controlled by symmetry is not always unique; in the monoclinic system, for example, one vector can be taken parallel to the symmetry direction but the other two vectors, perpendicular to it, are not uniquely determined by symmetry.

The choice of conventions for standardizing the setting of a lattice depends on the purpose for which it is used. The several sets of conventions rest on two conflicting principles: symmetry considerations and metric considerations. The following rules (i) to (vii) defining a *conventional basis* are taken from Donnay (1943; Donnay & Ondik, 1973); they deal with the conventions based on symmetry:

(i) Each basis vector is a lattice vector from the origin to the nearest node on the related row. The basis must define a right-handed coordinate system.

(ii) The basis vectors for a *cubic* lattice are parallel to the fourfold axes.

(iii*a*) In a *hexagonal* lattice, one basis vector, parallel to the sixfold axis, is labelled **c**. The remaining two basis vectors are taken along twofold axes and they must include an angle of 120°; from the two possible sets, the shorter vectors are chosen.

(iii*b*) For *rhombohedral* lattices, two descriptions are given in the present edition, as in earlier ones. The first description which gives the conventional cell uses 'hexagonal axes'. In this case, **c** is taken along the threefold axis. The remaining two vectors are chosen along twofold axes including an angle of 120°; they are oriented so that lattice points occur at $2/3, 1/3, 1/3$ and $1/3, 2/3, 2/3$ (obverse setting). The reverse setting $(0, 0, 0; 1/3, 2/3, 1/3; 2/3, 1/3, 2/3)$ is not used in the space-group tables (*cf.* Section 1.2.1, footnote †). The second description uses 'rhombohedral axes': **a**, **b** and **c** are the shortest non-coplanar lattice vectors symmetrically equivalent with respect to the threefold axis.

(iv) In a *tetragonal* lattice, the vector **c** is along the fourfold axis, and **a** and **b** are chosen along twofold axes perpendicular to each other. From the two possible sets, the shorter vectors are chosen.

(v) In an *orthorhombic* lattice, **a**, **b** and **c** must be taken along the twofold axes.

(vi) For *monoclinic* lattices, two 'settings' are given in the present edition. In one setting, the only symmetry direction is labelled **b** (*b*-unique setting). The basis vectors **a** and **c** are chosen to be the shortest two vectors in the net plane perpendicular to **b**, the angle β should be non-acute. This occurs if

$$0 \leq -2\mathbf{a} \cdot \mathbf{c} \leq \min(a^2, c^2). \qquad (9.1.4.1)$$

In the other setting, the symmetry direction is labelled **c** [*c*-unique setting; first introduced in *IT* (1952)]. In this case, **a** and **b** are the shortest two vectors in the net plane perpendicular to **c** and the angle γ should be non-acute. The *b*-unique setting is considered to be the standard setting.

(vii) The reduced basis is used to describe a *triclinic* (= *anorthic*) lattice (*cf.* Chapter 9.3).

The metric parameters of the conventional basis are called *lattice parameters*. For the purpose of identification, additional metric rules have to be employed to make the labelling unique; they can be found in the introduction to *Crystal Data* (Donnay & Ondik, 1973).

When the above rules have been applied, it may occur that not all lattice points can be described by integral coordinates. In such cases, the unit cell contains two, three or four lattice points. The additional points may be regarded as *centrings* of the conventional cell. They have simple rational coordinates. For a conventional basis, the number of lattice points per cell is 1, 2, 3 or 4 (see Tables 9.1.7.1 and 9.1.7.2).

In two dimensions, only two centring types are needed:

p : no centring (primitive);

c : face centred.

In three dimensions, the following centring types are used:

P : no centring (primitive);

I : body centred (*innenzentriert*);

F : all-face centred;

A, B, C : one-face centred, $(\mathbf{b}, \mathbf{c})$ or $(\mathbf{c}, \mathbf{a})$ or $(\mathbf{a}, \mathbf{b})$;

R : hexagonal cell rhombohedrally centred

[see rule (iii*b*) above].

In orthorhombic and monoclinic lattices, some differently centred cells can be transformed into each other without violating the symmetry conditions for the choice of the basis vectors. In these cases, the different centred cells belong to the same *centring mode.* In the orthorhombic case, the three types of one-face-centred cells belong to the same centring mode because the symbol of the cell depends on the labelling of the basis vectors; *C* is usually preferred to *A* and *B* in the standard setting; the centring mode is designated *S* (*seitenflächenzentriert*). In the monoclinic case (*b*-unique setting), *A*, *I* and *C* can be transformed into each other without changing the symmetry direction. *C* is used for the standard setting (*cf.* Section 2.2.3); it represents the centring mode *S*. The vectors **a**, **c** are conventionally chosen as short as the *C*-centring allows so that they need not be the shortest two vectors in their net plane and need not fulfil the inequalities (9.1.4.1).

In some situations, the *I*-centring of the monoclinic conventional cell may be more advantageous. If the vectors **a**, **c** are the shortest ones leading to the centring *I*, they obey the inequalities (9.1.4.1).

9.1.5. Remarks

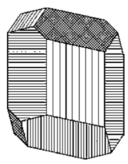
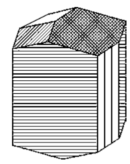
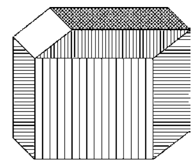
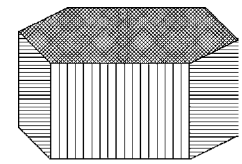
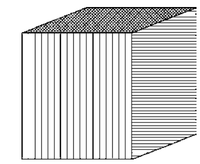
(i) For the handling of special problems such as subgroup relations, it may be convenient to use additional centred cells, *e.g.* a hexagonal cell centred at $2/3, 1/3, 0$ and $1/3, 2/3, 0$, which is called *H.* In this case, rule (iii*a*) above is violated as vectors **a** and **b** are now directed along the second set of twofold axes. Similarly, for tetragonal lattices, *C* may be used instead of *P,* or *F* instead of *I; cf.* Chapter 1.2.

(ii) Readers who have studied Section 8.1.4 may realize that the 'lattice bases' defined here are called 'primitive bases' there and that both 'primitive bases' and 'conventional bases' are special cases of bases used in crystallography.

9.1.6. Classifications

By means of the above-mentioned lattice properties, it is possible to classify lattices according to various criteria. Lattices can be

Table 9.1.6.1. *Representations of the five types of Voronoi polyhedra*

V_I	V_{II}	V_{III}	V_{IV}	V_V
				

subdivided with respect to their topological types of domains, resulting in two classes in two dimensions and five classes in three dimensions. They are called *Voronoi types* (see Table 9.1.6.1). If the classification involves topological *and* symmetry properties of the domains, 24 *Symmetrische Sorten* (Delaunay, 1933) are obtained in three dimensions and 5 in two dimensions. Other classifications consider either the centring type or the point group of the lattice.

The most important classification takes into account both the lattice point-group symmetry and the centring mode (Bravais, 1866). The resulting classes are called *Bravais types of lattices* or, for short, *Bravais lattices*. Two lattices belong to the same Bravais type if and only if they coincide both in their point-group symmetry and in the centring mode of their conventional cells. The Bravais lattice characterizes the translational subgroup of a space group. The number of Bravais lattices is 1 in one dimension, 5 in two dimensions, 14 in three dimensions and 64 in four dimensions. The Bravais lattices may be derived by topological (Delaunay, 1933) or algebraic procedures (Burckhardt, 1966; Neubüser *et al.*, 1971). It can be shown (Wondratschek *et al.*, 1971) that 'all Bravais types of the same crystal family can be

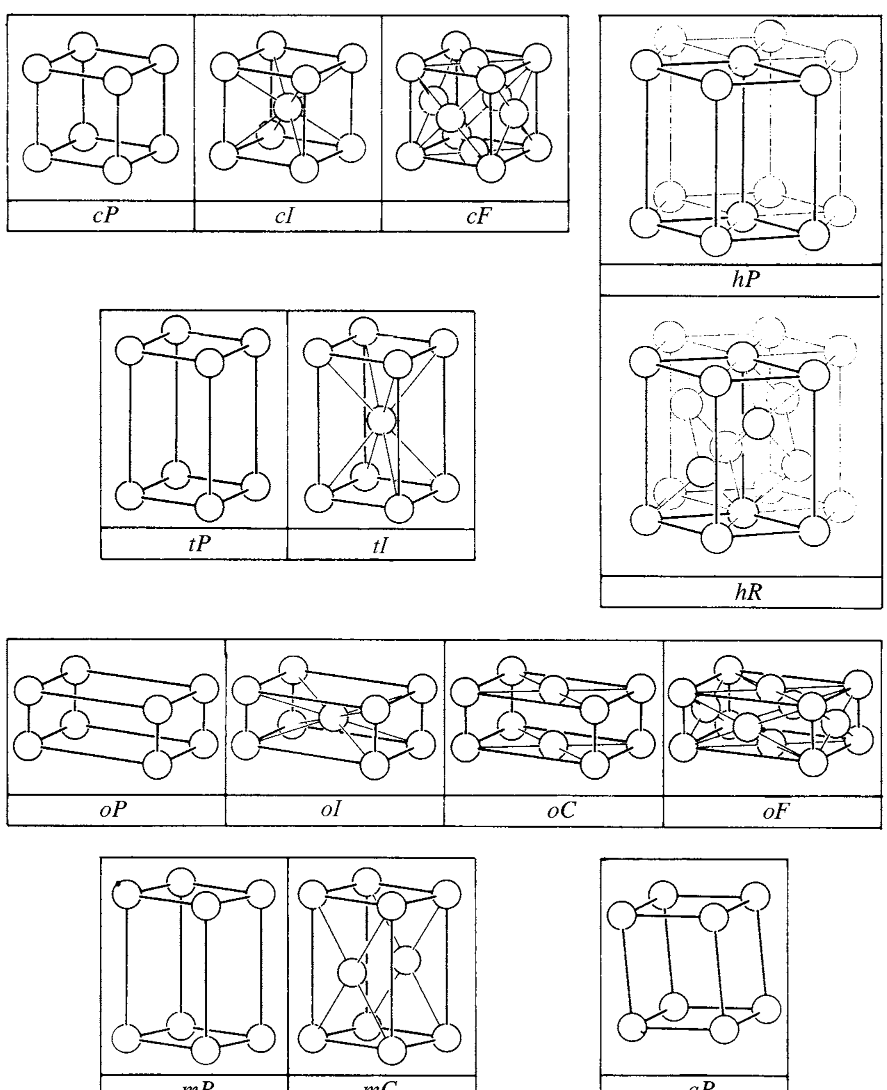
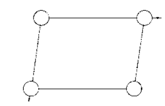
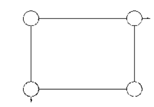
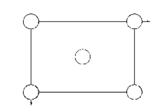
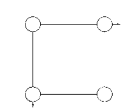
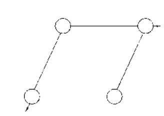


Fig. 9.1.7.1. Conventional cells of the three-dimensional Bravais lattices (for symbols see Table 9.1.7.2).

Table 9.1.7.1. *Two-dimensional Bravais lattices*

Bravais lattice*	Lattice parameters: Conventional	Lattice parameters: Primitive/ transformation to primitive cell	Metric tensor: Conventional	Metric tensor: Primitive	Metric tensor: Relations of the components	Projections
mp	a, b γ	a, b γ	$\begin{matrix} g_{11} & g_{12} \\ & g_{22} \end{matrix}$	$\begin{matrix} g_{11} & g_{12} \\ & g_{22} \end{matrix}$		
op	a, b $\gamma = 90°$	a, b $\gamma = 90°$	$\begin{matrix} g_{11} & 0 \\ & g_{22} \end{matrix}$	$\begin{matrix} g_{11} & 0 \\ & g_{22} \end{matrix}$		
oc		$a_1 = a_2, \gamma$ $\boldsymbol{P}(c)$†		$\begin{matrix} g'_{11} & g'_{12} \\ & g'_{22} \end{matrix}$	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{12} = 2(g'_{11} - g'_{12})$	
tp	$a_1 = a_2$ $\gamma = 90°$	$a_1 = a_2$ $\gamma = 90°$	$\begin{matrix} g_{11} & 0 \\ & g_{11} \end{matrix}$	$\begin{matrix} g_{11} & 0 \\ & g_{11} \end{matrix}$		
hp	$a_1 = a_2$ $\gamma = 120°$	$a_1 = a_2$ $\gamma = 120°$	$\begin{matrix} g_{11} & -\frac{1}{2} g_{11} \\ & g_{11} \end{matrix}$	$\begin{matrix} g_{11} & -\frac{1}{2} g_{11} \\ & g_{11} \end{matrix}$		

* The symbols for Bravais lattices were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985).
† $\boldsymbol{P}(c) = \frac{1}{2}(11/\bar{1}1)$.

obtained from each other by the process of centring'. As a consequence, different Bravais types of the same [crystal] family (*cf.* Section 8.1.4) differ in their centring mode. Thus, the Bravais types may be described by a lower-case letter designating the crystal family and an upper-case letter designating the centring mode. The relations between the point groups of the lattices and the crystal families are shown in Table 9.1.4.1. Since the hexagonal and rhombohedral Bravais types belong to the same crystal family, the rhombohedral lattice is described by *hR*, *h* indicating the family and *R* the centring type. This nomenclature was adopted for the 1969 reprint (*IT* 1969) of *IT* (1952) and for *Structure Reports* since 1975 (*cf.* Trotter, 1975).

9.1.7. Description of Bravais lattices

In Fig. 9.1.7.1, conventional cells for the 14 three-dimensional Bravais lattices are illustrated.

In Tables 9.1.7.1 and 9.1.7.2, the two- and three-dimensional Bravais lattices are described in detail. For each entry, the tables contain conditions that must be fulfilled by the lattice parameters and the metric tensor. These conditions are given with respect to two different basis systems, first the conventional basis related to symmetry, second a special primitive basis (see below). In columns 2 and 3, basis vectors not required by symmetry to be of the same length are designated by different letters. Columns 4 and 5 contain the metric tensors for the two related bases. Column 6 shows the relations between the components of the two tensors.

The last columns of Tables 9.1.7.1 and 9.1.7.2 show parallel projections of the appropriate conventional unit cells. Among the different possible choices of the primitive basis, as discussed in Sections 9.1.1–9.1.5, the special primitive basis mentioned above is obtained according to the following rules:

(i) For each type of centring, only one transformation matrix $\boldsymbol{P}$ is used to obtain the primitive cell as given in Tables 9.1.7.1 and 9.1.7.2. The transformation obeys equation (9.1.1.1).

(ii) Among the different possible transformations, those are preferred which result in a metric tensor with simple relations among its components, as defined in Tables 9.1.7.1 and 9.1.7.2.

If a primitive basis is chosen according to these rules, basis vectors of the conventional cell have parallel face-diagonal or body-diagonal orientation with respect to the basis vectors of the primitive cell. For cubic and rhombohedral lattices, the primitive basis vectors are selected such that they are symmetrically equivalent with respect to a threefold axis. In all cases, a face of the 'domain of influence' is perpendicular to each basis vector of these primitive cells.

9.1.8. Delaunay reduction

Further classifications use reduction theory. There are different approaches to the reduction of quadratic forms in mathematics. The two most important in our context are

(i) the Selling–Delaunay reduction (Selling, 1874),

(ii) the Eisenstein–Niggli reduction.

The investigations by Gruber (*cf.* Chapter 9.3) have shown the common root of both crystallographic approaches. As in Chapters 9.2 and 9.3 the Niggli reduction will be discussed in detail, we shall discuss the Delaunay reduction here.

We start with a lattice basis $(\mathbf{b}_i)_{1 \leq i \leq n}$ $(n = 2, 3)$. This basis is extended by a vector

$$\mathbf{b}_{n+1} = -(\mathbf{b}_1 + \ldots + \mathbf{b}_n).$$

All scalar products

$$\mathbf{b}_i \cdot \mathbf{b}_k \ (1 \leq i < k \leq n+1)$$

Table 9.1.7.2. *Three-dimensional Bravais lattices*

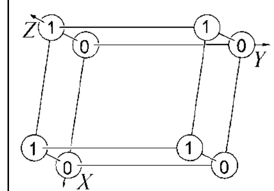
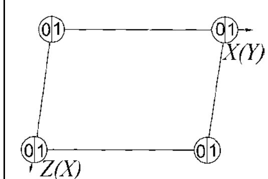
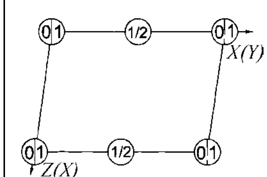
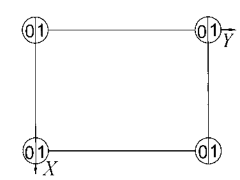
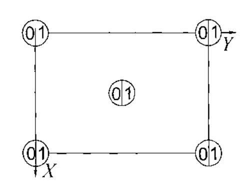
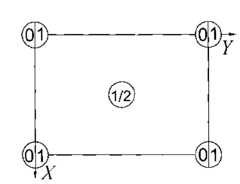
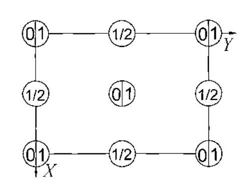
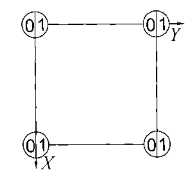
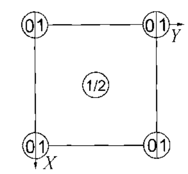
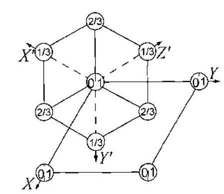
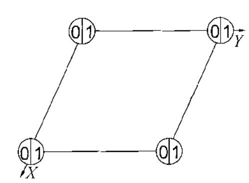
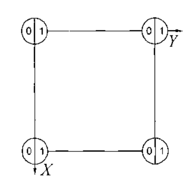
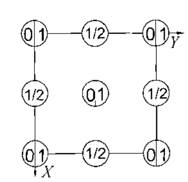
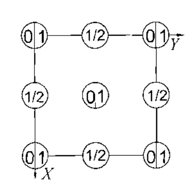
Bravais lattice*	Lattice parameters: Conventional	Lattice parameters: Primitive	Metric tensor: Conventional	Metric tensor: Primitive/transf.†	Metric tensor: Relations of the components	Projections
aP	a, b, c α, β, γ	a, b, c α, β, γ	$\begin{matrix} g_{11} & g_{12} & g_{13} \\ & g_{22} & g_{23} \\ & & g_{33} \end{matrix}$	$\begin{matrix} g_{11} & g_{12} & g_{13} \\ & g_{22} & g_{23} \\ & & g_{33} \end{matrix}$		
mP	a, b, c $\beta, \alpha = \gamma = 90^\circ$	a, b, c $\beta, \alpha = \gamma = 90^\circ$	$\begin{matrix} g_{11} & 0 & g_{13} \\ & g_{22} & 0 \\ & & g_{33} \end{matrix}$	$\begin{matrix} g_{11} & 0 & g_{13} \\ & g_{22} & 0 \\ & & g_{33} \end{matrix}$		
mC (mS)		$a_1 = a_2, c$ $\gamma, \alpha = \beta$		$\boldsymbol{P}(C)$ $\begin{matrix} g'_{11} & g'_{12} & g'_{13} \\ & g'_{11} & g'_{13} \\ & & g_{33} \end{matrix}$	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g'_{13} = \frac{1}{2} g_{13}$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{22} = 2(g'_{11} - g'_{12})$ $g_{13} = 2g'_{13}$	
oP	a, b, c $\alpha = \beta = \gamma = 90^\circ$	a, b, c $\alpha = \beta = \gamma = 90^\circ$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{22} & 0 \\ & & g_{33} \end{matrix}$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{22} & 0 \\ & & g_{33} \end{matrix}$		
oC (oS)		$a_1 = a_2, c$ $\gamma, \alpha = \beta = 90^\circ$		$\boldsymbol{P}(C)$ $\begin{matrix} g'_{11} & g'_{12} & 0 \\ & g'_{11} & 0 \\ & & g_{33} \end{matrix}$	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{22} = 2(g'_{11} - g'_{12})$	
oI		$a_1 = a_2 = a_3$ α, β, γ $\cos\alpha + \cos\beta$ $+ \cos\gamma = -1$		$\boldsymbol{P}(I)$ $\begin{matrix} -\tilde{g} & g'_{12} & g'_{13} \\ & -\tilde{g} & g'_{23} \\ & & -\tilde{g} \end{matrix}$ $\tilde{g} = g'_{12} + g'_{13} + g'_{23}$	$g'_{12} = \frac{1}{4}(-g_{11} - g_{22} + g_{33})$ $g'_{13} = \frac{1}{4}(-g_{11} + g_{22} - g_{33})$ $g'_{23} = \frac{1}{4}(g_{11} - g_{22} - g_{33})$ $g_{11} = -2(g'_{12} + g'_{13})$ $g_{22} = -2(g'_{12} + g'_{23})$ $g_{33} = -2(g'_{13} + g'_{23})$	
oF		a, b, c α, β, γ $\cos\alpha = \frac{-a^2 + b^2 + c^2}{2bc}$ $\cos\beta = \frac{a^2 + b^2 + c^2}{2ac}$ $\cos\gamma = \frac{a^2 + b^2 - c^2}{2ab}$		$\boldsymbol{P}(F)$ $\begin{matrix} \tilde{g}_1 & g'_{12} & g'_{13} \\ & \tilde{g}_2 & g'_{23} \\ & & \tilde{g}_3 \end{matrix}$ $\tilde{g}_1 = g'_{12} + g'_{13}$ $\tilde{g}_2 = g'_{12} + g'_{23}$ $\tilde{g}_3 = g'_{13} + g'_{23}$	$g'_{12} = \frac{1}{4} g_{33}$ $g'_{13} = \frac{1}{4} g_{22}$ $g'_{23} = \frac{1}{4} g_{11}$ $g_{11} = 4g'_{23}$ $g_{22} = 4g'_{13}$ $g_{33} = 4g'_{12}$	

Table 9.1.7.2. *Three-dimensional Bravais lattices* (*cont.*)

Bravais lattice*	Lattice parameters: Conventional	Lattice parameters: Primitive	Metric tensor: Conventional	Metric tensor: Primitive/transf.†	Metric tensor: Relations of the components	Projections
tP	$a_1 = a_2, c$ $\alpha = \beta = \gamma = 90°$	$a_1 = a_2, c$ $\alpha = \beta = \gamma = 90°$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{matrix}$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{matrix}$		
tI		$a_1 = a_2 = a_3$ $\gamma, \alpha = \beta$ $2\cos\alpha + \cos\gamma = -1$		$\boldsymbol{P}(I)$ $\begin{matrix} \bar{g} & g'_{12} & g'_{13} \\ & \bar{g} & g'_{13} \\ & & \bar{g} \end{matrix}$ $\bar{g} = -(g'_{12} + 2g'_{13})$	$g'_{12} = \frac{1}{4}(-2g_{11} + g_{33})$ $g'_{13} = -\frac{1}{4}g_{33}$ $g_{11} = 2(g'_{12} + g'_{13})$ $g_{33} = -4g'_{13}$	
hR	$a_1 = a_2, c$ $\alpha = \beta = 90°$ $\gamma = 120°$	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma$	$\begin{matrix} g_{11} & -\frac{1}{2}g_{11} & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{matrix}$	$\boldsymbol{P}(R)$ $\begin{matrix} g'_{11} & g'_{12} & g'_{12} \\ & g'_{11} & g'_{12} \\ & & g'_{11} \end{matrix}$	$g'_{11} = \frac{1}{9}(3g_{11} + g_{33})$ $g'_{12} = \frac{1}{9}(-\frac{3}{2}g_{11} + g_{33})$ $g_{11} = 2(g'_{11} - g'_{12})$ $g_{33} = 3(g'_{11} + 2g'_{12})$	
hP		$a_1 = a_2, c$ $\alpha = \beta = 90°$ $\gamma = 120°$		$\begin{matrix} g_{11} & -\frac{1}{2}g_{11} & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{matrix}$		
cP	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{11} \end{matrix}$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{11} \end{matrix}$		
cI		$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 109.5°$ $\cos\alpha = -\frac{1}{3}$		$\boldsymbol{P}(I)$ $\begin{matrix} g'_{11} & -\frac{1}{3}g'_{11} & -\frac{1}{3}g'_{11} \\ & g'_{11} & -\frac{1}{3}g'_{11} \\ & & g'_{11} \end{matrix}$	$g'_{11} = \frac{3}{4}g_{11}$ $g_{11} = \frac{4}{3}g'_{11}$	
cF		$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 60°$		$\boldsymbol{P}(F)$ $\begin{matrix} g'_{11} & \frac{1}{2}g'_{11} & \frac{1}{2}g'_{11} \\ & g'_{11} & \frac{1}{2}g'_{11} \\ & & g'_{11} \end{matrix}$	$g'_{11} = \frac{1}{2}g_{11}$ $g_{11} = 2g'_{11}$	

* See footnote to Table 9.1.7.1. Symbols in parentheses are standard symbols, see Table 2.1.2.1.

† $\boldsymbol{P}(C) = \frac{1}{2}(110/\bar{1}10/002), \boldsymbol{P}(I) = \frac{1}{2}(\bar{1}11/1\bar{1}1/11\bar{1}), \boldsymbol{P}(F) = \frac{1}{2}(011/101/110), \boldsymbol{P}(R) = \frac{1}{3}(\bar{1}2\bar{1}/\bar{2}11/111)$.

Table 9.1.8.1. *The 24 'Symmetrische Sorten'*

In the centred monoclinic lattices, the set $\{\mathbf{a}, \mathbf{c}, \mathbf{a}+\mathbf{c}\} = \{\mathbf{p}, \mathbf{q}, \mathbf{r}\}$ of the three shortest vectors in the **ac** plane is used to describe the metrical conditions. These vectors are renamed according to their relation to the projection of the centring point in the **ac** plane: **p** designates the vector that crosses the projection of the centring point, **q** is the shorter one of the two others and **r** labels the third one.

Delaunay symbol	Bravais type	Metrical conditions (parameters of conventional cells)	Voronoi type	Notation of the scalar products according to equation (9.1.8.1)						Transformation matrix $\boldsymbol{P}$
				12	13	14	23	24	34	
$K1$	cI	–	I	12	12	12	12	12	12	$011/101/110$
$K2$	cF	–	III	0	13	13	13	13	0	$1\bar{1}1/111/002$
$K3$	cP	–	V	0	0	14	14	14	0	$100/001/011$
				0	0	14	0	14	14	$100/010/001$
H	hP	–	IV	12	0	12	0	12	34	$100/010/001$
$R1$	hR	$2c^2 < 3a^2$	I	12	12	14	12	14	14	$101/\bar{1}11/0\bar{1}1$
$R2$	hR	$2c^2 > 3a^2$	III	0	13	13	13	24	0	$101/003/012$
$Q1$	tI	$c^2 < 2a^2$	I	12	13	13	13	13	12	$011/101/110$
$Q2$	tI	$c^2 > 2a^2$	II	0	13	13	13	13	34	$101/011/002$
$Q3$	tP	–	V	0	0	14	0	14	34	$100/010/001$
				0	0	14	14	24	0	$100/001/011$
				0	0	14	23	0	23	$001/110/010$
$O1$	oF	–	I	12	13	13	13	13	34	$1\bar{1}1/111/002$
$O2$	oI	$a^2+b^2 > c^2$	I	12	13	14	14	13	12	$011/101/110$
$O3$	oI	$a^2+b^2 < c^2$	II	0	13	13	23	23	34	$101/011/002$
$O4$	oI	$a^2+b^2 = c^2$	III	0	13	14	14	13	0	$011/101/110$
				0	13	13	23	23	0	$101/011/002$
$O5$	$o(AB)C$	–	IV	12	0	14	0	12	34	$200/110/001$
				12	0	14	0	14	34	$110/\bar{1}10/001$
$O6$	oP	–	V	0	0	14	0	24	34	$100/010/001$
				0	0	14	23	24	0	$100/001/011$
$M1$	$m(AC)I$	$b^2 > p^2$	I	12	13	14	13	14	34	$\bar{1}10/\bar{1}\bar{1}0/\bar{1}01$
$M2$	$m(AC)I$	$p^2 > b^2 > r^2 - q^2$	I	12	13	14	14	13	34	$01\bar{1}/110/10\bar{1}$
$M3$	$m(AC)I$	$r^2 - q^2 > b^2$	II	0	13	14	23	23	34	$\bar{1}01/\bar{1}10/\bar{2}00$
$M4$	$m(AC)I$	$b^2 = p^2$	II	0	13	14	14	13	34	$01\bar{1}/110/10\bar{1}$
				0	13	14	13	14	34	$\bar{1}10/\bar{1}\bar{1}0/\bar{1}01$
$M5$	$m(AC)I$	$b^2 = r^2 - q^2$	III	0	13	14	23	23	0	$\bar{1}01/\bar{1}10/\bar{2}00$
				0	13	14	23	13	0	$10\bar{1}/\bar{1}10/0\bar{1}\bar{1}$
$M6$	mP	–	IV	0	13	14	0	24	34	$100/010/001$
$T1$	aP	–	I	12	13	14	23	24	34	$100/010/001$
$T2$	aP	–	II	0	13	14	23	24	34	$100/010/001$
$T3$	aP	–	III	0	13	14	23	24	0	$100/010/001$

Table 9.1.9.1. *Example*

Transformation				Scalar products					
				12	13	14	23	24	34
$\mathbf{b}_1$	$\mathbf{b}_2$	$\mathbf{b}_3$	$\mathbf{b}_4$	−0.271	0.265	−22.02	−24.37	0.272	−32.51
$-\mathbf{b}_1$	$\mathbf{b}_1 + \mathbf{b}_2$	$\mathbf{b}_3$	$\mathbf{b}_1 + \mathbf{b}_4$	−21.75	−0.265	0	−24.10	~0	−32.24
$\mathbf{b}_1'$	$\mathbf{b}_3'$	$\mathbf{b}_4'$	$\mathbf{b}_2'$	13	14	12	34	23	24

are considered. The reduction is performed minimizing the sum

$$\sum = {\mathbf{b}_1}^2 + \ldots + {\mathbf{b}_{n+1}}^2. \qquad (9.1.8.1)$$

It can be shown that this sum can be reduced as long as one of the scalar products is still positive. If *e.g.* the scalar product $\mathbf{b}_1 \cdot \mathbf{b}_2$ is still positive, a transformation can be performed such that the sum $\sum'$ of the transformed $\mathbf{b}_i'^2$ is smaller than $\sum$:

$$\mathbf{b}_1' = -\mathbf{b}_1,\ \mathbf{b}_2' = \mathbf{b}_2,\ \mathbf{b}_3' = \mathbf{b}_1 + \mathbf{b}_3 \ \text{ and } \ \mathbf{b}_4' = \mathbf{b}_1 + \mathbf{b}_4.$$

In the two-dimensional case, $\mathbf{b}_3' = 2\mathbf{b}_1 + \mathbf{b}_3$ holds.

If all the scalar products are less than or equal to zero, the three shortest vectors forming the reduced basis are contained in the set

$$V = \{\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3, \mathbf{b}_4, \mathbf{b}_1 + \mathbf{b}_2, \mathbf{b}_2 + \mathbf{b}_3, \mathbf{b}_3 + \mathbf{b}_1\},$$

which corresponds to the maximal set of faces of the Dirichlet domain (14 faces).

For practical application, it is useful to classify the patterns of the resulting $n(n-1)/2$ scalar products regarding their equivalence or zero values. These classes of patterns correspond to the reduced bases and result in '*Symmetrische Sorten*' (Delaunay, 1933) that lead directly to the conventional crystallographic cells by fixed transformations (*cf.* Patterson & Love, 1957; Burzlaff & Zimmermann, 1993). Table 9.1.8.1 gives the list of the 24 '*symmetrische Sorten*'. Column 1 contains Delaunay's symbols, column 2 the symbol of the Bravais type. For monoclinic centred lattices, the matrix $\boldsymbol{P}$ of the last column transforms the primitive reduced cell into an *I*-centred cell, which has to be transformed to *A* or *C* according to the monoclinic standardization rules, if necessary. $\boldsymbol{P}$ operates on the basis in the following form:

$$(\mathbf{a}_r, \mathbf{b}_r, \mathbf{c}_r) \cdot \boldsymbol{P} = (\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c),$$

where $(\mathbf{a}_r, \mathbf{b}_r, \mathbf{c}_r)$ denotes the (1×3) matrix of the basis vectors of the reduced cell and $(\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c)$ the (1×3) matrix of the conventional cell.

Column 3 gives metrical conditions for the occurrence of certain Voronoi types. Column 5 indicates the relations among the scalar products of the reduced vector set. In some cases, different Selling patterns are given for one '*symmetrische Sorte*'. This procedure avoids a final reduction step (*cf.* Patterson & Love, 1957) and simplifies the computational treatment significantly. The number of '*symmetrische Sorten*', and thus the number of transformations which have to be applied, is smaller than the number of lattice characters according to Niggli. Note that the introduction of reduced bases using shortest lattice vectors causes complications in more than three dimensions (*cf.* Schwarzenberger, 1980).

9.1.9. Example

This example is discussed in Azároff & Buerger (1958, pp. 176–180).

The lattice parameters are given as $b_1 = 4.693$, $b_2 = 4.936$, $b_3 = 7.524$ Å, $\beta_{23} = 131.00$, $\beta_{31} = 89.57$, $\beta_{12} = 90.67°$. The scalar products resulting from these data are given in Table 9.1.9.1. The scalar product $\mathbf{b}_1 \cdot \mathbf{b}_3$ is positive. Thus the transformation

$$\mathbf{b}_1' = -\mathbf{b}_1,\ \mathbf{b}_3' = \mathbf{b}_3,\ \mathbf{b}_2' = \mathbf{b}_1 + \mathbf{b}_2,\ \mathbf{b}_4' = \mathbf{b}_1 + \mathbf{b}_4$$

is applied. The new scalar products are all non-positive as given in the second row of Table 9.1.9.1 (within the accuracy of the experimental data). Comparison with Table 9.1.8.1 leads to *M*6, Voronoi type IV and the monoclinic Bravais lattice *mP*.

The transformation related to this case leads to a monoclinic conventional cell but does not consider the possibility of shorter basis vectors. For this reason, it is necessary here to look at the other vectors of the set *V* in the $(\mathbf{b}_1'\mathbf{b}_3')$ plane, the only one of interest is $\mathbf{b}_1' + \mathbf{b}_3'$. The length of this vector is 4.936 Å, which is shorter than $\mathbf{b}_3'$ ($|\mathbf{b}_3'| = 6.771$ Å) and leads to the cell parameters $a = 4.693, b = 5.678, c = 4.936$ Å, $\alpha = 90, \beta = 90.67, \gamma = 90°$.

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9.2. Reduced bases

BY P. M. DE WOLFF

9.2.1. Introduction

Unit cells are usually chosen according to the conventions mentioned in Chapter 9.1 so one might think that there is no need for another standard choice. This is not true, however; conventions based on symmetry do not always permit unambiguous choice of the unit cell, and unconventional descriptions of a lattice do occur. They are often chosen for good reasons or they may arise from experimental limitations such as may occur, for example, in high-pressure work. So there is a need for normalized descriptions of crystal lattices.

Accordingly, the *reduced basis** (Eisenstein, 1851; Niggli, 1928), which is a primitive basis unique (apart from orientation) for any given lattice, is at present widely used as a means of classifying and identifying crystalline materials. A comprehensive survey of the principles, the techniques and the scope of such applications is given by Mighell (1976). The present contribution merely aims at an exposition of the basic concepts and a brief account of some applications.

The main criterion for the reduced basis is a metric one: choice of the shortest three non-coplanar lattice vectors as basis vectors. Therefore, the resulting bases are, in general, widely different from any symmetry-controlled basis, *cf.* Chapter 9.1.

9.2.2. Definition

A primitive basis **a**, **b**, **c** is called a 'reduced basis' if it is right-handed and if the components of the metric tensor **G** (*cf.* Chapter 9.1)

$$\begin{matrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{c} & \mathbf{c}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} \end{matrix} \qquad (9.2.2.1)$$

satisfy the conditions shown below. The matrix (9.2.2.1) for the reduced basis is called the *reduced form*.

Because of lattice symmetry there can be two or more possible orientations of the reduced basis in a given lattice but, apart from orientation, the reduced basis is unique.

Any basis, reduced or not, determines a unit cell – that is, the parallelepiped of which the basis vectors are edges. In order to test whether a given basis is the reduced one, it is convenient first to find the 'type' of the corresponding unit cell. The type of a cell depends on the sign of

$$T = (\mathbf{a}\cdot\mathbf{b})(\mathbf{b}\cdot\mathbf{c})(\mathbf{c}\cdot\mathbf{a}).$$

If $T > 0$, the cell is of type I, if $T \leq 0$ it is of type II. 'Type' is a property of the cell since T keeps its value when **a**, **b** or **c** is inverted. Geometrically speaking, such an inversion corresponds to moving the origin of the basis towards another corner of the cell. Corners with all three angles acute occur for cells of type I (one opposite pair, the remaining six corners having one acute and two obtuse angles). The other alternative, specified by main condition (ii) of Section 9.2.3, *viz* all three angles non-acute, occurs for cells of type II (one or more opposite pairs, the remaining corners having either one or two acute angles).

The conditions can all be stated analytically in terms of the components (9.2.2.1), as follows:

(*a*) Type-I cell

Main conditions:

$$\mathbf{a}\cdot\mathbf{a} \leq \mathbf{b}\cdot\mathbf{b} \leq \mathbf{c}\cdot\mathbf{c};\ |\mathbf{b}\cdot\mathbf{c}| \leq \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b};\ |\mathbf{a}\cdot\mathbf{c}| \leq \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a};\ |\mathbf{a}\cdot\mathbf{b}| \leq \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \qquad (9.2.2.2a)$$

$$\mathbf{b}\cdot\mathbf{c} > 0; \qquad \mathbf{a}\cdot\mathbf{c} > 0; \qquad \mathbf{a}\cdot\mathbf{b} > 0. \qquad (9.2.2.2b)$$

Special conditions:

$$\text{if } \mathbf{a}\cdot\mathbf{a} = \mathbf{b}\cdot\mathbf{b} \text{ then } \mathbf{b}\cdot\mathbf{c} \leq \mathbf{a}\cdot\mathbf{c} \qquad (9.2.2.3a)$$
$$\text{if } \mathbf{b}\cdot\mathbf{b} = \mathbf{c}\cdot\mathbf{c} \text{ then } \mathbf{a}\cdot\mathbf{c} \leq \mathbf{a}\cdot\mathbf{b} \qquad (9.2.2.3b)$$
$$\text{if } \mathbf{b}\cdot\mathbf{c} = \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b} \text{ then } \mathbf{a}\cdot\mathbf{b} \leq 2\mathbf{a}\cdot\mathbf{c} \qquad (9.2.2.3c)$$
$$\text{if } \mathbf{a}\cdot\mathbf{c} = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{b} \leq 2\mathbf{b}\cdot\mathbf{c} \qquad (9.2.2.3d)$$
$$\text{if } \mathbf{a}\cdot\mathbf{b} = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{c} \leq 2\mathbf{b}\cdot\mathbf{c}. \qquad (9.2.2.3e)$$

(*b*) Type-II cell

Main conditions:

$$\text{as } (9.2.2.2a) \qquad (9.2.2.4a)$$
$$(|\mathbf{b}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{b}|) \leq \tfrac{1}{2}(\mathbf{a}\cdot\mathbf{a} + \mathbf{b}\cdot\mathbf{b}) \qquad (9.2.2.4b)$$
$$\mathbf{b}\cdot\mathbf{c} \leq 0; \qquad \mathbf{a}\cdot\mathbf{c} \leq 0; \qquad \mathbf{a}\cdot\mathbf{b} \leq 0. \qquad (9.2.2.4c)$$

Special conditions:

$$\text{if } \mathbf{a}\cdot\mathbf{a} = \mathbf{b}\cdot\mathbf{b} \text{ then } |\mathbf{b}\cdot\mathbf{c}| \leq |\mathbf{a}\cdot\mathbf{c}| \qquad (9.2.2.5a)$$
$$\text{if } \mathbf{b}\cdot\mathbf{b} = \mathbf{c}\cdot\mathbf{c} \text{ then } |\mathbf{a}\cdot\mathbf{c}| \leq |\mathbf{a}\cdot\mathbf{b}| \qquad (9.2.2.5b)$$
$$\text{if } |\mathbf{b}\cdot\mathbf{c}| = \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b} \text{ then } \mathbf{a}\cdot\mathbf{b} = 0 \qquad (9.2.2.5c)$$
$$\text{if } |\mathbf{a}\cdot\mathbf{c}| = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{b} = 0 \qquad (9.2.2.5d)$$
$$\text{if } |\mathbf{a}\cdot\mathbf{b}| = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{c} = 0 \qquad (9.2.2.5e)$$
$$\text{if } (|\mathbf{b}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{b}|) = \tfrac{1}{2}(\mathbf{a}\cdot\mathbf{a} + \mathbf{b}\cdot\mathbf{b}) \text{ then } \mathbf{a}\cdot\mathbf{a} \leq 2|\mathbf{a}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{b}|. \qquad (9.2.2.5f)$$

The geometrical interpretation in the following sections is given in order to make the above conditions more explicit rather than to replace them, since the analytical form is obviously the most suitable one for actual verification.

9.2.3. Main conditions

The main conditions† express the following two requirements:

(i) Of all lattice vectors, none is shorter than **a**; of those not directed along **a**, none is shorter than **b**; of those not lying in the **ab** plane, none is shorter than **c**. This requirement is expressed analytically by (9.2.2.2*a*), and for type-II cells by (9.2.2.4*b*), which for type-I cells is redundant.

(ii) The three angles between basis vectors are either all acute or all non-acute, conditions (9.2.2.2*b*) and (9.2.2.4*c*). As shown in Section 9.2.2 for a given unit cell, the origin corner can always be

* Very often, the term 'reduced cell' is used to indicate this normalized lattice description. To avoid confusion, we shall use 'reduced basis', since it is actually a basis and some of the criteria are related precisely to the difference between unit cells and vector bases.

† In a book on reduced cells and on retrieval of symmetry information from lattice parameters, Gruber (1978) reformulated the main condition (i) as a minimum condition on the sum $s = a + b + c$. He also examined the surface areas of primitive unit cells in a given lattice, which are easily shown to be proportional to the corresponding sums $s^* = a^* + b^* + c^*$ for the reciprocal bases. He finds that if there are two or more non-congruent cells with minimum s ('Buerger cells'), these cells always have different values of s^*. Gruber (1989) proposes a new criterion to replace the conditions (9.2.2.2*a*)–(9.2.2.5*f*), *viz* that, among the cells with the minimum s value, the one with the smallest value of s^* be chosen (which need not be the absolute minimum of s^* since that may occur for cells that are not Buerger cells). The analytic form of this criterion is identical to (9.2.2.2*a*)–(9.2.2.5*e*); only (9.2.2.5*f*) is altered. For further details, see Chapter 9.3.

chosen so as to satisfy either the first alternative of this condition (if the cell is of type I) or the second (if the cell is of type II).

Condition (i) is by far the most essential one. It uniquely defines the lengths a, b and c, and limits the angles to the range $60 \leq \alpha, \beta, \gamma \leq 120°$. However, there are often different unit cells satisfying (i), *cf.* Gruber (1973). In order to find the reduced basis, starting from an arbitrary one given by its matrix (9.2.2.1), one can: (*a*) find some basis satisfying (i) and (ii) and if necessary modify it so as to fulfil the special conditions as well; (*b*) find all bases satisfying (i) and (ii) and test them one by one with regard to the special conditions until the reduced form is found. Method (*a*) relies mainly on an algorithm by Buerger (1957, 1960), *cf.* also Mighell (1976). Method (*b*) stems from a theorem and an algorithm, both derived by Delaunay (1933); the theorem states that the desired basis vectors **a**, **b** and **c** are among seven (or fewer) vectors – the distance vectors between parallel faces of the Voronoi domain – which follow directly from the algorithm. The method has been established and an example is given by Delaunay *et al.* (1973), *cf.* Section 9.1.3 where this method is described.

9.2.4. Special conditions

For a given lattice, the main condition (i) defines not only the lengths a, b, c of the reduced basis vectors but also the plane containing **a** and **b**, in the sense that departures from special conditions can be repaired by transformations which do not change this plane. An exception can occur when $b = c$; then such transformations must be supplemented by interchange(s) of **b** and **c** whenever either (9.2.2.3*b*) or (9.2.2.5*b*) is not fulfilled. All the other conditions can be conveniently illustrated by projections of part of the lattice onto the **ab** plane as shown in Figs. 9.2.4.1 to 9.2.4.5. Let us represent the vector lattice by a point lattice. In Fig. 9.2.4.1, the net in the **ab** plane (of which *OBAD* is a primitive mesh; $OA = a$, $OB = b$) is shown as well as the projection (normal to that plane) of the adjoining layer which is assumed to lie above the paper. In general, just one lattice node P_0 of that layer, projected in Fig. 9.2.4.1 as P, will be closer to the origin than all others. Then the vector $\overrightarrow{OP_0}$ is $\pm\mathbf{c}$ according to condition (i). It should be stressed that, though the **ab** plane is most often (see above) correctly established by (i), the vectors **a**, **b** and **c** still have to be chosen so as to comply with (ii), with the special conditions, and with right-handedness. The result will depend on the position of P with respect to the net. This dependence will now be investigated.

The inner hexagon shown, which is the two-dimensional Voronoi domain around O, limits the possible projected positions P of P_0. Its short edges, normal to OD, result from (9.2.2.4*b*); the other edges from (9.2.2.2*a*). If the spacing d between **ab** net planes is smaller than b, the region allowed for P is moreover limited inwardly by the circle around O with radius $(b^2 - d^2)^{1/2}$, corresponding to the projection of points P_0 for which $OP_0 = c = b$. The case $c = b$ has been dealt with, so in order to simplify the drawings we shall assume $d > b$. Then, for a given value of d, each point within the above-mentioned hexagonal domain, regarded as the projection of a lattice node P_0 in the next layer, completely defines a lattice based on $\overrightarrow{OA}$, $\overrightarrow{OB}$ and $\overrightarrow{OP_0}$. Diametrically opposite points like P and P' represent the same lattice in two orientations differing by a rotation of 180° in the plane of the figure. Therefore, the systematics of reduced bases can be shown completely in just half the domain. As a halving line, the n_a normal to OA is chosen. This is an important boundary in view of condition (ii), since it separates points P for which the angle between OP_0 and OA is acute from those for which it is obtuse.

Similarly, n_b, normal to OB, separates the sharp and obtuse values of the angles P_0OB. It follows that if P lies in the obtuse sector (cross-hatched area) between n_a and n_b, the reduced cell is of type I, with basis vectors $\mathbf{a}^{\mathrm{I}}$, $\mathbf{b}^{\mathrm{I}}$, and $OP_0 = +\mathbf{c}$. Otherwise (hatched

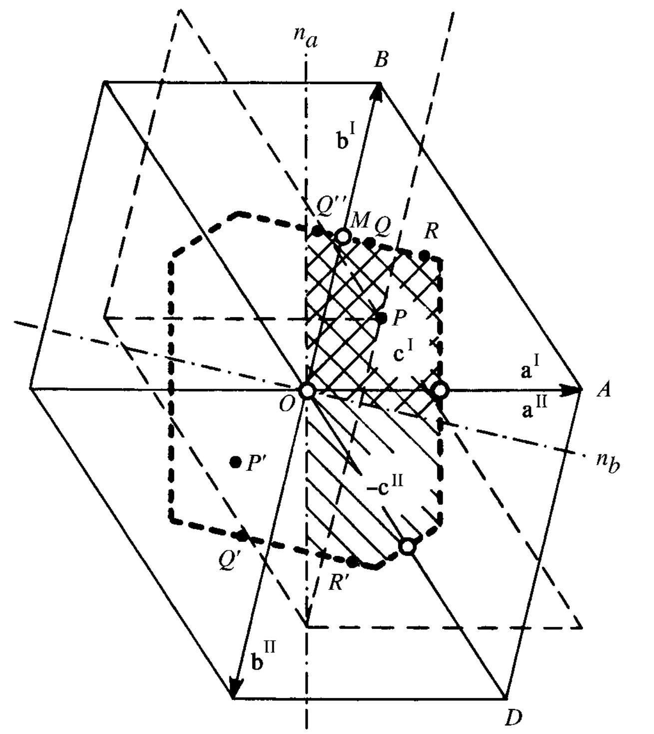

Fig. 9.2.4.1. The net of lattice points in the plane of the reduced basis vectors **a** and **b**; *OBAD* is a primitive mesh. The actual choice of **a** and **b** depends on the position of the point P, which is the projection of the point P_0 in the next layer (supposed to lie above the paper, thin dashed lines) closest to O. Hence, P is confined to the Voronoi domain (dashed hexagon) around O. For a given interlayer distance, P defines the complete lattice. In that sense, P and P' represent identical lattices; so do Q, Q' and Q'', and also R and R'. When P lies in a region marked $-c^{\mathrm{II}}$ (hatched), the reduced type-II basis is formed by $\mathbf{a}^{\mathrm{II}}$, $\mathbf{b}^{\mathrm{II}}$ and $\mathbf{c} = -\overrightarrow{OP}_0$. Regions marked c^{I} (cross-hatched) have the reduced type-I basis $\mathbf{a}^{\mathrm{I}}$, $\mathbf{b}^{\mathrm{I}}$ and $\mathbf{c} = +\overrightarrow{OP}_0$. Small circles in O, M *etc.* indicate twofold rotation points lying on the region borders (see text).

area), we have a type-II reduced cell, with $OP_0 = -\mathbf{c}$ and $+\mathbf{a}$ and $+\mathbf{b}$ as shown by $\mathbf{a}^{\mathrm{II}}$ and $\mathbf{b}^{\mathrm{II}}$.

Since type II includes the case of right angles, the borders of this region on n_a and n_b are inclusive. Other borderline cases are points like R and R', separated by **b** and thus describing the same lattice. By condition (9.2.2.5*c*) the reduced cell for such cases is excluded from type II (except for rectangular **a**, **b** nets, *cf.* Fig. 9.2.4.2); so the projection of **c** points to R, not R'. Accordingly, this part of the border is inclusive for the type-I region and exclusive (at R') for the type-II region as indicated in Fig. 9.2.4.3. Similarly, (9.2.2.5*d*) defines which part of the border normal to OA is inclusive.

The inclusive border is seen to end where it crosses OA, OB or OD. This is prescribed by the conditions (9.2.2.3*d*), (9.2.2.3*c*) and (9.2.2.5*f*), respectively. The explanation is given in Fig. 9.2.4.1 for (9.2.2.3*c*): The points Q and Q'' represent the same lattice because Q' (diametrically equivalent to Q as shown before) is separated from Q'' by the vector **b**. Hence, the point M halfway between O and B is a twofold rotation point just like O. For a primitive orthogonal **a**, **b** net, only type II occurs according to (9.2.2.5*c*) and (9.2.2.5*d*), *cf.* Fig. 9.2.4.2. A centred orthogonal **a**, **b** net of elongated character (shortest net vector in a symmetry direction, *cf.* Section 9.2.5) is depicted in Fig. 9.2.4.4. It yields type-I cells except when $\beta = 90°$ [condition (9.2.2.5*c*)]. Moreover, (9.2.2.3*c*) eliminates part of the type-I region as compared to Fig. 9.2.4.3. Finally, a centred net with compressed character (shortest two net vectors equal in length) requires criteria allowing unambiguous designation of **a** and **b**.

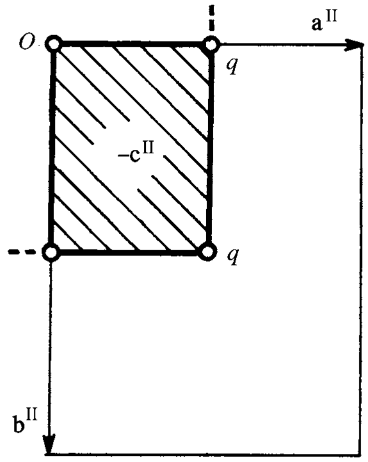

Fig. 9.2.4.2. The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. The type-I and type-II regions are marked as in Fig. 9.2.4.1. A heavy border line of a region stops short of an end point if the latter is not included in the region to which the border belongs. **a**, **b** net primitive orthogonal; special conditions (9.2.2.5*c*), (9.2.2.5*d*).

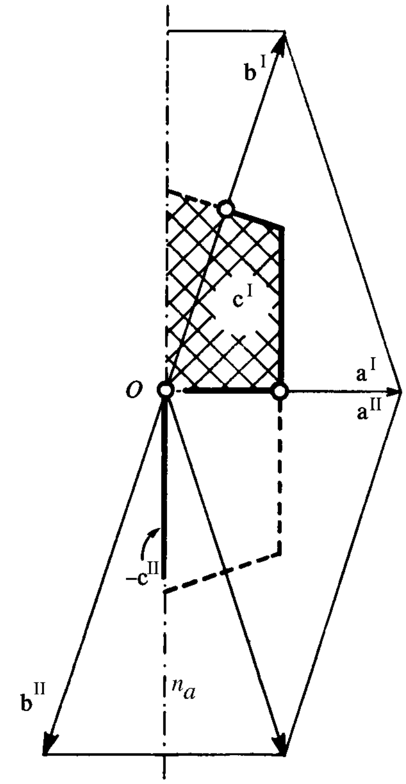

Fig. 9.2.4.4. The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. The type-I region is cross-hatched; the type-II region is a mere line. A heavy border line of a region stops short of an end point if the latter is not included in the region to which the border belongs. **a**, **b** net centred orthogonal (elongated); special conditions (9.2.2.3*e*), (9.2.2.5*e*).

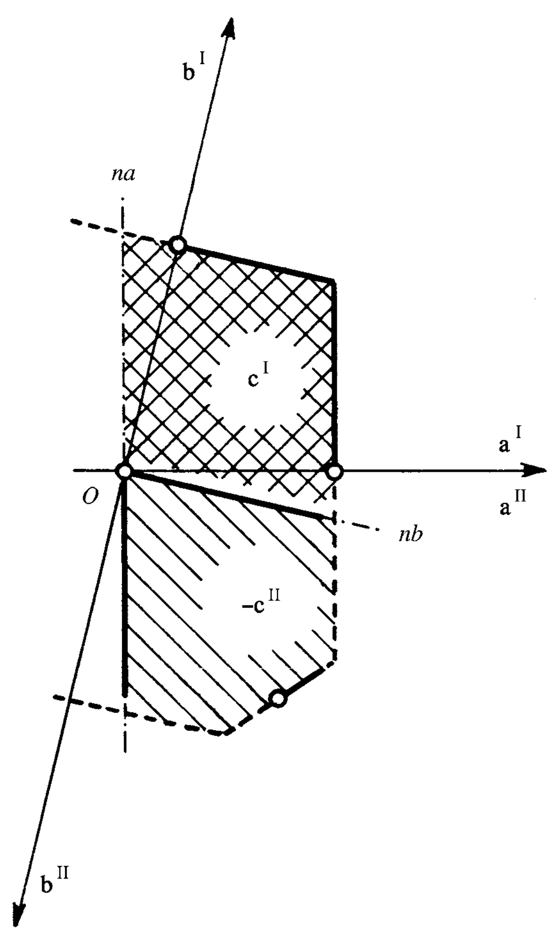

Fig. 9.2.4.3. The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. Type-I and type-II regions are marked as in Fig. 9.2.4.1. n_b belongs to the type-II region. A heavy border line of a region stops short of an end point if the latter is not included in the region to which the border belongs. **a**, **b** net oblique; special conditions (9.2.2.3*c*), (9.2.2.3*d*), (9.2.2.5*f*).

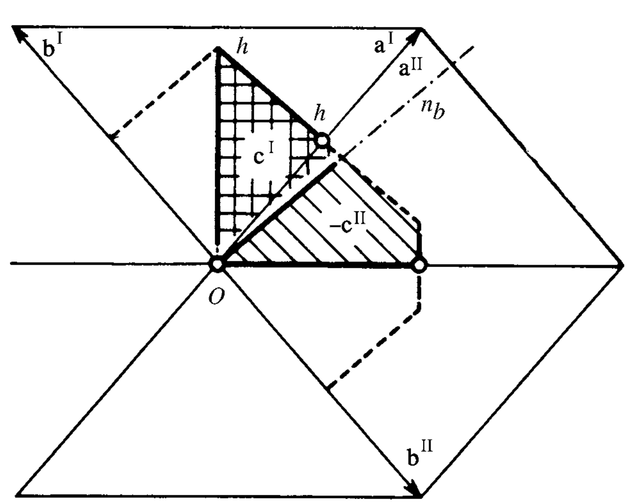

Fig. 9.2.4.5. The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. Type-I and type-II regions are marked as in Fig. 9.2.4.1. n_b belongs to the type-II region. A heavy border line of a region stops short of an end point if the latter is not included in the region to which the border belongs. **a**, **b** net centred orthogonal (compressed); special conditions (9.2.2.3*a*), (9.2.2.5*a*).

Table 9.2.5.1. *The parameters $D = \mathbf{b} \cdot \mathbf{c}$, $E = \mathbf{a} \cdot \mathbf{c}$ and $F = \mathbf{a} \cdot \mathbf{b}$ of the 44 lattice characters ($A = \mathbf{a} \cdot \mathbf{a}$, $B = \mathbf{b} \cdot \mathbf{b}$, $C = \mathbf{c} \cdot \mathbf{c}$)*

The character of a lattice given by its reduced form (9.2.2.1) is the first one that agrees when the 44 entries are compared with that reduced form in the sequence given below (suggested by Gruber). Such a logical order is not always obeyed by the widely used character numbers (first column), which therefore show some reversals, *e.g.* 4 and 5.

No.	Type	D	E	F	Lattice symmetry	Bravais type‡	Transformation to a conventional basis (*cf.* Table 9.2.5.2, footnote **)
$A = B = C$							
1	I	$A/2$	$A/2$	$A/2$	Cubic	cF	$1\bar{1}1/11\bar{1}/\bar{1}11$
2	I	D	D	D	Rhombohedral	hR	$1\bar{1}0/\bar{1}01/\bar{1}\bar{1}\bar{1}$
3	II	0	0	0	Cubic	cP	$100/010/001$
5	II	$-A/3$	$-A/3$	$-A/3$	Cubic	cI	$101/110/011$
4	II	D	D	D	Rhombohedral	hR	$1\bar{1}0/\bar{1}01/\bar{1}\bar{1}\bar{1}$
6	II	D*	D	F	Tetragonal	tI	$011/101/110$
7	II	D*	E	E	Tetragonal	tI	$101/110/011$
8	II	D*	E	F	Orthorhombic	oI	$\bar{1}\bar{1}0/\bar{1}0\bar{1}/0\bar{1}\bar{1}$
$A = B$, no conditions on C							
9	I	$A/2$	$A/2$	$A/2$	Rhombohedral	hR	$100/\bar{1}10/\bar{1}\bar{1}3$
10	I	D	D	F	Monoclinic	mC	$110/1\bar{1}0/00\bar{1}$
11	II	0	0	0	Tetragonal	tP	$100/010/001$
12	II	0	0	$-A/2$	Hexagonal	hP	$100/010/001$
13	II	0	0	F	Orthorhombic	oC	$110/\bar{1}10/001$
15	II	$-A/2$	$-A/2$	0	Tetragonal	tI	$100/010/112$
16	II	D*	D	F	Orthorhombic	oF	$\bar{1}\bar{1}0/1\bar{1}0/112$
14	II	D	D	F	Monoclinic	mC	$110/\bar{1}10/001$
17	II	D*	E	F	Monoclinic	mC	$1\bar{1}0/110/\bar{1}0\bar{1}$
$B = C$, no conditions on A							
18	I	$A/4$	$A/2$	$A/2$	Tetragonal	tI	$0\bar{1}1/1\bar{1}\bar{1}/100$
19	I	D	$A/2$	$A/2$	Orthorhombic	oI	$\bar{1}00/0\bar{1}1/\bar{1}11$
20	I	D	E	E	Monoclinic	mC	$011/01\bar{1}/\bar{1}00$
21	II	0	0	0	Tetragonal	tP	$010/001/100$
22	II	$-B/2$	0	0	Hexagonal	hP	$010/001/100$
23	II	D	0	0	Orthorhombic	oC	$011/0\bar{1}1/100$
24	II	D*	$-A/3$	$-A/3$	Rhombohedral	hR	$121/0\bar{1}1/100$
25	II	D	E	E	Monoclinic	mC	$011/0\bar{1}1/100$
No conditions on A, B, C							
26	I	$A/4$	$A/2$	$A/2$	Orthorhombic	oF	$100/\bar{1}20/\bar{1}02$
27	I	D	$A/2$	$A/2$	Monoclinic	mC	$\bar{1}20/\bar{1}00/0\bar{1}1$
28	I	D	$A/2$	$2D$	Monoclinic	mC	$\bar{1}00/\bar{1}02/010$
29	I	D	$2D$	$A/2$	Monoclinic	mC	$100/1\bar{2}0/00\bar{1}$
30	I	$B/2$	E	$2E$	Monoclinic	mC	$010/01\bar{2}/\bar{1}00$
31	I	D	E	F	Triclinic	aP	$100/010/001$
32	II	0	0	0	Orthorhombic	oP	$100/010/001$
40	II	$-B/2$	0	0	Orthorhombic	oC	$0\bar{1}0/012/\bar{1}00$
35	II	D	0	0	Monoclinic	mP	$0\bar{1}0/\bar{1}00/00\bar{1}$
36	II	0	$-A/2$	0	Orthorhombic	oC	$100/\bar{1}0\bar{2}/010$
33	II	0	E	0	Monoclinic	mP	$100/010/001$
38	II	0	0	$-A/2$	Orthorhombic	oC	$\bar{1}00/120/00\bar{1}$
34	II	0	0	F	Monoclinic	mP	$\bar{1}00/00\bar{1}/0\bar{1}0$
42	II	$-B/2$	$-A/2$	0	Orthorhombic	oI	$\bar{1}00/0\bar{1}0/112$
41	II	$-B/2$	E	0	Monoclinic	mC	$0\bar{1}\bar{2}/0\bar{1}0/\bar{1}00$
37	II	D	$-A/2$	0	Monoclinic	mC	$102/100/010$
39	II	D	0	$-A/2$	Monoclinic	mC	$\bar{1}\bar{2}0/\bar{1}00/00\bar{1}$
43	II	D†	E	F	Monoclinic	mI	$\bar{1}00/\bar{1}\bar{1}\bar{2}/0\bar{1}0$
44	II	D	E	F	Triclinic	aP	$100/010/001$

* $2|D + E + F| = A + B$.
† As footnote * plus $|2D + F| = B$.
‡ For symbols for Bravais types see footnote * to Table 9.1.7.1 and de Wolff *et al.* (1985). The capital letter of the symbols in this column indicates the centring type of the cell as obtained by the transformation in the last column. For this reason, the standard symbols mS and oS are not used here.

Table 9.2.5.2. *Lattice characters described by relations between conventional cell parameters*

Under each of the roman numerals below ‘Lattice characters in’, *numbers* of characters (*cf.* Table 9.2.5.1, first column) are listed for which the key parameter *p* lies in the interval defined by the same roman numeral below ‘Intervals of *p*’. For instance, a lattice with character No. 15 under IV has $p = c/a$; so it falls in the interval IV with $\sqrt{2} < c/a\ (< \infty)$; No. 33 under II has $p = b$; therefore the interval $a - c$ for II yields the relation $a < b < c$.

Lattice symmetry	Bravais type*	p = key parameter	Lattice characters in I	II	III	IV	Intervals of p (I)	(II)	(III)	(IV)		Conventions**
Tetragonal	tP	c/a	21	11	–	–	0	1	∞	–	–	
Tetragonal	tI	c/a	18	6	7	15	0	$\sqrt{(2/3)}$	1	$\sqrt{2}$	∞	
Hexagonal	hP	c/a	22	12	–	–	0	1	∞	–	–	
Rhombohedral	hR	c/a	24	4	2	9	0	$\sqrt{(3/8)}$	$\sqrt{(3/2)}$	$\sqrt{6}$	∞	Hexagonal axes
Orthorhombic	oP	–	32 no relations				–	–	–	–	–	$a < b < c$
Orthorhombic	oS											
$b < a/\sqrt{3}$		c	23	13	–	–	0	d†	∞	–	–	$a < b$
$b > a/\sqrt{3}$		c	40	36	38	–	0	a	d†	∞	–	
Orthorhombic	oI	r‡	8	19	42	–	0	a	b	∞	–	$a < b < c$
Orthorhombic	oF	b/a	16	26	–	–	1	$\sqrt{3}$	∞	–	–	$a < b < c$
Monoclinic	mP	b	35	33	34	–	0	a	c	∞	–	$a < c$¶
Monoclinic	mS											
Centred net $= 1$§		b/a	–	–	–	28, 29	0	$\sqrt{(1/3)}$	1	$\sqrt{3}$	∞	C centred¶
Centred net $= 2$		b/a	–	–	–	30						
Centred net $= 2, 3$		b/a	37, 41	20	25	–						
Centred net $= 1, 2, 3$		b/a	27, 39	10, 17	14	–						
Centred net $= 3$		b/a	43	–	–	–	1	∞	–	–	–	I centred¶
Triclinic	aP	α, β, γ	31	44	–	–	60°	90°	120°	–	–	$a < b < c$
Cubic	cP	–		3 no relations			–	–	–	–	–	
	cI	–		5 no relations			–	–	–	–	–	
	cF	–		1 no relations			–	–	–	–	–	

* For symbols for Bravais types see footnote * to Table 9.1.7.1 and de Wolff *et al.* (1985).
† $d = \frac{1}{2}\sqrt{(a^2 + b^2)}$.
‡ $r = \frac{1}{2}\sqrt{(a^2 + b^2 + c^2)}$.
§ This number specifies the centred net among the three orthogonal nets parallel to the twofold axis and passing through (1) the shortest, (2) the second shortest, and (3) the third shortest lattice vector perpendicular to the axis. For example, ‘2, 3’ means that either net (2) or net (3) is the centred one.
¶ Setting with unique axis *b*; $\beta > 90°$; $a < c$ for both *P* and *I* cells, $a < c$ or $a > c$ for *C* cells.
** These conventions refer to the cells obtained by the transformations of Table 9.2.5.1. They have been chosen for convenience in this table.

These are conditions (9.2.2.3*a*) and (9.2.2.5*a*), *cf.* Fig. 9.2.4.5. The simplicity of these bisecting conditions, similar to those for the case $b = c$ mentioned initially, is apparent from that figure when compared with Fig. 9.2.4.3. This compressed type of centred orthogonal **a**, **b** net is limited by the case of a hexagonal net (where it merges with the elongated type, Fig. 9.2.4.4) and by the centred quadratic net (where it merges with the primitive orthogonal net, Fig. 9.2.4.2). In the limit of the hexagonal net, the triangle *Ohh* in Figs. 9.2.4.4 and 9.2.4.5 is all that remains, it is of type I except for the point *O*. For the quadratic net, only the type-II region in Fig. 9.2.4.5, then a triangle with all edges inclusive, is left. It corresponds to the triangle *Oqq* in Fig. 9.2.4.2.

9.2.5. Lattice characters

Apart from being unique, the reduced cell has the further advantage of allowing a much finer differentiation between types of lattices than is given by the Bravais types. For two-dimensional lattices, this is apparent already in the last section where the centred orthogonal class is subdivided into nets with elongated character and those with compressed character, depending on whether the shortest net vector is, or is not, a symmetry direction. It is impossible to perform a continuous deformation – within the centred orthogonal type – of an elongated net into a compressed one, since one has to pass through either a hexagonal or a quadratic net.

In three dimensions, lattices are of the same character if, first, a continuous deformation of one into the other is possible without leaving the Bravais type. Secondly, it is required that all matrix elements of the reduced form (9.2.2.1) change continuously during such a deformation. These criteria lead to 44 different *lattice characters* (Niggli, 1928; Buerger, 1957). Each of them can be recognized easily from the relations between the elements of the reduced form given in Table 9.2.5.1 [adapted from Table 5.1.3.1 in *IT* (1969), which was recently improved by Mighell & Rodgers (1980)]. The numbers in column 1 of this table are at the same time used as a general notation of the lattice characters themselves. We speak, for example, about the lattice character No. 7 (which is part of the Bravais type *tI*) *etc*.

In Table 9.2.5.2, another description of lattice characters is given by grouping together all characters of a given Bravais type and by indicating for each character the corresponding interval of values of a suitable parameter *p*, expressed in the usual parameters of a conventional cell. In systems where no generally accepted convention exists, the choice of this cell has been made for convenience in the last column of this table.

The subdistinctions 'centred net $= 1, 2$ or 3' for the monoclinic centred type are closely related to the description in other conventions. For instance, they correspond to *C*-, *A*- or *I*-centred cells, respectively, if **b** is the unique axis and **a** and **c** are the shortest vectors $(a < c)$ perpendicular to **b**; note that in Table 9.2.5.2 only *C* and *I*, not *A*, cells are listed. From the multiple entries in Table 9.2.5.2 for this type, it follows that the description in terms of b/a is not exhaustive; the distinctions depend upon rather intricate relations (*cf.* Mighell *et al.*, 1975; Mighell & Rodgers, 1980).

No attempt has been made in Table 9.2.5.2 to specify whether the end points of p intervals are inclusive or not. For practical purposes, they can always be taken to be non-inclusive. Indeed, the end points correspond either to a different Bravais type or to a purely geometric singularity without physical significance. If p is very close to an interval limit of the latter kind, one should be aware of the fact that different measurements of such a lattice may yield different characters, with totally differing aspects of the reduced form.

9.2.6. Applications

9.2.6.1. *Classification*

The reduced basis can be used to derive the Bravais-lattice type and the conventional cell parameters, starting from an arbitrary description of the lattice. For this purpose, the reduced form is first derived from the given description, *e.g.* by means of the algorithm of Křivý & Gruber (1976). Subsequently it is compared with the reduced forms (Table 9.2.5.1) for the 44 lattice characters and transformed to the appropriate conventional cell. Thus the reduced cell is helpful as an accessory in classifications based on conventional cells.

Alternatively, the parameters of the reduced form itself (either of the direct lattice or of the reciprocal lattice) can be used as a basis for determinative classification.

9.2.6.2. *Comparison of lattices*

Two lattices, defined by their reduced cells, can be compared on a rigorous basis to find out whether they are identical lattices or are related by one cell being a subcell of the other (Santoro *et al.*, 1980).

Further properties of lattices are discussed in Chapter 9.3.

Acknowledgements

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9.3. Further properties of lattices

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9.3.1. Further kinds of reduced cells

In Section 9.2.2, a 'reduced basis' of a lattice is defined which permits a unique representation of this lattice. It was introduced into crystallography by Niggli (1928) and incorporated into *International Tables for X-ray Crystallography* (1969), Vol. I. Originating from algebra (Eisenstein, 1851), a reduced basis is defined in a rather complicated manner [conditions (9.2.2.2*a*) to (9.2.2.5*f*) in Section 9.2.2] and lacks any geometrical meaning. A cell spanned by a reduced basis is called the *Niggli cell*.

However, unique primitive cells may be introduced also in other ways that – unlike the Niggli cell* – have significant geometrical features based mainly on extremal principles (Gruber, 1989). We shall describe some of them below.

If a (primitive) cell of the lattice L fulfils the condition

$$a + b + c = \min$$

on the set of all primitive cells of L, we call it a *Buerger cell*. This cell need not be unique with regard to its shape in the lattice. There exist lattices with 1, 2, 3, 4 and 5 (but not more) Buerger cells differing in shape. The uniqueness can be achieved by various additional conditions. In this way, we can arrive at the following four reduced cells:

(i) the Buerger cell with minimum surface;†
(ii) the Buerger cell with maximum surface;
(iii) the Buerger cell with minimum deviation;‡
(iv) the Buerger cell with maximum deviation.

Equivalent definitions can be obtained by replacing the term 'surface' in (i) and (ii) by the expression

$$\sin\alpha + \sin\beta + \sin\gamma$$

or

$$\sin\alpha \sin\beta \sin\gamma,$$

and by replacing the 'deviation' in (iii) and (iv) by

$$|\cos\alpha| + |\cos\beta| + |\cos\gamma|$$

or

$$|\cos\alpha \cos\beta \cos\gamma|.$$

A Buerger cell can agree with more than one of the definitions

$$\text{(i), (ii), (iii), (iv).} \tag{9.3.1.1}$$

For example, if a lattice has only one Buerger cell, then this cell agrees with all the definitions in (9.3.1.1). However, there exist also Buerger cells that are in agreement with none of them. Thus, the definitions (9.3.1.1) do not imply a partition of Buerger cells into classes.

It appears that case (iv) coincides with the Niggli cell. This is important because this cell can now be defined by a simple geometrical property instead of a complicated system of conditions.

Further reduced cells can be obtained by applying the definitions (9.3.1.1) to the reciprocal lattice. Then, to a Buerger cell in the reciprocal lattice, there corresponds a primitive cell with absolute minimum surface§ in the direct lattice.

The reduced cells according to the definitions (9.3.1.1) can be recognized by means of a table and found in the lattice by means of algorithms. Detailed mutual relationships between them have been ascertained.

* See, however, later parts of this section.
† Meaning that this cell has the smallest surface of all Buerger cells of the lattice.
‡ The deviation of a cell is the number $|90° - \alpha| + |90° - \beta| + |90° - \gamma|$.
§ This cell need not be a Buerger cell.

9.3.2. Topological characteristic of lattice characters

In his thorough analysis of lattice characters, de Wolff (1988) remarks that so far they have not been defined as clearly as the Bravais types and that an exact general definition does not exist. Gruber (1992) tried to base such a definition on topological concepts.

The crucial notion is the decomposition of a set $\boldsymbol{M}$ of points of the n-dimensional Euclidean space E_n into equivalence classes called *components* of the set $\boldsymbol{M}$. They can be defined as follows: Two points X, Y of the set $\boldsymbol{M}$ belong to the same component if they can be connected by a *continuous* path which lies entirely in the set $\boldsymbol{M}$ (Fig. 9.3.2.1). This partition of the set $\boldsymbol{M}$ into components is unique and is determined solely by the set $\boldsymbol{M}$.

Now let us return to lattices. To any lattice L there is attached a point in E_5 called the *Niggli point* of L. It is the point

$$\left[\frac{\mathbf{a}\cdot\mathbf{a}}{\mathbf{c}\cdot\mathbf{c}}, \frac{\mathbf{b}\cdot\mathbf{b}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{b}\cdot\mathbf{c}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{a}\cdot\mathbf{c}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{a}\cdot\mathbf{b}}{\mathbf{c}\cdot\mathbf{c}}\right] \tag{9.3.2.1}$$

provided that the vectors **a**, **b**, **c** describe the Niggli cell of L and fulfil the conditions (9.2.2.2*a*) to (9.2.2.5*f*) of Section 9.2.2. If $\mathscr{L}$ is a set of lattices then the set of Niggli points of all lattices of $\mathscr{L}$ is called the *Niggli image* of $\mathscr{L}$.

Thus we can speak about the Niggli image of a Bravais type $\mathscr{T}$. This Niggli image is a part of E_5 and so can be partitioned into components. This division of Niggli points induces back a division of lattices of the Bravais type $\mathscr{T}$. It turns out that this division is identical with the division of $\mathscr{T}$ into lattice characters as introduced in Section 9.2.5. This fact, used conversely, can be considered an exact definition of the lattice characters: Two lattices of Bravais type $\mathscr{T}$ are said to be of the same lattice character if their Niggli points lie in the same component of the Niggli image of $\mathscr{T}$.

We can, of course, also speak about Niggli images of particular lattice characters. According to their definition, these images are connected sets. However, much more can be stated about them: these sets are even *convex* (Fig. 9.3.2.2). This means that any two points of the Niggli image of a lattice character can be connected by a *straight segment* lying totally in this Niggli image. From this property, it follows that the lattice characters may be defined also in the following equivalent way:

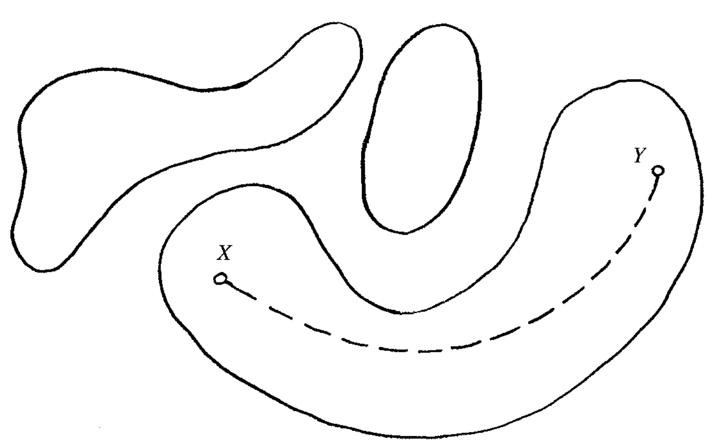

Fig. 9.3.2.1. A set $M \subset E_2$ consisting of three components.

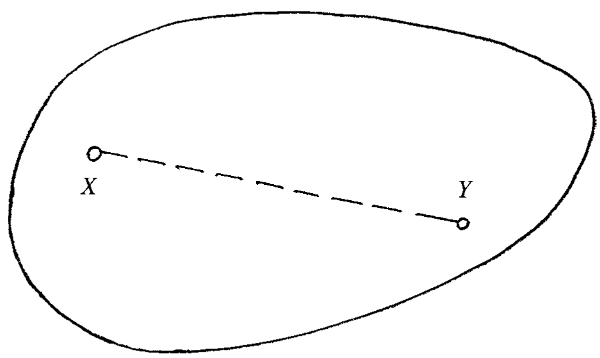

Fig. 9.3.2.2. A convex set in E_2.

We say that two lattices of the same Bravais type belong to the same lattice character if one of them can be deformed into the other in such a way that the Niggli point of the deformed lattice moves *linearly* from the initial to the final position while the Bravais type of the lattice remains unchanged.

Unlike convexity, nothing can be said whether the Niggli images of lattice characters are *open* sets (with regard to their dimension) or not. Both cases occur.

The lattice character of a lattice L can also be recognized [instead of by means of Table 9.2.5.1 or by Tables 1 and 3 in Gruber (1992)] by perpendicular projection of the **c** vector onto the **ab** plane provided the vectors **a**, **b**, **c** describe the Niggli cell of L and fulfil the conditions (9.2.2.2*a*) to (9.2.2.5*f*) in Section 9.2.2 (de Wolff & Gruber, 1991). See also Figs. 9.2.4.1 to 9.2.4.5.

9.3.3. A finer division of lattices

The 44 lattice characters form a subdivision of the 14 Bravais types. There is another commonly known subdivision of the Bravais types, namely the 24 Delaunay sorts (*symmetrische Sorten*) (Delaunay, 1933; *International Tables for X-ray Crystallography*, 1952, Vol. I; *cf.* Section 9.1.8). However, both divisions, being based on quite different principles, are incompatible: the 44 lattice characters do not form a subdivision of the 24 Delaunay sorts.

A natural problem arises to construct a division of lattices which would be a subdivision of both the lattice characters and the Delaunay sorts. However, we do not admit a purely mechanical intersection of both these divisions; we insist that their common subdivision be crystallographically meaningful.

Such a division was proposed recently (Gruber, 1997*a*). It uses the fact that the Niggli points of all lattices lie in two five-dimensional polyhedra, say Ω^+ and Ω^-. The underlying idea, originating from H. Wondratschek, is based on the distribution of Niggli points among the vertices, edges, faces, three- and four-dimensional hyperfaces, and the interior of Ω^+ and Ω^-. This leads to a natural division of Niggli points and further to a division of lattices. This division has 67 classes, but is not suitable for crystallography because it does not constitute a subdivision of the Bravais types.

A modification of the idea is necessary. It consists of representing a lattice L by several points (instead of by one Niggli point) and the addition of two minor conditions. One of them concerns the diagonals of the Niggli cell and the other the bases of L which describe the Niggli cell.

Though these conditions are of little importance in themselves, they lead to a very useful notion, *viz* the division of all lattices into 127 classes which is a subdivision of both the lattice characters and the Delaunay sorts. The equivalence classes of this division are called *genera*. They form, in a certain sense, building blocks of both lattice characters and Delaunay sorts and show their mutual relationship.

The distribution of genera along the Bravais types is the following (the number of genera is given in parentheses): *cP*(1), *cI*(1), *cF*(1), *tP*(2), *tI*(5), *oP*(1), *oC*(8), *oI*(7), *oF*(3), *hP*(3), *hR*(4), *mP*(5), *mC*(43), *aP*(43). Thus, genera seem to be especially suitable for a finer classification of lattices of low symmetry.

The genus of a given lattice L can be determined – provided that the Niggli point of L is known – by means of a table containing explicit descriptions of all genera. These descriptions are formed by open linear systems of inequalities. Consequently, the ranges of conventional parameters of genera are open unlike those concerning the lattice characters.

Genera are denoted by symbols derived from the geometrical shape of Ω^+ and Ω^-. They can be visualized in the three-dimensional cross sections of these bodies. This gives a fairly good illustration of the relationships between genera.

However, the most important feature of genera seems to be the fact that lattices of the same genus agree in a surprisingly great number of crystallographically significant properties, such as the number of Buerger cells, the densest directions and planes, the symmetry of these planes *etc.* Even the formulae for the conventional cells are the same. The genus appears to be a remarkably strong bond between lattices.

9.3.4. Conventional cells

Conventional cells are dealt with in Chapter 9.1. They are illustrated in Fig. 9.1.7.1 and described in Table 9.1.7.2. This description, however, is not exhaustive enough for determining the Bravais type. In mathematical terms, the conditions in Table 9.1.7.2 are necessary but not sufficient. For example, the C-centred cell with

$$a = 6, \quad b = 8, \quad c = 5, \quad \cos\beta = -7/15, \quad \alpha = \gamma = 90^\circ \tag{9.3.4.1}$$

has the typical shape of a conventional cell of an *mC* lattice. But the lattice generated by the C-centred cell (9.3.4.1) is actually *hR* with the conventional rhombohedral basis vectors

$$\mathbf{c}, \quad (\mathbf{a}+\mathbf{b})/2, \quad (\mathbf{a}-\mathbf{b})/2.$$

It is a natural goal to establish a system of conditions for the conventional cells which would be not only necessary but also sufficient. This is done in Table 9.3.4.1. In order to make the conditions as simple as possible, the usual *mC* description of the monoclinic centred lattices is replaced by the *mI* description. The relation between the two descriptions is simple:

$$\mathbf{a}_I = -\mathbf{c}_C, \quad \mathbf{b}_I = \mathbf{b}_C, \quad \mathbf{c}_I = \mathbf{a}_C + \mathbf{c}_C.$$

The exact meaning of Table 9.3.4.1 is as follows: Suppose that a Bravais type different from *aP* is given and that its symbol appears in column 1 in the *i*th entry of Table 9.3.4.1. Then a lattice L is of this Bravais type if and only if there exists a cell (**a**, **b**, **c**) in L such that

(i) the centring of (**a**, **b**, **c**) agrees with the centring mode given in column 2 in the *i*th entry, and

(ii) the parameters of the cell (**a**, **b**, **c**) fulfil the conditions listed in column 3 in the *i*th entry of Table 9.3.4.1.

9.3.5. Conventional characters

Lattice characters were defined in Section 9.3.2 by dividing the Niggli image of a certain Bravais type $\mathscr{T}$ into components. Doing

Table 9.3.4.1. *Conventional cells*

Bravais type	Centring mode of the cell (**a**, **b**, **c**)	Conditions
cP	*P*	$a = b = c$, $\alpha = \beta = \gamma = 90°$
cI	*I*	$a = b = c$, $\alpha = \beta = \gamma = 90°$
cF	*F*	$a = b = c$, $\alpha = \beta = \gamma = 90°$
tP	*P*	$a = b \neq c$, $\alpha = \beta = \gamma = 90°$
tI	*I*	$c/\sqrt{2} \neq a = b \neq c$,* $\alpha = \beta = \gamma = 90°$
oP	*P*	$a < b < c$,† $\alpha = \beta = \gamma = 90°$
oI	*I*	$a < b < c$, $\alpha = \beta = \gamma = 90°$
oF	*F*	$a < b < c$, $\alpha = \beta = \gamma = 90°$
oC	*C*	$a < b \neq a\sqrt{3}$,‡ $\alpha = \beta = \gamma = 90°$
hP	*P*	$a = b$, $\alpha = \beta = 90°,\ \gamma = 120°$
hR	*P*	$a = b = c$, $\alpha = \beta = \gamma$, $\alpha \neq 60°,\ \alpha \neq 90°,\ \alpha \neq \omega$§
mP	*P*	$-2c\cos\beta < a < c$,¶ $\alpha = \gamma = 90° < \beta$
mI	*I*	$-c\cos\beta < a < c$,** $\alpha = \gamma = 90° < \beta, \qquad (9.3.4.2)$ but not $a^2 + b^2 = c^2$, $a^2 + ac\cos\beta = b^2$,†† (9.3.4.3) nor $a^2 + b^2 = c^2$, $b^2 + ac\cos\beta = a^2$,‡‡ (9.3.4.4) nor $c^2 + 3b^2 = 9a^2$, $c = -3a\cos\beta$,§§ (9.3.4.5) nor $a^2 + 3b^2 = 9c^2$, $a = -3c\cos\beta$¶¶ (9.3.4.6)

Note: All remaining cases are covered by Bravais type *aP*.

* For $a = c/\sqrt{2}$, the lattice is *cF* with conventional basis vectors $\mathbf{c}, \mathbf{a} + \mathbf{b}, \mathbf{a} - \mathbf{b}$.
† The labelling of the basis vectors according to their length is the reason for unconventional Hermann–Mauguin symbols: for example, the Hermann–Mauguin symbol *Pmna* may be changed to *Pncm*, *Pbmn*, *Pman*, *Pcnm* or *Pnmb*. Analogous facts apply to the *oI*, *oC*, *oF*, *mP* and *mI* Bravais types.
‡ For $b = a\sqrt{3}$, the lattice is *hP* with conventional vectors $\mathbf{a}, (\mathbf{b} - \mathbf{a})/2, \mathbf{c}$.
§ $\omega = \arccos(-1/3) = 109°28'16''$. For $\alpha = 60°$, the lattice is *cF* with conventional vectors $-\mathbf{a} + \mathbf{b} + \mathbf{c},\ \mathbf{a} - \mathbf{b} + \mathbf{c},\ \mathbf{a} + \mathbf{b} - \mathbf{c}$; for $\alpha = \omega$, the lattice is *cI* with conventional vectors $\mathbf{a} + \mathbf{b}, \mathbf{a} + \mathbf{c}, \mathbf{b} + \mathbf{c}$.
¶ This means that **a**, **c** are shortest non-coplanar lattice vectors in their plane.
** This means that **a**, **c** are shortest non-coplanar lattice vectors in their plane on condition that the cell (**a**, **b**, **c**) is body-centred.
†† If (9.3.4.2) and (9.3.4.3) hold, the lattice is *hR* with conventional vectors $\mathbf{a}, (\mathbf{a} + \mathbf{b} - \mathbf{c})/2, (\mathbf{a} - \mathbf{b} - \mathbf{c})/2$, making the rhombohedral angle smaller than 60°.
‡‡ If (9.3.4.2) and (9.3.4.4) hold, the lattice is *hR* with conventional vectors $\mathbf{a}, (\mathbf{a} + \mathbf{b} + \mathbf{c})/2, (\mathbf{a} - \mathbf{b} + \mathbf{c})/2$, making the rhombohedral angle between 60 and 90°.
§§ If (9.3.4.2) and (9.3.4.5) hold, the lattice is *hR* with conventional vectors $-\mathbf{a}, (\mathbf{a} + \mathbf{b} + \mathbf{c})/2, (\mathbf{a} - \mathbf{b} + \mathbf{c})/2$, making the rhombohedral angle between 90° and ω.
¶¶ If (9.3.4.2) and (9.3.4.6) hold, the lattice is *hR* with conventional vectors $-\mathbf{c}, (\mathbf{a} + \mathbf{b} + \mathbf{c})/2, (\mathbf{a} - \mathbf{b} + \mathbf{c})/2$, making the rhombohedral angle greater than ω.

Table 9.3.5.1. *Conventional characters*

Bravais type	Conditions	Conventional character
cP		{3}
cI		{5}
cF		{1}
tP	$a < c$	{11}
	$c < a$	{21}
tI	$a < c/\sqrt{2}$	{15}
	$c/\sqrt{2} < a < c$	{7}
	$c < a$	{6, 18}
oP		{32}
oI		{8, 19, 42}
oF		{16, 26}
oC	$b < a\sqrt{3}$	{13, 23}
	$a\sqrt{3} < b$	{36, 38, 40}
hP		{12, 22}
*hR**	$\alpha < 60°$	{9}
	$60° < \alpha < 90°$	{2}
	$90° < \alpha < \omega$†	{4}
	$\omega < \alpha$	{24}
mP		{33, 34, 35}
mC		{10, 14, 17, 20, 25, 27, 28, 29, 30, 37, 39, 41, 43}
aP	$\alpha < 90°$	{31}
	$90° \leq \alpha$	{44}

* The angle α refers to the rhombohedral description of the *hR* lattices.
† $\omega = \arccos(-1/3) = 109°28'16''$.

the same – instead of with the Niggli points – with the parameters of conventional cells* of lattices of the Bravais type $\mathcal{T}$ we obtain a division of the range† of these parameters into components. This leads to a further division of lattices of the Bravais type $\mathcal{T}$ into equivalence classes. We call these classes – in analogy to the Niggli characters – *conventional characters*. There are 22 of them.

Two lattices of the same Bravais type belong to the same conventional character if and only if one lattice can be deformed into the other in such a way that the conventional parameters of the deformed lattice change *continuously* from the initial to the final position without change of the Bravais type. The word 'continuously' cannot be replaced by the stronger term 'linearly' because the range of conventional parameters of the monoclinic centred lattices is not convex.

Conventional characters form a superdivision of the lattice characters. Therefore, no special notation of conventional characters need be invented: we write them simply as sets of lattice characters which constitute the conventional character. Denoting the lattice characters by integral numbers from 1 to 44 (according to the convention in Section 9.2.5), we obtain for the conventional characters symbols like $\{8, 19, 42\}$ or $\{7\}$.

Conventional characters are described in Table 9.3.5.1.

9.3.6. Sublattices

A sublattice L' of an n-dimensional lattice L is a proper subset of L which itself is a lattice of the same dimension as L. A sublattice L' of

* For *aP* lattices, these parameters are derived from the Niggli point [see (9.3.2.1)].
† This range is a subset of E_k, where $k \leq 6$.

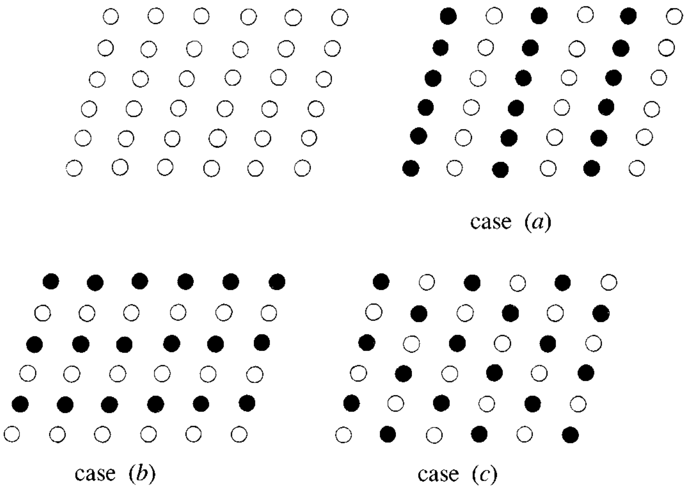

Fig. 9.3.6.1. Three possible decompositions of a two-dimensional lattice L into sublattices of index 2.

L causes a decomposition of the set L into, say, i mutually congruent sublattices, L' itself being one of them (Fig. 9.3.6.1). The number i is called the *index* of the sublattice L' and indicates how many times L' is 'diluted' with respect to L.

Sublattices are defined in a natural way in those lattices that have centred conventional cells, being generated by the vertices of these cells ('decentring'). They are primitive and belong to the same crystal family as the given lattice. Thus, in the *cI*, *cF*, *tI*, *oI*, *oF*, *oC*, *mC* and *hR* * lattices, we can meet sublattices of indices 2, 4, 2, 2, 4, 2, 2 and 3, respectively.

Theoretically (though hardly in crystallographic practice), the Bravais type of centred lattices can also be determined by testing all their sublattices with the suspected index and finding in any of these sublattices the Niggli cell.

All sublattices of index i of an n-dimensional lattice L can be constructed by a procedure suggested by Cassels (1971). If $\mathbf{a}_1, \ldots, \mathbf{a}_n$ is a primitive basis of the lattice L then primitive bases $\mathbf{a}'_1, \ldots, \mathbf{a}'_n$ of all sublattices of index i of the lattice L can be found by the relations

$$[\mathbf{a}'_1, \ldots, \mathbf{a}'_n] = [\mathbf{a}_1, \ldots, \mathbf{a}_n]\boldsymbol{R}^T,$$

where the matrix $\boldsymbol{R} = [r_{ij}]$ fulfils

$$\begin{aligned} 0 &= r_{ij} && \text{for} \quad 1 \le i < j \le n, \\ 0 &\le r_{ij} < r_{jj} && \text{for} \quad 1 \le j < i \le n, \\ r_{11} &\ldots r_{nn} = i. \end{aligned} \qquad (9.3.6.1)$$

The number $D_{n,i}$ of these matrices is equal to the number of decompositions of an n-dimensional lattice L into sublattices of index i. To determine this number, it is not necessary to construct explicitly the matrices fulfilling (9.3.6.1). The following formulae (Gruber, 1997*b*) can be used:

(i) If $i = p^q$, where $p > 1$ is a prime number, then

$$D_{n,i} = \underbrace{\frac{p^n - 1}{p - 1} \times \frac{p^{n+1} - 1}{p^2 - 1} \times \frac{p^{n+2} - 1}{p^3 - 1} \times \ldots}_{q \text{ times}}.$$

(ii) If $i = p_1^{q_1} \ldots p_m^{q_m}$ ($p_1, \ldots, p_m$ mutually different prime numbers, $m > 1$), we deal with any factor $p_j^{q_j}$ ($j = 1, \ldots, m$) according to point (i) and multiply all these numbers to obtain the number $D_{n,i}$.

For example, for $n = 3$ and $i = 2$, 3, 4 and 6, we obtain for $D_{n,i}$ the values 7, 13, 35 and 91, respectively.

In all considerations so far, the symmetry of the lattice L was irrelevant. We took L simply as a set of points and its sublattices as its subsets. (Thus, for illustrating sublattices, the 'triclinic' lattices are most apt; *cf.* 'derivative lattices' in Chapter 13.2.)

However, this is not exactly the crystallographic point of view. If, for example, the mesh of the lattice L in Fig. 9.3.6.1 were a square, the sublattices in cases (*a*) and (*b*) would have the same symmetry (though being different subsets of L) and therefore would be considered by crystallographers as one case only. The number $D_{n,i}$ would be reduced. From this aspect, the problem is treated in Chapter 13.1 in group-theoretical terms which are more suitable for this purpose than the set-theory language used here.

* When choosing their hexagonal description.

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9.1

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10.1. Crystallographic and noncrystallographic point groups

BY TH. HAHN AND H. KLAPPER

10.1.1. Introduction and definitions

A *point group** is a group of symmetry operations all of which leave at least one point unmoved. Thus, all operations containing translations are excluded. Point groups can be subdivided into crystallographic and noncrystallographic point groups. A *crystallographic* point group is a point group that maps a point lattice onto itself. Consequently, rotations and rotoinversions are restricted to the well known crystallographic cases 1, 2, 3, 4, 6 and $\bar{1}$, $\bar{2} = m, \bar{3}, \bar{4}, \bar{6}$ (*cf.* Chapter 1.3); matrices for these symmetry operations are listed in Tables 11.2.2.1 and 11.2.2.2. No such restrictions apply to the *noncrystallographic* point groups.

The numbers of the crystallographic point groups are finite: 2 for one dimension, 10 for two dimensions and 32 for three dimensions. The numbers of noncrystallographic point groups for dimensions $n \geq 2$ are infinite. The two- and three-dimensional crystallographic point groups and their crystal systems are summarized in Tables 10.1.1.1 and 10.1.1.2. They are described in detail in Section 10.1.2. The two one-dimensional point groups are discussed in Section 2.2.17. The noncrystallographic point groups are treated in Section 10.1.4.

Crystallographic point groups occur:

(i) in vector space as symmetries of the external shapes of crystals, *i.e.* of the set of vectors normal to the crystal faces (morphological symmetry);

(ii) in point space as site symmetries of points in lattices or in crystal structures and as symmetries of atomic groups and coordination polyhedra.

General point groups, *i.e.* crystallographic *and* noncrystallographic point groups, occur as:

(iii) symmetries of (rigid) molecules (molecular symmetry):

(iv) symmetries of physical properties of crystals (*e.g.* tensor symmetries); here noncrystallographic point groups with axes of order infinity are of particular importance, as in the symmetries of spheres or rotation ellipsoids:

(v) approximate symmetries of the local environment of a point in a crystal structure, *i.e.* as *local* site symmetries. Examples are sphere-like atoms or ions in crystals, as well as icosahedral atomic groups. These noncrystallographic symmetries, however, are only approximate, even for the close neighbourhood of a site.

A (geometric) *crystal class* is the set of all crystals having the same point-group symmetry. The word 'class', therefore, denotes a classificatory pigeon-hole and should not be used as synonymous with the point group of a particular crystal. The symbol of a crystal class is that of the common point group. (For geometric and arithmetic crystal classes of space groups, see Sections 8.2.3 and 8.2.4.)

Of particular importance for the structure determination of crystals are the 11 *centrosymmetric crystallographic point groups*, because they describe the possible symmetries of the diffraction record of a crystal: $\bar{1}$; $2/m$; mmm; $4/m$; $4/mmm$; $\bar{3}$; $\bar{3}m$; $6/m$; $6/mmm$; $m\bar{3}$; $m\bar{3}m$. This is due to Friedel's rule, which states that, provided anomalous dispersion is neglected, the diffraction record of any crystal is centrosymmetric, even if the crystal is noncentrosymmetric. The symmetry of the diffraction record determines the *Laue class* of the crystal; this is further explained in Part 3. For a given crystal, its Laue class is obtained if a symmetry centre is added to its point group, as shown in Table 10.2.1.1.

In two dimensions, six 'centrosymmetric' crystallographic point groups and hence six two-dimensional Laue classes exist: 2; $2mm$; 4; $4mm$; 6; $6mm$. These point groups are, for instance, the only possible symmetries of zero-layer X-ray photographs.

Among the centrosymmetric crystallographic point groups in three dimensions, the *lattice point groups* (holohedral point groups, *holohedries*) are of special importance because they constitute the seven possible point symmetries of lattices, *i.e.* the site symmetries of their nodes. In three dimensions, the seven holohedries are: $\bar{1}$; $2/m$; mmm; $4/mmm$; $\bar{3}m$; $6/mmm$; $m\bar{3}m$. Note that $\bar{3}m$ is the point symmetry of the rhombohedral lattice and $6/mmm$ the point symmetry of the hexagonal lattice; both occur in the hexagonal crystal family (*cf.* Chapter 2.1). Point groups that are, within a crystal family, subgroups of a holohedry are called merohedries; they are called specifically hemihedries for subgroups of index 2, tetartohedries for index 4 and ogdohedries for index 8.

In two dimensions, four holohedries exist: 2; $2mm$; $4mm$; $6mm$. Note that the hexagonal crystal family in two dimensions contains only one lattice type, with point symmetry $6mm$.

Another classification of the crystallographic point groups is that into isomorphism classes. Here all those point groups that have the same kind of group table appear in one class. These isomorphism classes are also known under the name of *abstract point groups*.

There are 18 abstract crystallographic point groups in three dimensions: the point groups in each of the following lines are isomorphous and belong to the same abstract group:

$$
\begin{array}{rl@{\qquad}rl}
\text{Order} \ 1: & 1 & \text{Order} \ 8: & 422, 4mm, \bar{4}2m \\
2: & \bar{1}, 2, m & 12: & 6/m \\
3: & 3 & 12: & \bar{3}m, 622, 6mm, \bar{6}2m \\
4: & 2/m, 222, mm2 & 12: & 23 \\
4: & 4, \bar{4} & 16: & 4/mmm \\
6: & \bar{3}, 6, \bar{6} & 24: & 6/mmm \\
6: & 32, 3m & 24: & m\bar{3} \\
8: & mmm & 24: & 432, \bar{4}3m \\
8: & 4/m & 48: & m\bar{3}m.
\end{array}
$$

In two dimensions, the ten crystallographic point groups form nine abstract groups; the groups 2 and m are isomorphous and belong to the same abstract group, the remaining eight point groups correspond to one abstract group each.

Table 10.1.1.1. *The ten two-dimensional crystallographic point groups, arranged according to crystal system*

Dashed lines separate point groups with different Laue classes within one crystal system.

General symbol	Crystal system: Oblique (top) Rectangular (bottom)		Square	Hexagonal	
n	1	2	4	3	6
nmm	m	$2mm$	$4mm$	$3m$	$6mm$

* For reasons of simplicity, in this chapter the same term 'point group' is used for a 'particular point group' *and* a 'type of point group'. For space groups, this distinction is explained in Section 8.2.2. For a different use of the term 'point group' see Section 8.1.6.

Table 10.1.1.2. *The 32 three-dimensional crystallographic point groups, arranged according to crystal system (cf. Chapter 2.1)*

Full Hermann–Mauguin (left) and Schoenflies symbols (right). Dashed lines separate point groups with different Laue classes within one crystal system.

General symbol	Crystal system: Triclinic		Monoclinic (top) Orthorhombic (bottom)		Tetragonal		Trigonal		Hexagonal		Cubic	
n	1	C_1	2	C_2	4	C_4	3	C_3	6	C_6	23	T
$\bar{n}$	$\bar{1}$	C_i	$m \equiv \bar{2}$	C_s	$\bar{4}$	S_4	$\bar{3}$	C_{3i}	$\bar{6} \equiv 3/m$	C_{3h}	–	–
n/m			$2/m$	C_{2h}	$4/m$	C_{4h}	–	–	$6/m$	C_{6h}	$2/m\bar{3}$	T_h
$n22$			222	D_2	422	D_4	32	D_3	622	D_6	432	O
nmm			$mm2$	C_{2v}	$4mm$	C_{4v}	$3m$	C_{3v}	$6mm$	C_{6v}	–	–
$\bar{n}2m$			–	–	$\bar{4}2m$	D_{2d}	$\bar{3}2/m$	D_{3d}	$\bar{6}2m$	D_{3h}	$\bar{4}3m$	T_d
$n/m\,2/m\,2/m$			$2/m\,2/m\,2/m$	D_{2h}	$4/m\,2/m\,2/m$	D_{4h}	–	–	$6/m\,2/m\,2/m$	D_{6h}	$4/m\,\bar{3}\,2/m$	O_h

10.1.2. Crystallographic point groups

10.1.2.1. *Description of point groups*

In crystallography, point groups usually are described

(i) by means of their Hermann–Mauguin or Schoenflies symbols;

(ii) by means of their stereographic projections;

(iii) by means of the matrix representations of their symmetry operations, frequently listed in the form of Miller indices (*hkl*) of the equivalent general crystal faces;

(iv) by means of drawings of actual crystals, natural or synthetic. Descriptions (i) through (iii) are given in this section, whereas for crystal drawings and actual photographs reference is made to textbooks of crystallography and mineralogy; this also applies to the construction and the properties of the stereographic projection.

In Tables 10.1.2.1 and 10.1.2.2, the two- and three-dimensional crystallographic point groups are listed and described. The tables are arranged according to crystal systems and Laue classes. Within each crystal system and Laue class, the sequence of the point groups corresponds to that in the space-group tables of this volume: pure rotation groups are followed by groups containing reflections, rotoinversions and inversions. The holohedral point group is always given last.

In Tables 10.1.2.1 and 10.1.2.2, some point groups are described in *two or three versions*, in order to bring out the relations to the corresponding space groups (*cf.* Section 2.2.3):

(*a*) The three monoclinic point groups 2, m and $2/m$ are given with two settings, one with 'unique axis b' and one with 'unique axis c'.

(*b*) The two point groups $\bar{4}2m$ and $\bar{6}m2$ are described for two orientations with respect to the crystal axes, as $\bar{4}2m$ and $\bar{4}m2$ and as $\bar{6}m2$ and $\bar{6}2m$.

(*c*) The five trigonal point groups 3, $\bar{3}$, 32, $3m$ and $\bar{3}m$ are treated with two axial systems, 'hexagonal axes' and 'rhombohedral axes'.

(*d*) The hexagonal-axes description of the three trigonal point groups 32, $3m$ and $\bar{3}m$ is given for two orientations, as 321 and 312, as $3m1$ and $31m$, and as $\bar{3}m1$ and $\bar{3}1m$; this applies also to the two-dimensional point group $3m$.

The presentation of the point groups is similar to that of the space groups in Part 7. The *headline* contains the short Hermann–Mauguin and the Schoenflies symbols. The full Hermann–Mauguin symbol, if different, is given below the short symbol. No Schoenflies symbols exist for two-dimensional groups. For an explanation of the symbols see Section 2.2.4 and Chapter 12.1.

Next to the headline, a pair of *stereographic projections* is given. The diagram on the left displays a general crystal or point form, that on the right shows the 'framework of symmetry elements'. Except as noted below, the c axis is always normal to the plane of the figure, the a axis points down the page and the b axis runs horizontally from left to right. For the five trigonal point groups, the c axis is normal to the page only for the description with 'hexagonal axes'; if described with 'rhombohedral axes', the direction [111] is normal and the positive a axis slopes towards the observer. The conventional coordinate systems used for the various crystal systems are listed in Table 2.1.2.1 and illustrated in Figs. 2.2.6.1 to 2.2.6.10.

In the *right-hand projection*, the graphical symbols of the symmetry elements are the same as those used in the space-group diagrams; they are listed in Chapter 1.4. Note that the symbol of a symmetry centre, a small circle, is also used for a face-pole in the left-hand diagram. Mirror planes are indicated by heavy solid lines or circles; thin lines are used for the projection circle, for symmetry axes in the plane and for some special zones in the cubic system.

In the *left-hand projection*, the projection circle and the coordinate axes are indicated by thin solid lines, as are again some special zones in the cubic system. The dots and circles in this projection can be interpreted in two ways.

(i) As *general face poles*, where they represent general crystal faces which form a polyhedron, the 'general crystal form' (face form) $\{hkl\}$ of the point group (see below). In two dimensions, edges, edge poles, edge forms and polygons take the place of faces, face poles, crystal forms (face forms) and polyhedra in three dimensions.

Face poles marked as dots lie above the projection plane and represent faces which intersect the positive c axis* (positive Miller index l), those marked as circles lie below the projection plane (negative Miller index l). In two dimensions, edge poles always lie on the pole circle.

(ii) As *general points* (centres of atoms) that span a polyhedron or polygon, the 'general crystallographic point form' x, y, z. This interpretation is of interest in the study of coordination polyhedra, atomic groups and molecular shapes. The polyhedron or polygon of a point form is dual to the polyhedron of the corresponding crystal form.†

The general, special and limiting *crystal forms* and *point forms* constitute the main part of the table for each point group. The theoretical background is given below under *Crystal and point forms*; the explanation of the listed data is to be found under *Description of crystal and point forms.*

* This does not apply to 'rhombohedral axes': here the positive directions of all three axes slope upwards from the plane of the paper: *cf.* Fig. 2.2.6.9.

† Dual polyhedra have the same number of edges, but the numbers of faces and vertices are interchanged; *cf.* textbooks of geometry.

The last entry for each point group contains the *Symmetry of special projections*, *i.e.* the plane point group that is obtained if the three-dimensional point group is projected along a symmetry direction. The special projection directions are the same as for the space groups; they are listed in Section 2.2.14. The relations between the axes of the three-dimensional point group and those of its two-dimensional projections can easily be derived with the help of the stereographic projection. No projection symmetries are listed for the two-dimensional point groups.

Note that the symmetry of a projection along a certain direction may be higher than the symmetry of the crystal face normal to that direction. For example, in point group $\bar{1}$ all faces have face symmetry 1, whereas projections along any direction have symmetry 2; in point group 422, the faces (001) and $(00\bar{1})$ have face symmetry 4, whereas the projection along [001] has symmetry 4*mm*.

10.1.2.2. *Crystal and point forms*

For a point group $\mathcal{P}$ a *crystal form* is a set of all symmetrically equivalent faces; a *point form* is a set of all symmetrically equivalent points. Crystal and point forms in point groups correspond to 'crystallographic orbits' in space groups; *cf.* Section 8.3.2.

Two kinds of crystal and point forms with respect to $\mathcal{P}$ can be distinguished. They are defined as follows:

(i) *General form*: A *face* is called 'general' if only the identity operation transforms the face onto itself. Each complete set of symmetrically equivalent 'general faces' is a *general crystal form.* The *multiplicity* of a general form, *i.e.* the number of its faces, is the order of $\mathcal{P}$. In the stereographic projection, the poles of general faces do *not* lie on symmetry elements of $\mathcal{P}$.

A *point* is called 'general' if its *site symmetry*, *i.e.* the group of symmetry operations that transforms this point onto itself, is 1. A *general point form* is a complete set of symmetrically equivalent 'general points'.

(ii) *Special form*: A *face* is called 'special' if it is transformed onto itself by at least one symmetry operation of $\mathcal{P}$, in addition to the identity. Each complete set of symmetrically equivalent 'special faces' is called a *special crystal form.* The *face symmetry* of a special face is the group of symmetry operations that transforms this face onto itself; it is a subgroup of $\mathcal{P}$. The multiplicity of a special crystal form is the multiplicity of the general form divided by the order of the face-symmetry group. In the stereographic projection, the poles of special faces lie on symmetry elements of $\mathcal{P}$. The Miller indices of a special crystal form obey restrictions like $\{hk0\}$, $\{hhl\}$, $\{100\}$.

A *point* is called 'special' if its *site symmetry* is higher than 1. A special point form is a complete set of symmetrically equivalent 'special points'. The multiplicity of a special point form is the multiplicity of the general form divided by the order of the site-symmetry group. It is thus the same as that of the corresponding special crystal form. The coordinates of the points of a special point form obey restrictions, like $x, y, 0$; x, x, z; $x, 0, 0$. The point $0, 0, 0$ is not considered to be a point form.

In two dimensions, point groups 1, 2, 3, 4 and 6 and, in three dimensions, point groups 1 and $\bar{1}$ have no special crystal and point forms.

General and special crystal and point forms can be represented by their sets of equivalent Miller indices $\{hkl\}$ and point coordinates x, y, z. Each set of these 'triplets' stands for infinitely many crystal forms or point forms which are obtained by independent variation of the values and signs of the Miller indices h, k, l or the point coordinates x, y, z.

It should be noted that for crystal forms, owing to the well known 'law of rational indices', the indices h, k, l must be integers; no such restrictions apply to the coordinates x, y, z, which can be rational or irrational numbers.

Example

In point group 4, the general crystal form $\{hkl\}$ stands for the set of all possible tetragonal pyramids, pointing either upwards or downwards, depending on the sign of l; similarly, the general point form x, y, z includes all possible squares, lying either above or below the origin, depending on the sign of z. For the limiting cases $l = 0$ or $z = 0$, see below.

In order to survey the infinite number of possible forms of a point group, they are classified into *Wyckoff positions of crystal and point forms,* for short *Wyckoff positions*. This name has been chosen in analogy to the Wyckoff positions of space groups; *cf.* Sections 2.2.11 and 8.3.2. In point groups, the term 'position' can be visualized as the position of the face poles and points in the stereographic projection. Each 'Wyckoff position' is labelled by a *Wyckoff letter*.

Definition

A 'Wyckoff position of crystal and point forms' consists of all those crystal forms (point forms) of a point group $\mathcal{P}$ for which the face poles (points) are positioned on the same set of conjugate symmetry elements of $\mathcal{P}$; *i.e.* for each face (point) of one form there is one face (point) of every other form of the same 'Wyckoff position' that has exactly the same face (site) symmetry.

Each point group contains one 'general Wyckoff position' comprising all *general* crystal and point forms. In addition, up to two 'special Wyckoff positions' may occur in two dimensions and up to six in three dimensions. They are characterized by the different sets of conjugate face and site symmetries and correspond to the seven positions of a pole in the interior, on the three edges, and at the three vertices of the so-called 'characteristic triangle' of the stereographic projection.

Examples

(1) All tetragonal pyramids $\{hkl\}$ and tetragonal prisms $\{hk0\}$ in point group 4 have face symmetry 1 and belong to the same general 'Wyckoff position' 4*b*, with Wyckoff letter *b*.
(2) All tetragonal pyramids *and* tetragonal prisms in point group 4*mm* belong to two special 'Wyckoff positions', depending on the orientation of their face-symmetry groups *m* with respect to the crystal axes: For the 'oriented face symmetry' *.m.*, the forms $\{h0l\}$ and $\{100\}$ belong to Wyckoff position 4*c*; for the oriented face symmetry *..m*, the forms $\{hhl\}$ and $\{110\}$ belong to Wyckoff position 4*b*. The face symmetries *.m.* and *..m* are not conjugate in point group 4*mm*. For the analogous 'oriented site symmetries' in space groups, see Section 2.2.12.

It is instructive to subdivide the crystal forms (point forms) of one Wyckoff position further, into *characteristic* and *noncharacteristic* forms. For this, one has to consider two symmetries that are connected with each crystal (point) form:

(i) the point group $\mathcal{P}$ by which a form is generated (*generating point group*), *i.e.* the point group in which it occurs;

(ii) the full symmetry (inherent symmetry) of a form (considered as a polyhedron by itself), here called *eigensymmetry* $\mathcal{C}$. The *eigensymmetry point group* $\mathcal{C}$ is either the generating point group itself or a supergroup of it.

Examples

(1) Each tetragonal pyramid $\{hkl\}$ $(l \neq 0)$ of Wyckoff position 4*b* in point group 4 has generating symmetry 4 and *eigensymmetry*

$4mm$; each tetragonal prism $\{hk0\}$ of the same Wyckoff position has generating symmetry 4 again, but *eigensymmetry* $4/mmm$.

(2) A cube $\{100\}$ may have generating symmetry 23, $m\bar{3}$, 432, $\bar{4}3m$ or $m\bar{3}m$, but its *eigensymmetry* is always $m\bar{3}m$.

The *eigensymmetries* and the generating symmetries of the 47 crystal forms (point forms) are listed in Table 10.1.2.3. With the help of this table, one can find the various point groups in which a given crystal form (point form) occurs, as well as the face (site) symmetries that it exhibits in these point groups; for experimental methods see Sections 10.2.2 and 10.2.3.

With the help of the two groups $\mathcal{P}$ and $\mathcal{C}$, each crystal or point form occurring in a particular point group can be assigned to one of the following two categories:

(i) *characteristic* form, if *eigensymmetry* $\mathcal{C}$ and generating symmetry $\mathcal{P}$ are the same;

(ii) *noncharacteristic* form, if $\mathcal{C}$ is a proper supergroup of $\mathcal{P}$.

The importance of this classification will be apparent from the following examples.

Examples

(1) A pedion and a pinacoid are noncharacteristic forms in all crystallographic point groups in which they occur:

(2) all other crystal or point forms occur as characteristic forms in their *eigensymmetry* group $\mathcal{C}$;

(3) a tetragonal pyramid is noncharacteristic in point group 4 and characteristic in $4mm$;

(4) a hexagonal prism can occur in nine point groups (12 Wyckoff positions) as a noncharacteristic form; in $6/mmm$, it occurs in two Wyckoff positions as a characteristic form.

The general forms of the 13 point groups with no, or only one, symmetry direction ('monoaxial groups') $1, 2, 3, 4, 6, \bar{1}, m, \bar{3}, \bar{4}, \bar{6} = 3/m, 2/m, 4/m, 6/m$ are always noncharacteristic, *i.e.* their *eigensymmetries* are enhanced in comparison with the generating point groups. The general positions of the other 19 point groups always contain characteristic crystal forms that may be used to determine the point group of a crystal uniquely (*cf.* Section 10.2.2).*

So far, we have considered the occurrence of one crystal or point form in different point groups and different Wyckoff positions. We now turn to the occurrence of different kinds of crystal or point forms in one and the same Wyckoff position of a particular point group.

In a Wyckoff position, crystal forms (point forms) of different *eigensymmetries* may occur; the crystal forms (point forms) with the lowest *eigensymmetry* (which is always well defined) are called *basic forms* (German: *Grundformen*) of that Wyckoff position. The crystal and point forms of higher *eigensymmetry* are called *limiting forms* (German: *Grenzformen*) (*cf.* Table 10.1.2.3). These forms are always noncharacteristic.

Limiting forms† occur for certain restricted values of the Miller indices or point coordinates. They always have the same multiplicity and oriented face (site) symmetry as the corresponding basic forms because they belong to the same Wyckoff position. The enhanced *eigensymmetry* of a limiting form may or may not be accompanied by a change in the topology‡ of its polyhedra, compared with that of a basic form. In every case, however, the name of a limiting form is different from that of a basic form.

The face poles (or points) of a limiting form lie on symmetry elements of a supergroup of the point group that are not symmetry elements of the point group itself. There may be several such supergroups.

Examples

(1) In point group 4, the (noncharacteristic) crystal forms $\{hkl\}$ $(l \neq 0)$ (tetragonal pyramids) of *eigensymmetry* $4mm$ are basic forms of the general Wyckoff position $4b$, whereas the forms $\{hk0\}$ (tetragonal prisms) of higher *eigensymmetry* $4/mmm$ are 'limiting general forms'. The face poles of forms $\{hk0\}$ lie on the horizontal mirror plane of the supergroup $4/m$.

(2) In point group $4mm$, the (characteristic) special crystal forms $\{h0l\}$ with *eigensymmetry* $4mm$ are 'basic forms' of the special Wyckoff position $4c$, whereas $\{100\}$ with *eigensymmetry* $4/mmm$ is a 'limiting special form'. The face poles of $\{100\}$ are located on the intersections of the vertical mirror planes of the point group $4mm$ with the horizontal mirror plane of the supergroup $4/mmm$, *i.e.* on twofold axes of $4/mmm$.

Whereas basic and limiting forms belonging to one 'Wyckoff position' are always clearly distinguished, closer inspection shows that a Wyckoff position may contain different 'types' of limiting forms. We need, therefore, a further criterion to classify the limiting forms of one Wyckoff position into types: A *type of limiting form of a Wyckoff position* consists of all those limiting forms for which the face poles (points) are located on the same set of additional conjugate symmetry elements of the holohedral point group (for the trigonal point groups, the hexagonal holohedry $6/mmm$ has to be taken). Different types of limiting forms may have the same *eigensymmetry* and the same topology, as shown by the examples below. The occurrence of two topologically different polyhedra as two 'realizations' of one type of limiting form in point groups 23, $m\bar{3}$ and 432 is explained below in Section 10.1.2.4, *Notes on crystal and point forms*, item (viii).

Examples

(1) In point group 32, the limiting general crystal forms are of four types:

(i) ditrigonal prisms, *eigensymmetry* $\bar{6}2m$ (face poles on horizontal mirror plane of holohedry $6/mmm$);

(ii) trigonal dipyramids, *eigensymmetry* $\bar{6}2m$ (face poles on one kind of vertical mirror plane);

(iii) rhombohedra, *eigensymmetry* $\bar{3}m$ (face poles on second kind of vertical mirror plane);

(iv) hexagonal prisms, *eigensymmetry* $6/mmm$ (face poles on horizontal twofold axes).

Types (i) and (ii) have the same *eigensymmetry* but different topologies; types (i) and (iv) have the same topology but different *eigensymmetries;* type (iii) differs from the other three types in both *eigensymmetry* and topology.

(2) In point group 222, the face poles of the three types of general limiting forms, rhombic prisms, are located on the three (non-equivalent) symmetry planes of the holohedry *mmm.* Geometrically, the axes of the prisms are directed along the three non-equivalent orthorhombic symmetry directions. The three types

* For a survey of these relations, as well as of the 'limiting forms', it is helpful to consider the (seven) *normalizers* of the crystallographic point groups in the group of all rotations and reflections (orthogonal group, sphere group); normalizers of the crystallographic and noncrystallographic point groups are listed in Tables 15.4.1.1 and 15.4.1.2.

† The treatment of 'limiting forms' in the literature is quite ambiguous. In some textbooks, limiting forms are omitted or treated as special forms in their own right: other authors define only limiting *general* forms and consider limiting *special* forms as if they were new special forms. For additional reading, see P. Niggli (1941, pp. 80–98).

‡ The topology of a polyhedron is determined by the numbers of its vertices, edges and faces, by the number of vertices of each face and by the number of faces meeting in each vertex.

of limiting forms have the same *eigensymmetry* and the same topology but different orientations.

Similar cases occur in point groups 422 and 622 (*cf.* Table 10.1.2.3, footnote *).

Not considered in this volume are limiting forms of another kind, namely those that require either special metrical conditions for the axial ratios or irrational indices or coordinates (which always can be closely approximated by rational values). For instance, a rhombic disphenoid can, for special axial ratios, appear as a tetragonal or even as a cubic tetrahedron; similarly, a rhombohedron can degenerate to a cube. For special irrational indices, a ditetragonal prism changes to a (noncrystallographic) octagonal prism, a dihexagonal pyramid to a dodecagonal pyramid or a crystallographic pentagon-dodecahedron to a regular pentagon-dodecahedron. These kinds of limiting forms are listed by A. Niggli (1963).

In conclusion, each general or special Wyckoff position always contains one set of basic crystal (point) forms. In addition, it may contain one or more sets of limiting forms of different types. As a rule,† each type comprises polyhedra of the same *eigensymmetry* and topology and, hence, of the same name, for instance 'ditetragonal pyramid'. The name of the *basic general* forms is often used to designate the corresponding crystal class, for instance 'ditetragonal-pyramidal class'; some of these names are listed in Table 10.1.2.4.

10.1.2.3. *Description of crystal and point forms*

The main part of each point-group table describes the general and special *crystal and point forms* of that point group, in a manner analogous to the *positions* in a space group. The general Wyckoff position is given at the top, followed downwards by the special Wyckoff positions with decreasing multiplicity. Within each Wyckoff position, the first block refers to the basic forms, the subsequent blocks list the various types of limiting form, if any.

The columns, from left to right, contain the following data (further details are to be found below in Section 10.1.2.4, *Notes on crystal and point forms*):

Column 1: *Multiplicity* of the 'Wyckoff position', *i.e.* the number of equivalent faces and points of a crystal or point form.

Column 2: *Wyckoff letter.* Each general or special 'Wyckoff position' is designated by a 'Wyckoff letter', analogous to the Wyckoff letter of a position in a space group (*cf.* Section 2.2.11).

Column 3: *Face symmetry* or *site symmetry*, given in the form of an 'oriented point-group symbol', analogous to the oriented site-symmetry symbols of space groups (*cf.* Section 2.2.12). The face symmetry is also the symmetry of etch pits, striations and other face markings. For the two-dimensional point groups, this column contains the *edge symmetry*, which can be either 1 or *m.*

Column 4: *Name of crystal form.* If more than one name is in common use, several are listed. The names of the limiting forms are also given. The crystal forms, their names, *eigensymmetries* and occurrence in the point groups are summarized in Table 10.1.2.3, which may be useful for determinative purposes, as explained in Sections 10.2.2 and 10.2.3. There are 47 different types of crystal form. Frequently, 48 are quoted because 'sphenoid' and 'dome' are considered as two different forms. It is customary, however, to regard them as the same form, with the name 'dihedron'.

Name of point form (printed in italics). There exists no general convention on the names of the point forms. Here, only one name is given, which does not always agree with that of other authors. The names of the point forms are also contained in Table 10.1.2.3. Note that the same point form, 'line segment', corresponds to both sphenoid and dome. The letter in parentheses after each name of a point form is explained below.

Column 5: *Miller indices* (*hkl*) for the symmetrically equivalent faces (edges) of a crystal form. In the trigonal and hexagonal crystal systems, when referring to hexagonal axes, Bravais–Miller indices (*hkil*) are used, with $h + k + i = 0$.

Coordinates x, y, z for the symmetrically equivalent points of a point form are not listed explicitly because they can be obtained from data in this volume as follows: after the name of the point form, a letter is given in parentheses. This is the Wyckoff letter of the corresponding position in the symmorphic P space group that belongs to the point group under consideration. The coordinate triplets of this (general or special) position apply to the point form of the point group.

The triplets of Miller indices (*hkl*) and point coordinates x, y, z are arranged in such a way as to show analogous sequences; they are both based on the same set of generators, as described in Sections 2.2.10 and 8.3.5. For all point groups, except those referred to a hexagonal coordinate system, the correspondence between the (*hkl*) and the x, y, z triplets is immediately obvious.‡

The sets of symmetrically equivalent crystal faces also represent the sets of equivalent reciprocal-lattice points, as well as the sets of equivalent X-ray (neutron) reflections.

Examples

(1) In point group $\bar{4}$, the general crystal form 4*b* is listed as (hkl) $(\bar{h}\bar{k}l)$ $(k\bar{h}\bar{l})$ $(\bar{k}h\bar{l})$: the corresponding general position 4*h* of the symmorphic space group $P\bar{4}$ reads x, y, z; $\bar{x}, \bar{y}, z$; $y, \bar{x}, \bar{z}$; $\bar{y}, x, \bar{z}$.

(2) In point group 3, the general crystal form 3*b* is listed as $(hkil)$ $(ihkl)$ $(kihl)$ with $i = -(h + k)$; the corresponding general position 3*d* of the symmorphic space group $P3$ reads x, y, z; $\bar{y}, x - y, z$; $-x + y, \bar{x}, z$.

(3) The Miller indices of the *cubic point groups* are arranged in one, two or four blocks of (3×4) entries. The first block (upper left) belongs to point group 23. The second block (upper right) belongs to the diagonal twofold axes in 432 and $m\bar{3}m$ or to the diagonal mirror plane in $\bar{4}3m$. In point groups $m\bar{3}$ and $m\bar{3}m$, the lower one or two blocks are derived from the upper blocks by application of the inversion.

10.1.2.4. *Notes on crystal and point forms*

(i) As mentioned in Section 10.1.2.2, each set of Miller indices of a given point group represents infinitely many face forms with the same name. Exceptions occur for the following cases.

Some special crystal forms occur with only *one* representative. Examples are the pinacoid $\{001\}$, the hexagonal prism $\{10\bar{1}0\}$ and the cube $\{100\}$. The Miller indices of these forms consist of fixed numbers and signs and contain no variables.

In a few noncentrosymmetric point groups, a special crystal form is realized by *two* representatives: they are related by a centre of symmetry that is not part of the point-group symmetry. These cases are

(*a*) the two pedions (001) and $(00\bar{1})$;

† For the exceptions in the cubic crystal system *cf.* Section 10.1.2.4, *Notes on crystal and point forms*, item (viii)

‡ The matrices of corresponding triplets $(\tilde{h}\tilde{k}\tilde{l})$ and $\tilde{x}, \tilde{y}, \tilde{z}$, *i.e.* of triplets generated by the same symmetry operation from (*hkl*) and x, y, z, are inverse to each other, provided the x, y, z and $\tilde{x}, \tilde{y}, \tilde{z}$ are regarded as columns and the (*hkl*) and $(\tilde{h}\tilde{k}\tilde{l})$ as rows: this is due to the contravariant and covariant nature of the point coordinates and Miller indices, respectively. Note that for orthogonal matrices the inverse matrix equals the transposed matrix; in crystallography, this applies to all coordinate systems (including the rhombohedral one), except for the hexagonal system. The matrices for the symmetry operations occurring in the crystallographic point groups are listed in Tables 11.2.2.1 and 11.2.2.2.

(*b*) the two trigonal prisms $\{10\bar{1}0\}$ and $\{\bar{1}010\}$; similarly for two dimensions;

(*c*) the two trigonal prisms $\{11\bar{2}0\}$ and $\{\bar{1}\bar{1}20\}$; similarly for two dimensions;

(*d*) the positive and negative tetrahedra $\{111\}$ and $\{\bar{1}\bar{1}\bar{1}\}$.

In the point-group tables, both representatives of these forms are listed, separated by 'or', for instance '(001) or $(00\bar{1})$'.

(ii) In crystallography, the terms tetragonal, trigonal, hexagonal, as well as tetragon, trigon and hexagon, imply that the cross sections of the corresponding polyhedra, or the polygons, are *regular* tetragons (squares), trigons or hexagons. Similarly, ditetragonal, ditrigonal, dihexagonal, as well as ditetragon, ditrigon and dihexagon, refer to *semi-regular* cross sections or polygons.

(iii) Crystal forms can be 'open' or 'closed'. A crystal form is 'closed' if its faces form a closed polyhedron; the minimum number of faces for a closed form is 4. Closed forms are disphenoids, dipyramids, rhombohedra, trapezohedra, scalenohedra and all cubic forms; open forms are pedions, pinacoids, sphenoids (domes), pyramids and prisms.

A point form is always closed. It should be noted, however, that a point form dual to a *closed* face form is a *three*-dimensional polyhedron, whereas the dual of an *open* face form is a *two*- or *one*-dimensional polygon, which, in general, is located 'off the origin' but may be centred at the origin (here called 'through the origin').

(iv) Crystal forms are well known; they are described and illustrated in many textbooks. Crystal forms are 'isohedral' polyhedra that have all faces equivalent but may have more than one kind of vertex; they include regular polyhedra. The in-sphere of the polyhedron touches all the faces.

Crystallographic point forms are less known; they are described in a few places only, notably by A. Niggli (1963), by Fischer *et al.* (1973), and by Burzlaff & Zimmermann (1977). The latter publication contains drawings of the polyhedra of all point forms. Point forms are 'isogonal' polyhedra (polygons) that have all vertices equivalent but may have more than one kind of face;* again, they include regular polyhedra. The circumsphere of the polyhedron passes through all the vertices.

In most cases, the names of the point-form polyhedra can easily be derived from the corresponding crystal forms: the duals of *n*-gonal pyramids are regular *n*-gons off the origin, those of *n*-gonal prisms are regular *n*-gons through the origin. The duals of di-*n*-gonal pyramids and prisms are truncated (regular) *n*-gons, whereas the duals of *n*-gonal dipyramids are *n*-gonal prisms.

In a few cases, however, the relations are not so evident. This applies mainly to some cubic point forms [see item (v) below]. A further example is the rhombohedron, whose dual is a trigonal antiprism (in general, the duals of *n*-gonal streptohedra are *n*-gonal antiprisms).† The duals of *n*-gonal trapezohedra are polyhedra intermediate between *n*-gonal prisms and *n*-gonal antiprisms; they are called here 'twisted *n*-gonal antiprisms'. Finally, the duals of di-*n*-gonal scalenohedra are *n*-gonal antiprisms 'sliced off' perpendicular to the prism axis by the pinacoid $\{001\}$.‡

(v) Some cubic point forms have to be described by 'combinations' of 'isohedral' polyhedra because no common names exist for 'isogonal' polyhedra. The maximal number of polyhedra required is three. The *shape* of the combination that describes the point form depends on the relative sizes of the polyhedra involved, *i.e.* on the relative values of their central distances. Moreover, in some cases even the *topology* of the point form may change.

Example

'Cube truncated by octahedron' and 'octahedron truncated by cube'. Both forms have 24 vertices, 14 faces and 36 edges but the faces of the first combination are octagons and trigons, those of the second are hexagons and tetragons. These combinations represent different special point forms x, x, z and $0, y, z$. One form can change into the other only *via* the (semi-regular) cuboctahedron $0, y, y$, which has 12 vertices, 14 faces and 24 edges.

The unambiguous description of the cubic point forms by combinations of 'isohedral' polyhedra requires restrictions on the relative sizes of the polyhedra of a combination. The permissible range of the size ratios is limited on the one hand by vanishing, on the other hand by splitting of vertices of the combination. Three cases have to be distinguished:

(*a*) The relative sizes of the polyhedra of the combination can vary *independently.* This occurs whenever three edges meet in one vertex. In Table 10.1.2.2, the names of these point forms contain the term 'truncated'.

Examples

(1) 'Octahedron truncated by cube' (24 vertices, dual to tetrahexahedron).
(2) 'Cube truncated by two tetrahedra' (24 vertices, dual to hexatetrahedron), implying independent variation of the relative sizes of the two truncating tetrahedra.

(*b*) The relative sizes of the polyhedra are *interdependent.* This occurs for combinations of three polyhedra whenever four edges meet in one vertex. The names of these point forms contain the symbol '&'.

Example

'Cube & two tetrahedra' (12 vertices, dual to tetragon-tritetrahedron); here the interdependence results from the requirement that in the combination a cube edge is reduced to a vertex in which faces of the two tetrahedra meet. The location of this vertex on the cube edge is free. A higher symmetrical 'limiting' case of this combination is the 'cuboctahedron', where the two tetrahedra have the same sizes and thus form an octahedron.

(*c*) The relative sizes of the polyhedra are *fixed.* This occurs for combinations of three polyhedra if five edges meet in one vertex. These point forms are designated by special names (snub tetrahedron, snub cube, irregular icosahedron), or their names contain the symbol '+'.

The cuboctahedron appears here too, as a limiting form of the snub tetrahedron (dual to pentagon-tritetrahedron) and of the irregular icosahedron (dual to pentagon-dodecahedron) for the special coordinates $0, y, y$.

(vi) Limiting crystal forms result from general or special crystal forms for special values of certain geometrical parameters of the form.

Examples

(1) A pyramid degenerates into a prism if its apex angle becomes 0, *i.e.* if the apex moves towards infinity.

(*continued on page* 795)

* Thus, the name 'prism' for a *point form* implies combination of the prism with a pinacoid.

† A tetragonal tetrahedron is a digonal streptohedron; hence, its dual is a 'digonal antiprism', which is again a tetragonal tetrahedron.

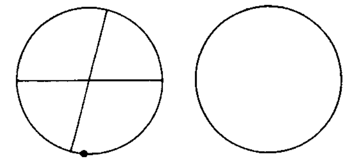
‡ The dual of a tetragonal (= di-digonal) scalenohedron is a 'digonal antiprism', which is 'cut off' by the pinacoid $\{001\}$.

Table 10.1.2.1. *The ten two-dimensional crystallographic point groups*

General, special and limiting edge forms and *point forms* (italics), oriented edge and site symmetries, and Miller indices (hk) of equivalent edges [for hexagonal groups Bravais–Miller indices (hki) are used if referred to hexagonal axes]; for point coordinates see text.

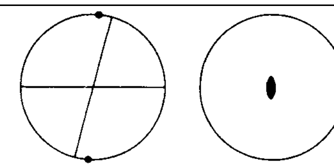
OBLIQUE SYSTEM

1



1	*a*	1	Single edge *Single point* (*a*)	(hk)

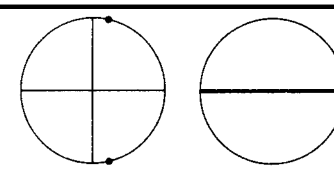
2



2	*a*	1	Pair of parallel edges *Line segment through origin* (*e*)	(hk) $(\bar{h}\bar{k})$

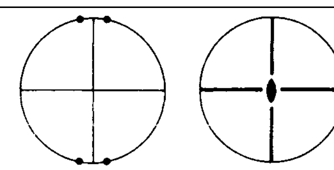
RECTANGULAR SYSTEM

m



2	*b*	1	Pair of edges *Line segment* (*c*)	(hk) $(\bar{h}k)$
			Pair of parallel edges *Line segment through origin*	(10) $(\bar{1}0)$
1	*a*	*.m.*	Single edge *Single point* (*a*)	(01) or $(0\bar{1})$

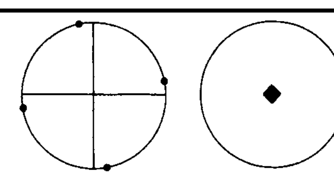
2*mm*



4	*c*	1	Rhomb *Rectangle* (*i*)	(hk) $(\bar{h}\bar{k})$ $(\bar{h}k)$ $(h\bar{k})$
2	*b*	*.m.*	Pair of parallel edges *Line segment through origin* (*g*)	(01) $(0\bar{1})$
2	*a*	*..m*	Pair of parallel edges *Line segment through origin* (*e*)	(10) $(\bar{1}0)$

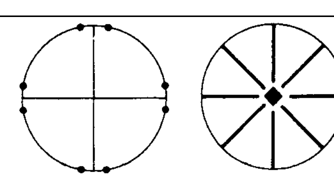
SQUARE SYSTEM

4



4	*a*	1	Square *Square* (*d*)	(hk) $(\bar{h}\bar{k})$ $(\bar{k}h)$ $(k\bar{h})$

4*mm*

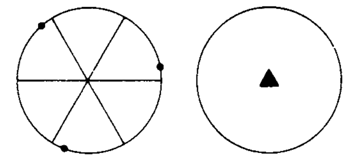


8	*c*	1	Ditetragon *Truncated square* (*g*)	(hk) $(\bar{h}\bar{k})$ $(\bar{k}h)$ $(k\bar{h})$ $(\bar{h}k)$ $(h\bar{k})$ (kh) $(\bar{k}\bar{h})$
4	*b*	*..m*	Square *Square* (*f*)	(11) $(\bar{1}\bar{1})$ $(\bar{1}1)$ $(1\bar{1})$
4	*a*	*.m.*	Square *Square* (*d*)	(10) $(\bar{1}0)$ (01) $(0\bar{1})$

Table 10.1.2.1. *The ten two-dimensional crystallographic point groups* (*cont.*)

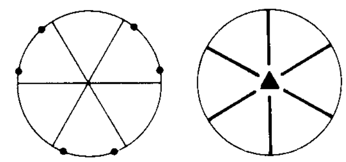
HEXAGONAL SYSTEM

3



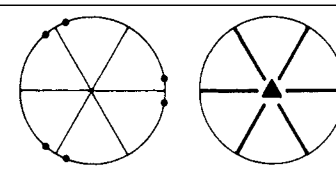
3	*a*	1	Trigon *Trigon* (*d*)	(hki) (ihk) (kih)

3*m*1



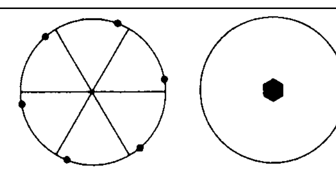
6	*b*	1	Ditrigon *Truncated trigon* (*e*)	(hki) (ihk) (kih) $(\bar{k}\bar{h}\bar{i})$ $(\bar{i}\bar{k}\bar{h})$ $(\bar{h}\bar{i}\bar{k})$
			Hexagon *Hexagon*	$(11\bar{2})$ $(\bar{2}11)$ $(1\bar{2}1)$ $(\bar{1}\bar{1}2)$ $(2\bar{1}\bar{1})$ $(\bar{1}2\bar{1})$
3	*a*	*.m.*	Trigon *Trigon* (*d*)	$(10\bar{1})$ $(\bar{1}10)$ $(0\bar{1}1)$ or $(\bar{1}01)$ $(1\bar{1}0)$ $(01\bar{1})$

31*m*



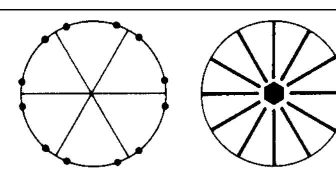
6	*b*	1	Ditrigon *Truncated trigon* (*d*)	(hki) (ihk) (kih) (khi) (ikh) (hik)
			Hexagon *Hexagon*	$(10\bar{1})$ $(\bar{1}10)$ $(0\bar{1}1)$ $(01\bar{1})$ $(\bar{1}01)$ $(1\bar{1}0)$
3	*a*	*..m*	Trigon *Trigon* (*c*)	$(11\bar{2})$ $(\bar{2}11)$ $(1\bar{2}1)$ or $(\bar{1}\bar{1}2)$ $(2\bar{1}\bar{1})$ $(\bar{1}2\bar{1})$

6



6	*a*	1	Hexagon *Hexagon* (*d*)	(hki) (ihk) (kih) $(\bar{h}\bar{k}\bar{i})$ $(\bar{i}\bar{h}\bar{k})$ $(\bar{k}\bar{i}\bar{h})$

6*mm*



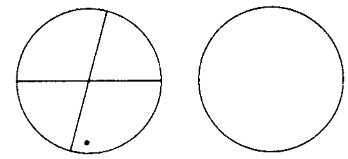
12	*c*	1	Dihexagon *Truncated hexagon* (*f*)	(hki) (ihk) (kih) $(\bar{h}\bar{k}\bar{i})$ $(\bar{i}\bar{h}\bar{k})$ $(\bar{k}\bar{i}\bar{h})$ $(\bar{k}\bar{h}\bar{i})$ $(\bar{i}\bar{k}\bar{h})$ $(\bar{h}\bar{i}\bar{k})$ (khi) (ikh) (hik)
6	*b*	*.m.*	Hexagon *Hexagon* (*e*)	$(10\bar{1})$ $(\bar{1}10)$ $(0\bar{1}1)$ $(\bar{1}01)$ $(1\bar{1}0)$ $(01\bar{1})$
6	*a*	*..m*	Hexagon *Hexagon* (*d*)	$(11\bar{2})$ $(\bar{2}11)$ $(1\bar{2}1)$ $(\bar{1}\bar{1}2)$ $(2\bar{1}\bar{1})$ $(\bar{1}2\bar{1})$

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups*

General, special and limiting face forms and *point forms* (italics), oriented face and site symmetries, and Miller indices (hkl) of equivalent faces [for trigonal and hexagonal groups Bravais–Miller indices ($hkil$) are used if referred to hexagonal axes]; for point coordinates see text.

TRICLINIC SYSTEM

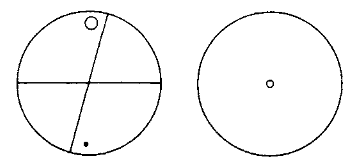
1 C_1



1	*a*	1	Pedion or monohedron *Single point* (*a*)	(hkl)

Symmetry of special projections
Along any direction
1

$\bar{1}$ C_i

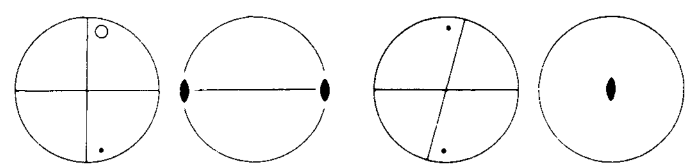


2	*a*	1	Pinacoid or parallelohedron *Line segment through origin* (*i*)	(hkl) ($\bar{h}\bar{k}\bar{l}$)

Symmetry of special projections
Along any direction
2

MONOCLINIC SYSTEM

2 C_2

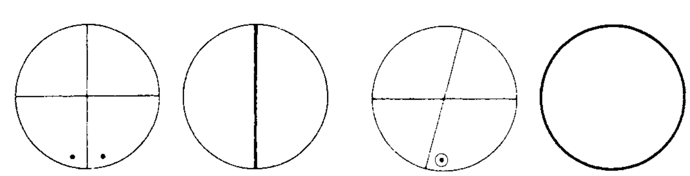


				Unique axis *b*	Unique axis *c*
2	*b*	1	Sphenoid or dihedron *Line segment* (*e*)	(hkl) ($\bar{h}k\bar{l}$)	(hkl) ($\bar{h}\bar{k}l$)
			Pinacoid or parallelohedron *Line segment through origin*	($h0l$) ($\bar{h}0\bar{l}$)	($hk0$) ($\bar{h}\bar{k}0$)
1	*a*	2	Pedion or monohedron *Single point* (*a*)	(010) or (0$\bar{1}$0)	(001) or (00$\bar{1}$)

Symmetry of special projections

	Along [100]	Along [010]	Along [001]
Unique axis *b*	*m*	2	*m*
c	*m*	*m*	2

m C_s



				Unique axis *b*	Unique axis *c*
2	*b*	1	Dome or dihedron *Line segment* (*c*)	(hkl) ($h\bar{k}l$)	(hkl) ($hk\bar{l}$)
			Pinacoid or parallelohedron *Line segment through origin*	(010) (0$\bar{1}$0)	(001) (00$\bar{1}$)
1	*a*	*m*	Pedion or monohedron *Single point* (*a*)	($h0l$)	($hk0$)

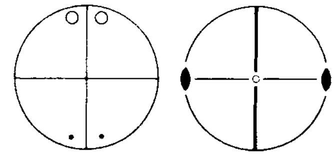
Symmetry of special projections

	Along [100]	Along [010]	Along [001]
Unique axis *b*	*m*	1	*m*
c	*m*	*m*	1

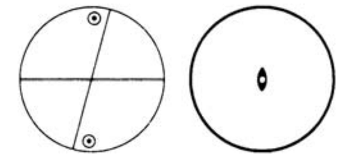
Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

MONOCLINIC SYSTEM (*cont.*)

$2/m$ C_{2h}



Unique axis *b*



Unique axis *c*

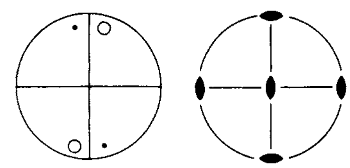
				Unique axis *b*	Unique axis *c*
4	*c*	1	Rhombic prism *Rectangle through origin* (*o*)	(hkl) $(\bar{h}k\bar{l})$ $(\bar{h}\bar{k}\bar{l})$ $(h\bar{k}l)$	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{h}\bar{k}\bar{l})$ $(hk\bar{l})$
2	*b*	*m*	Pinacoid or parallelohedron *Line segment through origin* (*m*)	$(h0l)$ $(\bar{h}0\bar{l})$	$(hk0)$ $(\bar{h}\bar{k}0)$
2	*a*	2	Pinacoid or parallelohedron *Line segment through origin* (*i*)	(010) $(0\bar{1}0)$	(001) $(00\bar{1})$

Symmetry of special projections

	Along [100]	Along [010]	Along [001]
Unique axis *b*	2*mm*	2	2*mm*
c	2*mm*	2*mm*	2

ORTHORHOMBIC SYSTEM

222 D_2



4	*d*	1	Rhombic disphenoid or rhombic tetrahedron *Rhombic tetrahedron* (*u*)	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{h}k\bar{l})$ $(h\bar{k}\bar{l})$
			Rhombic prism *Rectangle through origin*	$(hk0)$ $(\bar{h}\bar{k}0)$ $(\bar{h}k0)$ $(h\bar{k}0)$
			Rhombic prism *Rectangle through origin*	$(h0l)$ $(\bar{h}0l)$ $(\bar{h}0\bar{l})$ $(h0\bar{l})$
			Rhombic prism *Rectangle through origin*	$(0kl)$ $(0\bar{k}l)$ $(0k\bar{l})$ $(0\bar{k}\bar{l})$
2	*c*	..2	Pinacoid or parallelohedron *Line segment through origin* (*q*)	(001) $(00\bar{1})$
2	*b*	.2.	Pinacoid or parallelohedron *Line segment through origin* (*m*)	(010) $(0\bar{1}0)$
2	*a*	2..	Pinacoid or parallelohedron *Line segment through origin* (*i*)	(100) $(\bar{1}00)$

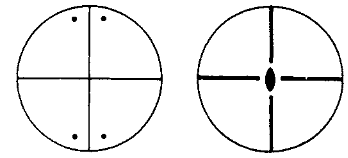
Symmetry of special projections

Along [100]	Along [010]	Along [001]
2*mm*	2*mm*	2*mm*

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

ORTHORHOMBIC SYSTEM (*cont.*)

$mm2$ $\quad C_{2v}$

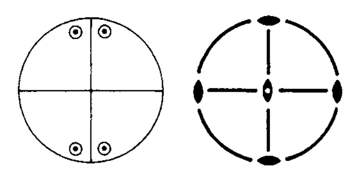


4	*d*	1	Rhombic pyramid *Rectangle* (*i*)	(hkl) $(\bar{h}\bar{k}l)$ $(h\bar{k}l)$ $(\bar{h}kl)$
			Rhombic prism *Rectangle through origin*	$(hk0)$ $(\bar{h}\bar{k}0)$ $(h\bar{k}0)$ $(\bar{h}k0)$
2	*c*	*m..*	Dome or dihedron *Line segment* (*g*)	$(0kl)$ $(0\bar{k}l)$
			Pinacoid or parallelohedron *Line segment through origin*	(010) $(0\bar{1}0)$
2	*b*	*.m.*	Dome or dihedron *Line segment* (*e*)	$(h0l)$ $(\bar{h}0l)$
			Pinacoid or parallelohedron *Line segment through origin*	(100) $(\bar{1}00)$
1	*a*	*mm*2	Pedion or monohedron *Single point* (*a*)	(001) or $(00\bar{1})$

Symmetry of special projections

Along [100]	Along [010]	Along [001]
m	*m*	2*mm*

$\dfrac{2}{m}\dfrac{2}{m}\dfrac{2}{m}$ ($m\,m\,m$) $\quad D_{2h}$



8	*g*	1	Rhombic dipyramid *Quad* (α)	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{h}k\bar{l})$ $(h\bar{k}\bar{l})$ $(\bar{h}\bar{k}\bar{l})$ $(hk\bar{l})$ $(h\bar{k}l)$ $(\bar{h}kl)$
4	*f*	*..m*	Rhombic prism *Rectangle through origin* (*y*)	$(hk0)$ $(\bar{h}\bar{k}0)$ $(\bar{h}k0)$ $(h\bar{k}0)$
4	*e*	*.m.*	Rhombic prism *Rectangle through origin* (*w*)	$(h0l)$ $(\bar{h}0l)$ $(\bar{h}0\bar{l})$ $(h0\bar{l})$
4	*d*	*m..*	Rhombic prism *Rectangle through origin* (*u*)	$(0kl)$ $(0\bar{k}l)$ $(0k\bar{l})$ $(0\bar{k}\bar{l})$
2	*c*	*mm*2	Pinacoid or parallelohedron *Line segment through origin* (*q*)	(001) $(00\bar{1})$
2	*b*	*m*2*m*	Pinacoid or parallelohedron *Line segment through origin* (*m*)	(010) $(0\bar{1}0)$
2	*a*	2*mm*	Pinacoid or parallelohedron *Line segment through origin* (*i*)	(100) $(\bar{1}00)$

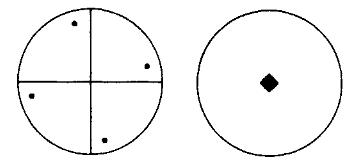
Symmetry of special projections

Along [100]	Along [010]	Along [001]
2*mm*	2*mm*	2*mm*

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

TETRAGONAL SYSTEM

4 C_4

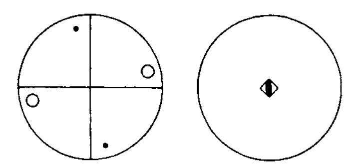


4	*b*	1	Tetragonal pyramid *Square* (*d*)	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{k}hl)$ $(k\bar{h}l)$
			Tetragonal prism *Square through origin*	$(hk0)$ $(\bar{h}\bar{k}0)$ $(\bar{k}h0)$ $(k\bar{h}0)$
1	*a*	4..	Pedion or monohedron *Single point* (*a*)	(001) or $(00\bar{1})$

Symmetry of special projections

Along [001]	Along [100]	Along [110]
4	*m*	*m*

$\bar{4}$ S_4

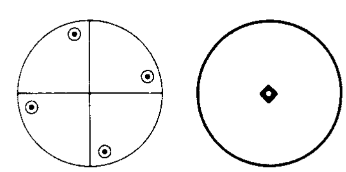


4	*b*	1	Tetragonal disphenoid or tetragonal tetrahedron *Tetragonal tetrahedron* (*h*)	(hkl) $(\bar{h}\bar{k}l)$ $(k\bar{h}\bar{l})$ $(\bar{k}h\bar{l})$
			Tetragonal prism *Square through origin*	$(hk0)$ $(\bar{h}\bar{k}0)$ $(k\bar{h}0)$ $(\bar{k}h0)$
2	*a*	2..	Pinacoid or parallelohedron *Line segment through origin* (*e*)	(001) $(00\bar{1})$

Symmetry of special projections

Along [001]	Along [100]	Along [110]
4	*m*	*m*

$4/m$ C_{4h}



8	*c*	1	Tetragonal dipyramid *Tetragonal prism* (*l*)	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{k}hl)$ $(k\bar{h}l)$ $(\bar{h}\bar{k}\bar{l})$ $(hk\bar{l})$ $(k\bar{h}\bar{l})$ $(\bar{k}h\bar{l})$
4	*b*	*m*..	Tetragonal prism *Square through origin* (*j*)	$(hk0)$ $(\bar{h}\bar{k}0)$ $(\bar{k}h0)$ $(k\bar{h}0)$
2	*a*	4..	Pinacoid or parallelohedron *Line segment through origin* (*g*)	(001) $(00\bar{1})$

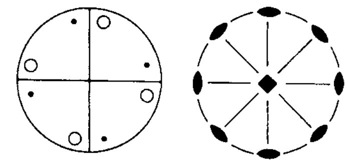
Symmetry of special projections

Along [001]	Along [100]	Along [110]
4	2*mm*	2*mm*

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

TETRAGONAL SYSTEM (*cont.*)

422 D_4

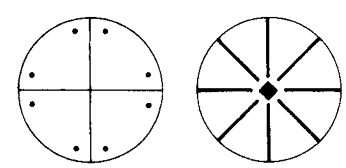


8	*d*	1	Tetragonal trapezohedron *Twisted tetragonal antiprism* (*p*)	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{k}hl)$ $(k\bar{h}l)$ $(\bar{h}k\bar{l})$ $(h\bar{k}\bar{l})$ $(kh\bar{l})$ $(\bar{k}\bar{h}\bar{l})$
			Ditetragonal prism *Truncated square through origin*	$(hk0)$ $(\bar{h}\bar{k}0)$ $(\bar{k}h0)$ $(k\bar{h}0)$ $(\bar{h}k0)$ $(h\bar{k}0)$ $(kh0)$ $(\bar{k}\bar{h}0)$
			Tetragonal dipyramid *Tetragonal prism*	$(h0l)$ $(\bar{h}0l)$ $(0hl)$ $(0\bar{h}l)$ $(\bar{h}0\bar{l})$ $(h0\bar{l})$ $(0h\bar{l})$ $(0\bar{h}\bar{l})$
			Tetragonal dipyramid *Tetragonal prism*	(hhl) $(\bar{h}\bar{h}l)$ $(\bar{h}hl)$ $(h\bar{h}l)$ $(\bar{h}h\bar{l})$ $(h\bar{h}\bar{l})$ $(hh\bar{l})$ $(\bar{h}\bar{h}\bar{l})$
4	*c*	.2.	Tetragonal prism *Square through origin* (*l*)	(100) $(\bar{1}00)$ (010) $(0\bar{1}0)$
4	*b*	..2	Tetragonal prism *Square through origin* (*j*)	(110) $(\bar{1}\bar{1}0)$ $(\bar{1}10)$ $(1\bar{1}0)$
2	*a*	4..	Pinacoid or parallelohedron *Line segment through origin* (*g*)	(001) $(00\bar{1})$

Symmetry of special projections

Along [001]	Along [100]	Along [110]
4*mm*	2*mm*	2*mm*

4*mm* C_{4v}



8	*d*	1	Ditetragonal pyramid *Truncated square* (*g*)	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{k}hl)$ $(k\bar{h}l)$ $(h\bar{k}l)$ $(\bar{h}kl)$ $(\bar{k}\bar{h}l)$ (khl)
			Ditetragonal prism *Truncated square through origin*	$(hk0)$ $(\bar{h}\bar{k}0)$ $(\bar{k}h0)$ $(k\bar{h}0)$ $(h\bar{k}0)$ $(\bar{h}k0)$ $(\bar{k}\bar{h}0)$ $(kh0)$
4	*c*	*.m.*	Tetragonal pyramid *Square* (*e*)	$(h0l)$ $(\bar{h}0l)$ $(0hl)$ $(0\bar{h}l)$
			Tetragonal prism *Square through origin*	(100) $(\bar{1}00)$ (010) $(0\bar{1}0)$
4	*b*	*..m*	Tetragonal pyramid *Square* (*d*)	(hhl) $(\bar{h}\bar{h}l)$ $(\bar{h}hl)$ $(h\bar{h}l)$
			Tetragonal prism *Square through origin*	(110) $(\bar{1}\bar{1}0)$ $(\bar{1}10)$ $(1\bar{1}0)$
1	*a*	4*mm*	Pedion or monohedron *Single point* (*a*)	(001) or $(00\bar{1})$

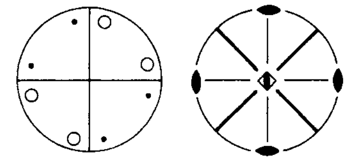
Symmetry of special projections

Along [001]	Along [100]	Along [110]
4*mm*	*m*	*m*

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

TETRAGONAL SYSTEM (*cont.*)

$\bar{4}2m$ D_{2d}

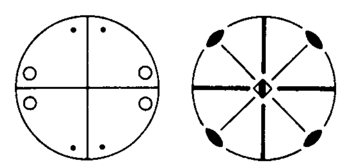


8	*d*	1	Tetragonal scalenohedron *Tetragonal tetrahedron cut off by pinacoid* (*o*)	(hkl) $(\bar{h}\bar{k}l)$ $(k\bar{h}\bar{l})$ $(\bar{k}h\bar{l})$ $(\bar{h}k\bar{l})$ $(h\bar{k}\bar{l})$ $(\bar{k}\bar{h}l)$ (khl)
			Ditetragonal prism *Truncated square through origin*	$(hk0)$ $(\bar{h}\bar{k}0)$ $(k\bar{h}0)$ $(\bar{k}h0)$ $(\bar{h}k0)$ $(h\bar{k}0)$ $(\bar{k}\bar{h}0)$ $(kh0)$
			Tetragonal dipyramid *Tetragonal prism*	$(h0l)$ $(\bar{h}0l)$ $(0\bar{h}\bar{l})$ $(0h\bar{l})$ $(\bar{h}0\bar{l})$ $(h0\bar{l})$ $(0\bar{h}l)$ $(0hl)$
4	*c*	*..m*	Tetragonal disphenoid or tetragonal tetrahedron *Tetragonal tetrahedron* (*n*)	(hhl) $(\bar{h}\bar{h}l)$ $(h\bar{h}\bar{l})$ $(\bar{h}h\bar{l})$
			Tetragonal prism *Square through origin*	(110) $(\bar{1}\bar{1}0)$ $(1\bar{1}0)$ $(\bar{1}10)$
4	*b*	.2.	Tetragonal prism *Square through origin* (*i*)	(100) $(\bar{1}00)$ $(0\bar{1}0)$ (010)
2	*a*	2*.mm*	Pinacoid or parallelohedron *Line segment through origin* (*g*)	(001) $(00\bar{1})$

Symmetry of special projections

Along [001]	Along [100]	Along [110]
4*mm*	2*mm*	*m*

$\bar{4}m2$ D_{2d}



8	*d*	1	Tetragonal scalenohedron *Tetragonal tetrahedron cut off by pinacoid* (*l*)	(hkl) $(\bar{h}\bar{k}l)$ $(k\bar{h}\bar{l})$ $(\bar{k}h\bar{l})$ $(h\bar{k}l)$ $(\bar{h}kl)$ $(kh\bar{l})$ $(\bar{k}\bar{h}\bar{l})$
			Ditetragonal prism *Truncated square through origin*	$(hk0)$ $(\bar{h}\bar{k}0)$ $(k\bar{h}0)$ $(\bar{k}h0)$ $(h\bar{k}0)$ $(\bar{h}k0)$ $(kh0)$ $(\bar{k}\bar{h}0)$
			Tetragonal dipyramid *Tetragonal prism*	(hhl) $(\bar{h}\bar{h}l)$ $(h\bar{h}\bar{l})$ $(\bar{h}h\bar{l})$ $(h\bar{h}l)$ $(\bar{h}hl)$ $(hh\bar{l})$ $(\bar{h}\bar{h}\bar{l})$
4	*c*	*.m.*	Tetragonal disphenoid or tetragonal tetrahedron *Tetragonal tetrahedron* (*j*)	$(h0l)$ $(\bar{h}0l)$ $(0\bar{h}\bar{l})$ $(0h\bar{l})$
			Tetragonal prism *Square through origin*	(100) $(\bar{1}00)$ $(0\bar{1}0)$ (010)
4	*b*	..2	Tetragonal prism *Square through origin* (*h*)	(110) $(\bar{1}\bar{1}0)$ $(1\bar{1}0)$ $(\bar{1}10)$
2	*a*	2*mm.*	Pinacoid or parallelohedron *Line segment through origin* (*e*)	(001) $(00\bar{1})$

Symmetry of special projections

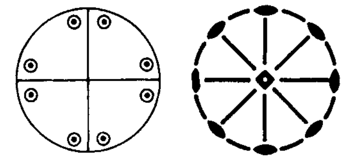
Along [001]	Along [100]	Along [110]
4*mm*	*m*	2*mm*

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

TETRAGONAL SYSTEM (*cont.*)

$4/mmm$ $\quad D_{4h}$

$\dfrac{4}{m}\dfrac{2}{m}\dfrac{2}{m}$



16	*g*	1	Ditetragonal dipyramid *Edge-truncated tetragonal prism* (*u*)	(hkl) $(\bar h\bar kl)$ $(\bar khl)$ $(k\bar hl)$ $(\bar hk\bar l)$ $(h\bar k\bar l)$ $(kh\bar l)$ $(\bar k\bar h\bar l)$ $(\bar h\bar k\bar l)$ $(hk\bar l)$ $(k\bar h\bar l)$ $(\bar kh\bar l)$ $(h\bar kl)$ $(\bar hkl)$ $(\bar k\bar hl)$ (khl)
8	*f*	*.m.*	Tetragonal dipyramid *Tetragonal prism* (*s*)	$(h0l)$ $(\bar h0l)$ $(0hl)$ $(0\bar hl)$ $(\bar h0\bar l)$ $(h0\bar l)$ $(0h\bar l)$ $(0\bar h\bar l)$
8	*e*	*..m*	Tetragonal dipyramid *Tetragonal prism* (*r*)	(hhl) $(\bar h\bar hl)$ $(\bar hhl)$ $(h\bar hl)$ $(\bar hh\bar l)$ $(h\bar h\bar l)$ $(hh\bar l)$ $(\bar h\bar h\bar l)$
8	*d*	*m..*	Ditetragonal prism *Truncated square through origin* (*p*)	$(hk0)$ $(\bar h\bar k0)$ $(\bar kh0)$ $(k\bar h0)$ $(\bar hk0)$ $(h\bar k0)$ $(kh0)$ $(\bar k\bar h0)$
4	*c*	*m2m.*	Tetragonal prism *Square through origin* (*l*)	(100) $(\bar 100)$ (010) $(0\bar 10)$
4	*b*	*m.m*2	Tetragonal prism *Square through origin* (*j*)	(110) $(\bar 1\bar 10)$ $(\bar 110)$ $(1\bar 10)$
2	*a*	4*mm*	Pinacoid or parallelohedron *Line segment through origin* (*g*)	(001) $(00\bar 1)$

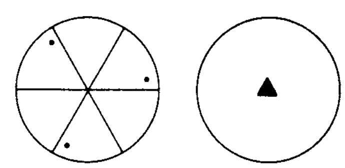
Symmetry of special projections

Along [001]	Along [100]	Along [110]
4*mm*	2*mm*	2*mm*

TRIGONAL SYSTEM

3 $\quad C_3$

HEXAGONAL AXES



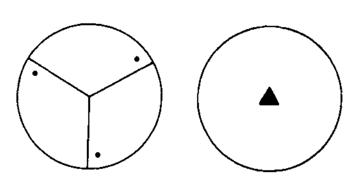
3	*b*	1	Trigonal pyramid *Trigon* (*d*)	$(hkil)$ $(ihkl)$ $(kihl)$
			Trigonal prism *Trigon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$
1	*a*	3..	Pedion or monohedron *Single point* (*a*)	(0001) or $(000\bar 1)$

Symmetry of special projections

Along [001]	Along [100]	Along [210]
3	1	1

3 $\quad C_3$

RHOMBOHEDRAL AXES



3	*b*	1	Trigonal pyramid *Trigon* (*b*)	(hkl) (lhk) (klh)
			Trigonal prism *Trigon through origin*	$(hk(\overline{h+k}))$ $((\overline{h+k})hk)$ $(k(\overline{h+k})h)$
1	*a*	3.	Pedion or monohedron *Single point* (*a*)	(111) or $(\bar 1\bar 1\bar 1)$

Symmetry of special projections

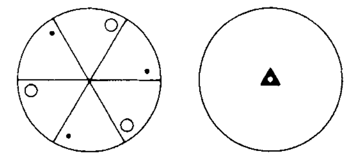
Along [111]	Along $[1\bar 10]$	Along $[2\bar 1\bar 1]$
3	1	1

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

TRIGONAL SYSTEM (*cont.*)

$\bar{3}$ C_{3i}

HEXAGONAL AXES



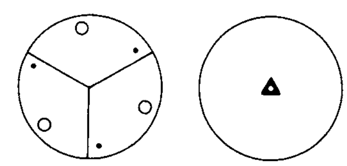
6	*b*	1	Rhombohedron *Trigonal antiprism* (*g*)	$(hkil)$ $(ihkl)$ $(kihl)$ $(\bar{h}\bar{k}\bar{i}\bar{l})$ $(\bar{i}\bar{h}\bar{k}\bar{l})$ $(\bar{k}\bar{i}\bar{h}\bar{l})$
			Hexagonal prism *Hexagon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(\bar{h}\bar{k}\bar{i}0)$ $(\bar{i}\bar{h}\bar{k}0)$ $(\bar{k}\bar{i}\bar{h}0)$
2	*a*	3..	Pinacoid or parallelohedron *Line segment through origin* (*c*)	(0001) $(000\bar{1})$

Symmetry of special projections

Along [001]	Along [100]	Along [210]
6	2	2

$\bar{3}$ C_{3i}

RHOMBOHEDRAL AXES



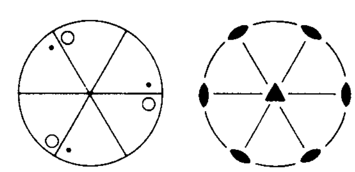
6	*b*	1	Rhombohedron *Trigonal antiprism* (*f*)	(hkl) (lhk) (klh) $(\bar{h}\bar{k}\bar{l})$ $(\bar{l}\bar{h}\bar{k})$ $(\bar{k}\bar{l}\bar{h})$
			Hexagonal prism *Hexagon through origin*	$(hk(\overline{h+k}))$ $((\overline{h+k})hk)$ $(k(\overline{h+k})h)$ $(\bar{h}\bar{k}(h+k))$ $((h+k)\bar{h}\bar{k})$ $(\bar{k}(h+k)\bar{h})$
2	*a*	3.	Pinacoid or parallelohedron *Line segment through origin* (*c*)	(111) $(\bar{1}\bar{1}\bar{1})$

Symmetry of special projections

Along [111]	Along [1$\bar{1}$0]	Along [2$\bar{1}\bar{1}$]
6	2	2

321 D_3

HEXAGONAL AXES



6	*c*	1	Trigonal trapezohedron *Twisted trigonal antiprism* (*g*)	$(hkil)$ $(ihkl)$ $(kihl)$ $(khi\bar{l})$ $(hik\bar{l})$ $(ikh\bar{l})$
			Ditrigonal prism *Truncated trigon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(khi0)$ $(hik0)$ $(ikh0)$
			Trigonal dipyramid *Trigonal prism*	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(hh\overline{2h}\bar{l})$ $(h\overline{2h}h\bar{l})$ $(\overline{2h}hh\bar{l})$
			Rhombohedron *Trigonal antiprism*	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(0h\bar{h}\bar{l})$ $(h\bar{h}0\bar{l})$ $(\bar{h}0h\bar{l})$
			Hexagonal prism *Hexagon through origin*	$(10\bar{1}0)$ $(\bar{1}100)$ $(0\bar{1}10)$ $(01\bar{1}0)$ $(1\bar{1}00)$ $(\bar{1}010)$
3	*b*	.2.	Trigonal prism *Trigon through origin* (*e*)	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ or $(\bar{1}\bar{1}20)$ $(2\bar{1}\bar{1}0)$ $(\bar{1}2\bar{1}0)$
2	*a*	3..	Pinacoid or parallelohedron *Line segment through origin* (*c*)	(0001) $(000\bar{1})$

Symmetry of special projections

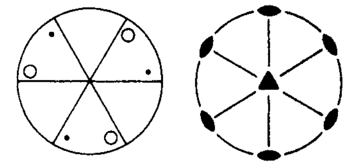
Along [001]	Along [100]	Along [210]
3*m*	2	1

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

TRIGONAL SYSTEM (*cont.*)

312 D_3

HEXAGONAL AXES



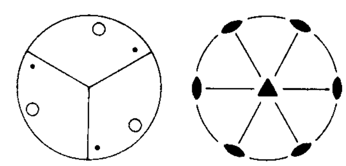
6	*c*	1	Trigonal trapezohedron *Twisted trigonal antiprism* (*l*)	$(hkil)$ $(ihkl)$ $(kihl)$ $(\bar{k}\bar{h}\bar{i}\bar{l})$ $(\bar{h}\bar{i}\bar{k}\bar{l})$ $(\bar{i}\bar{k}\bar{h}\bar{l})$
			Ditrigonal prism *Truncated trigon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(\bar{k}\bar{h}\bar{i}0)$ $(\bar{h}\bar{i}\bar{k}0)$ $(\bar{i}\bar{k}\bar{h}0)$
			Trigonal dipyramid *Trigonal prism*	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(0\bar{h}h\bar{l})$ $(\bar{h}h0\bar{l})$ $(h0\bar{h}\bar{l})$
			Rhombohedron *Trigonal antiprism*	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(\bar{h}\bar{h}2h\bar{l})$ $(\bar{h}2h\bar{h}\bar{l})$ $(2h\bar{h}\bar{h}\bar{l})$
			Hexagonal prism *Hexagon through origin*	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ $(\bar{1}\bar{1}20)$ $(\bar{1}2\bar{1}0)$ $(2\bar{1}\bar{1}0)$
3	*b*	..2	Trigonal prism *Trigon through origin* (*j*)	$(10\bar{1}0)$ $(\bar{1}100)$ $(0\bar{1}10)$ or $(\bar{1}010)$ $(1\bar{1}00)$ $(01\bar{1}0)$
2	*a*	3..	Pinacoid or parallelohedron *Line segment through origin* (*g*)	(0001) $(000\bar{1})$

Symmetry of special projections

Along [001]	Along [100]	Along [210]
$3m$	1	2

32 D_3

RHOMBOHEDRAL AXES



6	*c*	1	Trigonal trapezohedron *Twisted trigonal antiprism* (*f*)	(hkl) (lhk) (klh) $(\bar{k}\bar{h}\bar{l})$ $(\bar{h}\bar{l}\bar{k})$ $(\bar{l}\bar{k}\bar{h})$
			Ditrigonal prism *Truncated trigon through origin*	$(hk(\overline{h+k}))$ $((\overline{h+k})hk)$ $(k(\overline{h+k})h)$ $(\bar{k}\bar{h}(h+k))$ $(\bar{h}(h+k)\bar{k})$ $((h+k)\bar{k}\bar{h})$
			Trigonal dipyramid *Trigonal prism*	$(hk(2k-h))$ $((2k-h)hk)$ $(k(2k-h)h)$ $(\bar{k}\bar{h}(h-2k))$ $(\bar{h}(h-2k)\bar{k})$ $((h-2k)\bar{k}\bar{h})$
			Rhombohedron *Trigonal antiprism*	(hhl) (lhh) (hlh) $(\bar{h}\bar{h}\bar{l})$ $(\bar{h}\bar{l}\bar{h})$ $(\bar{l}\bar{h}\bar{h})$
			Hexagonal prism *Hexagon through origin*	$(11\bar{2})$ $(\bar{2}11)$ $(1\bar{2}1)$ $(\bar{1}\bar{1}2)$ $(\bar{1}2\bar{1})$ $(2\bar{1}\bar{1})$
3	*b*	.2	Trigonal prism *Trigon through origin* (*d*)	$(01\bar{1})$ $(\bar{1}01)$ $(1\bar{1}0)$ or $(0\bar{1}1)$ $(10\bar{1})$ $(\bar{1}10)$
2	*a*	3.	Pinacoid or parallelohedron *Line segment through origin* (*c*)	(111) $(\bar{1}\bar{1}\bar{1})$

Symmetry of special projections

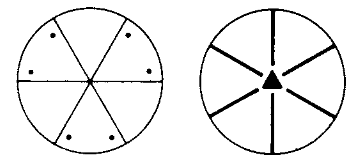
Along [111]	Along [1$\bar{1}$0]	Along [2$\bar{1}\bar{1}$]
$3m$	2	1

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

TRIGONAL SYSTEM (*cont.*)

$3m1$ $\quad C_{3v}$

HEXAGONAL AXES



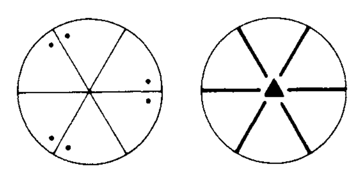
6	*c*	1	Ditrigonal pyramid	$(hkil)$	$(ihkl)$	$(kihl)$
			Truncated trigon (*e*)	$(\bar{k}\bar{h}\bar{i}l)$	$(\bar{h}\bar{i}\bar{k}l)$	$(\bar{i}\bar{k}\bar{h}l)$
			Ditrigonal prism	$(hki0)$	$(ihk0)$	$(kih0)$
			Truncated trigon through origin	$(\bar{k}\bar{h}\bar{i}0)$	$(\bar{h}\bar{i}\bar{k}0)$	$(\bar{i}\bar{k}\bar{h}0)$
			Hexagonal pyramid	$(hh\overline{2h}l)$	$(\overline{2h}hhl)$	$(h\overline{2h}hl)$
			Hexagon	$(\bar{h}\bar{h}2hl)$	$(\bar{h}2h\bar{h}l)$	$(2h\bar{h}\bar{h}l)$
			Hexagonal prism	$(11\bar{2}0)$	$(\bar{2}110)$	$(1\bar{2}10)$
			Hexagon through origin	$(\bar{1}\bar{1}20)$	$(\bar{1}2\bar{1}0)$	$(2\bar{1}\bar{1}0)$
3	*b*	*.m.*	Trigonal pyramid	$(h0\bar{h}l)$	$(\bar{h}h0l)$	$(0\bar{h}hl)$
			Trigon (*d*)			
			Trigonal prism	$(10\bar{1}0)$	$(\bar{1}100)$	$(0\bar{1}10)$
			Trigon through origin	or $(\bar{1}010)$	$(1\bar{1}00)$	$(01\bar{1}0)$
1	*a*	3*m.*	Pedion or monohedron	(0001) or $(000\bar{1})$		
			Single point (*a*)			

Symmetry of special projections

Along [001]	Along [100]	Along [210]
$3m$	1	m

$31m$ $\quad C_{3v}$

HEXAGONAL AXES



6	*c*	1	Ditrigonal pyramid	$(hkil)$	$(ihkl)$	$(kihl)$
			Truncated trigon (*d*)	$(khil)$	$(hikl)$	$(ikhl)$
			Ditrigonal prism	$(hki0)$	$(ihk0)$	$(kih0)$
			Truncated trigon through origin	$(khi0)$	$(hik0)$	$(ikh0)$
			Hexagonal pyramid	$(h0\bar{h}l)$	$(\bar{h}h0l)$	$(0\bar{h}hl)$
			Hexagon	$(0h\bar{h}l)$	$(h\bar{h}0l)$	$(\bar{h}0hl)$
			Hexagonal prism	$(10\bar{1}0)$	$(\bar{1}100)$	$(0\bar{1}10)$
			Hexagon through origin	$(01\bar{1}0)$	$(1\bar{1}00)$	$(\bar{1}010)$
3	*b*	*..m*	Trigonal pyramid	$(hh\overline{2h}l)$	$(\overline{2h}hhl)$	$(h\overline{2h}hl)$
			Trigon (*c*)			
			Trigonal prism	$(11\bar{2}0)$	$(\bar{2}110)$	$(1\bar{2}10)$
			Trigon through origin	or $(\bar{1}\bar{1}20)$	$(2\bar{1}\bar{1}0)$	$(\bar{1}2\bar{1}0)$
1	*a*	3.*m*	Pedion or monohedron	(0001) or $(000\bar{1})$		
			Single point (*a*)			

Symmetry of special projections

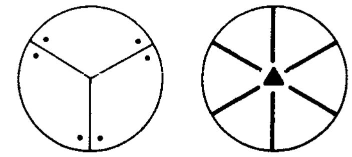
Along [001]	Along [100]	Along [210]
$3m$	m	1

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

TRIGONAL SYSTEM (*cont.*)

$3m$ C_{3v}

RHOMBOHEDRAL AXES



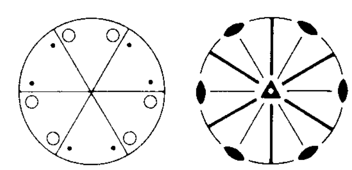
6	*c*	1	Ditrigonal pyramid *Truncated trigon* (*c*)	(hkl) (lhk) (klh) (khl) (hlk) (lkh)
			Ditrigonal prism *Truncated trigon through origin*	$(hk\overline{h+k})$ $(\overline{h+k}hk)$ $(k\overline{h+k}h)$ $(kh\overline{h+k})$ $(h\overline{h+k}k)$ $(\overline{h+k}kh)$
			Hexagonal pyramid *Hexagon*	$(hk(2k-h))$ $((2k-h)hk)$ $(k(2k-h)h)$ $(kh(2k-h))$ $(h(2k-h)k)$ $((2k-h)kh)$
			Hexagonal prism *Hexagon through origin*	$(01\bar{1})$ $(\bar{1}01)$ $(1\bar{1}0)$ $(10\bar{1})$ $(0\bar{1}1)$ $(\bar{1}10)$
3	*b*	*.m*	Trigonal pyramid *Trigon* (*b*)	(hhl) (lhh) (hlh)
			Trigonal prism *Trigon through origin*	$(11\bar{2})$ $(\bar{2}11)$ $(1\bar{2}1)$ or $(\bar{1}\bar{1}2)$ $(2\bar{1}\bar{1})$ $(\bar{1}2\bar{1})$
1	*a*	$3m.$	Pedion or monohedron *Single point* (*a*)	(111) or $(\bar{1}\bar{1}\bar{1})$

Symmetry of special projections

Along [111]	Along $[1\bar{1}0]$	Along $[2\bar{1}\bar{1}]$
$3m$	1	m

$\bar{3}m1$ $\bar{3}\frac{2}{m}1$ D_{3d}

HEXAGONAL AXES



12	*d*	1	Ditrigonal scalenohedron or hexagonal scalenohedron *Trigonal antiprism sliced off by pinacoid* (*j*)	$(hkil)$ $(ihkl)$ $(kihl)$ $(khi\bar{l})$ $(hik\bar{l})$ $(ikh\bar{l})$ $(\bar{h}\bar{k}\bar{i}\bar{l})$ $(\bar{i}\bar{h}\bar{k}\bar{l})$ $(\bar{k}\bar{i}\bar{h}\bar{l})$ $(\bar{k}\bar{h}\bar{i}l)$ $(\bar{h}\bar{i}\bar{k}l)$ $(\bar{i}\bar{k}\bar{h}l)$
			Dihexagonal prism *Truncated hexagon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(khi0)$ $(hik0)$ $(ikh0)$ $(\bar{h}\bar{k}\bar{i}0)$ $(\bar{i}\bar{h}\bar{k}0)$ $(\bar{k}\bar{i}\bar{h}0)$ $(\bar{k}\bar{h}\bar{i}0)$ $(\bar{h}\bar{i}\bar{k}0)$ $(\bar{i}\bar{k}\bar{h}0)$
			Hexagonal dipyramid *Hexagonal prism*	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(hh\overline{2h}\bar{l})$ $(h\overline{2h}h\bar{l})$ $(\overline{2h}hh\bar{l})$ $(\bar{h}\bar{h}2h\bar{l})$ $(2h\bar{h}\bar{h}\bar{l})$ $(\bar{h}2h\bar{h}\bar{l})$ $(\bar{h}\bar{h}2hl)$ $(\bar{h}2h\bar{h}l)$ $(2h\bar{h}\bar{h}l)$
6	*c*	*.m.*	Rhombohedron *Trigonal antiprism* (*i*)	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(0h\bar{h}\bar{l})$ $(h\bar{h}0\bar{l})$ $(\bar{h}0h\bar{l})$
			Hexagonal prism *Hexagon through origin*	$(10\bar{1}0)$ $(\bar{1}100)$ $(0\bar{1}10)$ $(01\bar{1}0)$ $(1\bar{1}00)$ $(\bar{1}010)$
6	*b*	.2.	Hexagonal prism *Hexagon through origin* (*g*)	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ $(\bar{1}\bar{1}20)$ $(\bar{1}2\bar{1}0)$ $(2\bar{1}\bar{1}0)$
2	*a*	$3m.$	Pinacoid or parallelohedron *Line segment through origin* (*c*)	(0001) $(000\bar{1})$

Symmetry of special projections

Along [001]	Along [100]	Along [210]
$6mm$	2	$2mm$

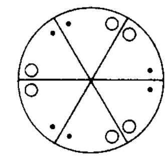
Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

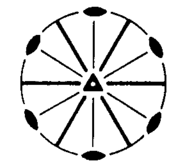
TRIGONAL SYSTEM (*cont.*)

$\bar{3}1m$ D_{3d}

$\bar{3}1\frac{2}{m}$

HEXAGONAL AXES





12	*d*	1	Ditrigonal scalenohedron or hexagonal scalenohedron	$(hkil)$	$(ihkl)$	$(kihl)$
			Trigonal antiprism sliced off by pinacoid (*l*)	$(\bar{k}\bar{h}\bar{i}\bar{l})$	$(\bar{h}\bar{i}\bar{k}\bar{l})$	$(\bar{i}\bar{k}\bar{h}\bar{l})$
				$(\bar{h}\bar{k}\bar{i}\bar{l})$	$(\bar{i}\bar{h}\bar{k}\bar{l})$	$(\bar{k}\bar{i}\bar{h}\bar{l})$
				$(khil)$	$(hikl)$	$(ikhl)$
			Dihexagonal prism	$(hki0)$	$(ihk0)$	$(kih0)$
			Truncated hexagon through origin	$(\bar{k}\bar{h}\bar{i}0)$	$(\bar{h}\bar{i}\bar{k}0)$	$(\bar{i}\bar{k}\bar{h}0)$
				$(\bar{h}\bar{k}\bar{i}0)$	$(\bar{i}\bar{h}\bar{k}0)$	$(\bar{k}\bar{i}\bar{h}0)$
				$(khi0)$	$(hik0)$	$(ikh0)$
			Hexagonal dipyramid	$(h0\bar{h}l)$	$(\bar{h}h0l)$	$(0\bar{h}hl)$
			Hexagonal prism	$(0\bar{h}h\bar{l})$	$(\bar{h}h0\bar{l})$	$(h0\bar{h}\bar{l})$
				$(\bar{h}0h\bar{l})$	$(h\bar{h}0\bar{l})$	$(0h\bar{h}\bar{l})$
				$(0h\bar{h}l)$	$(h\bar{h}0l)$	$(\bar{h}0hl)$
6	*c*	..*m*	Rhombohedron	$(hh\overline{2h}l)$	$(\overline{2h}hhl)$	$(h\overline{2h}hl)$
			Trigonal antiprism (*k*)	$(\bar{h}\bar{h}2h\bar{l})$	$(\bar{h}2h\bar{h}\bar{l})$	$(2h\bar{h}\bar{h}\bar{l})$
			Hexagonal prism	$(11\bar{2}0)$	$(\bar{2}110)$	$(1\bar{2}10)$
			Hexagon through origin	$(\bar{1}\bar{1}20)$	$(\bar{1}2\bar{1}0)$	$(2\bar{1}\bar{1}0)$
6	*b*	..2	Hexagonal prism	$(10\bar{1}0)$	$(\bar{1}100)$	$(0\bar{1}10)$
			Hexagon through origin (*i*)	$(\bar{1}010)$	$(1\bar{1}00)$	$(01\bar{1}0)$
2	*a*	3.*m*	Pinacoid or parallelohedron	(0001)	$(000\bar{1})$	
			Line segment through origin (*e*)			

Symmetry of special projections

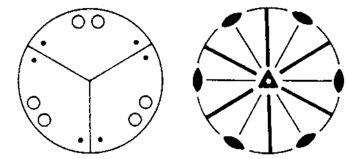
Along [001]	Along [100]	Along [210]
6*mm*	2*mm*	2

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont*.)

TRIGONAL SYSTEM (*cont*.)

$\bar{3}m$ D_{3d}

$\bar{3}\frac{2}{m}$



RHOMBOHEDRAL AXES

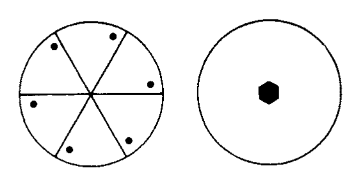
12	*d*	1	Ditrigonal scalenohedron or hexagonal scalenohedron *Trigonal antiprism sliced off by pinacoid* (*i*)	(hkl) (lhk) (klh) $(\bar{k}\bar{h}\bar{l})$ $(\bar{h}\bar{l}\bar{k})$ $(\bar{l}\bar{k}\bar{h})$ $(\bar{h}\bar{k}\bar{l})$ $(\bar{l}\bar{h}\bar{k})$ $(\bar{k}\bar{l}\bar{h})$ (khl) (hlk) (lkh)
			Dihexagonal prism *Truncated hexagon through origin*	$(hk(\overline{h+k}))$ $((\overline{h+k})hk)$ $(k(\overline{h+k})h)$ $(\bar{k}\bar{h}(h+k))$ $(\bar{h}(h+k)\bar{k})$ $((h+k)\bar{k}\bar{h})$ $(\bar{h}\bar{k}(h+k))$ $((h+k)\bar{h}\bar{k})$ $(\bar{k}(h+k)\bar{h})$ $(kh(\overline{h+k}))$ $(h(\overline{h+k})k)$ $((\overline{h+k})kh)$
			Hexagonal dipyramid *Hexagonal prism*	$(hk(2k-h))$ $((2k-h)hk)$ $(k(2k-h)h)$ $(\bar{k}\bar{h}(h-2k))$ $(\bar{h}(h-2k)\bar{k})$ $((h-2k)\bar{k}\bar{h})$ $(\bar{h}\bar{k}(h-2k))$ $((h-2k)\bar{h}\bar{k})$ $(\bar{k}(h-2k)\bar{h})$ $(kh(2k-h))$ $(h(2k-h)k)$ $((2k-h)kh)$
6	*c*	*.m*	Rhombohedron *Trigonal antiprism* (*h*)	(hhl) (lhh) (hlh) $(\bar{h}\bar{h}\bar{l})$ $(\bar{h}\bar{l}\bar{h})$ $(\bar{l}\bar{h}\bar{h})$
			Hexagonal prism *Hexagon through origin*	$(11\bar{2})$ $(\bar{2}11)$ $(1\bar{2}1)$ $(\bar{1}\bar{1}2)$ $(\bar{1}2\bar{1})$ $(2\bar{1}\bar{1})$
6	*b*	.2	Hexagonal prism *Hexagon through origin* (*f*)	$(01\bar{1})$ $(\bar{1}01)$ $(1\bar{1}0)$ $(0\bar{1}1)$ $(10\bar{1})$ $(\bar{1}10)$
2	*a*	3*m*	Pinacoid or parallelohedron *Line segment through origin* (*c*)	(111) $(\bar{1}\bar{1}\bar{1})$

Symmetry of special projections

Along [111]	Along $[1\bar{1}0]$	Along $[2\bar{1}\bar{1}]$
6*mm*	2	2*mm*

HEXAGONAL SYSTEM

6 C_6



6	*b*	1	Hexagonal pyramid *Hexagon* (*d*)	$(hkil)$ $(ihkl)$ $(kihl)$ $(\bar{h}\bar{k}\bar{i}l)$ $(\bar{i}\bar{h}\bar{k}l)$ $(\bar{k}\bar{i}\bar{h}l)$
			Hexagonal prism *Hexagon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(\bar{h}\bar{k}\bar{i}0)$ $(\bar{i}\bar{h}\bar{k}0)$ $(\bar{k}\bar{i}\bar{h}0)$
1	*a*	6..	Pedion or monohedron *Single point* (*a*)	(0001) or $(000\bar{1})$

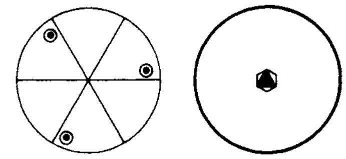
Symmetry of special projections

Along [001]	Along [100]	Along [210]
6	*m*	*m*

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

HEXAGONAL SYSTEM (*cont.*)

$\bar{6}$ C_{3h}

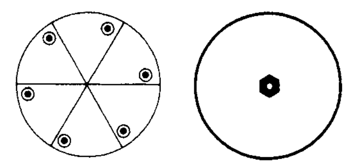


6	*c*	1	Trigonal dipyramid *Trigonal prism* (*l*)	$(hkil)$ $(ihkl)$ $(kihl)$ $(hki\bar{l})$ $(ihk\bar{l})$ $(kih\bar{l})$
3	*b*	*m*..	Trigonal prism *Trigon through origin* (*j*)	$(hki0)$ $(ihk0)$ $(kih0)$
2	*a*	3..	Pinacoid or parallelohedron *Line segment through origin* (*g*)	(0001) $(000\bar{1})$

Symmetry of special projections

Along [001]	Along [100]	Along [210]
3	*m*	*m*

$6/m$ C_{6h}

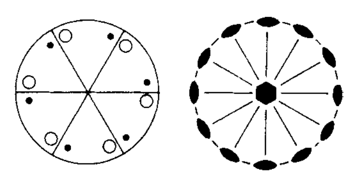


12	*c*	1	Hexagonal dipyramid *Hexagonal prism* (*l*)	$(hkil)$ $(ihkl)$ $(kihl)$ $(\bar{h}\bar{k}\bar{i}l)$ $(\bar{i}\bar{h}\bar{k}l)$ $(\bar{k}\bar{i}\bar{h}l)$ $(hki\bar{l})$ $(ihk\bar{l})$ $(kih\bar{l})$ $(\bar{h}\bar{k}\bar{i}\bar{l})$ $(\bar{i}\bar{h}\bar{k}\bar{l})$ $(\bar{k}\bar{i}\bar{h}\bar{l})$
6	*b*	*m*..	Hexagonal prism *Hexagon through origin* (*j*)	$(hki0)$ $(ihk0)$ $(kih0)$ $(\bar{h}\bar{k}\bar{i}0)$ $(\bar{i}\bar{h}\bar{k}0)$ $(\bar{k}\bar{i}\bar{h}0)$
2	*a*	6..	Pinacoid or parallelohedron *Line segment through origin* (*e*)	(0001) $(000\bar{1})$

Symmetry of special projections

Along [001]	Along [100]	Along [210]
6	2*mm*	2*mm*

622 D_6



12	*d*	1	Hexagonal trapezohedron *Twisted hexagonal antiprism* (*n*)	$(hkil)$ $(ihkl)$ $(kihl)$ $(\bar{h}\bar{k}\bar{i}l)$ $(\bar{i}\bar{h}\bar{k}l)$ $(\bar{k}\bar{i}\bar{h}l)$ $(khi\bar{l})$ $(hik\bar{l})$ $(ikh\bar{l})$ $(\bar{k}\bar{h}\bar{i}\bar{l})$ $(\bar{h}\bar{i}\bar{k}\bar{l})$ $(\bar{i}\bar{k}\bar{h}\bar{l})$
			Dihexagonal prism *Truncated hexagon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(\bar{h}\bar{k}\bar{i}0)$ $(\bar{i}\bar{h}\bar{k}0)$ $(\bar{k}\bar{i}\bar{h}0)$ $(khi0)$ $(hik0)$ $(ikh0)$ $(\bar{k}\bar{h}\bar{i}0)$ $(\bar{h}\bar{i}\bar{k}0)$ $(\bar{i}\bar{k}\bar{h}0)$
			Hexagonal dipyramid *Hexagonal prism*	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(\bar{h}0hl)$ $(h\bar{h}0l)$ $(0h\bar{h}l)$ $(0h\bar{h}\bar{l})$ $(h\bar{h}0\bar{l})$ $(\bar{h}0h\bar{l})$ $(0\bar{h}h\bar{l})$ $(\bar{h}h0\bar{l})$ $(h0\bar{h}\bar{l})$
			Hexagonal dipyramid *Hexagonal prism*	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(\bar{h}\bar{h}2hl)$ $(2h\bar{h}\bar{h}l)$ $(\bar{h}2h\bar{h}l)$ $(hh\overline{2h}\bar{l})$ $(h\overline{2h}h\bar{l})$ $(\overline{2h}hh\bar{l})$ $(\bar{h}\bar{h}2h\bar{l})$ $(\bar{h}2h\bar{h}\bar{l})$ $(2h\bar{h}\bar{h}\bar{l})$
6	*c*	..2	Hexagonal prism *Hexagon through origin* (*l*)	$(10\bar{1}0)$ $(\bar{1}100)$ $(0\bar{1}10)$ $(\bar{1}010)$ $(1\bar{1}00)$ $(01\bar{1}0)$
6	*b*	.2.	Hexagonal prism *Hexagon through origin* (*j*)	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ $(\bar{1}\bar{1}20)$ $(2\bar{1}\bar{1}0)$ $(\bar{1}2\bar{1}0)$
2	*a*	6..	Pinacoid or parallelohedron *Line segment through origin* (*e*)	(0001) $(000\bar{1})$

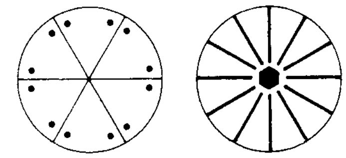
Symmetry of special projections

Along [001]	Along [100]	Along [210]
6*mm*	2*mm*	2*mm*

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

HEXAGONAL SYSTEM (*cont.*)

$6mm$ $\quad C_{6v}$

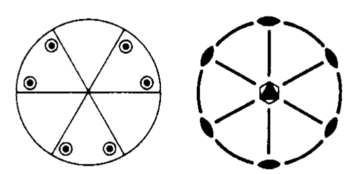


12	*d*	1	Dihexagonal pyramid *Truncated hexagon* (*f*)	$(hkil)$ $(ihkl)$ $(kihl)$ $(\bar{h}\bar{k}\bar{i}l)$ $(\bar{i}\bar{h}\bar{k}l)$ $(\bar{k}\bar{i}\bar{h}l)$ $(khil)$ $(hikl)$ $(ikhl)$ $(\bar{k}\bar{h}\bar{i}l)$ $(\bar{h}\bar{i}\bar{k}l)$ $(\bar{i}\bar{k}\bar{h}l)$
			Dihexagonal prism *Truncated hexagon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(\bar{h}\bar{k}\bar{i}0)$ $(\bar{i}\bar{h}\bar{k}0)$ $(\bar{k}\bar{i}\bar{h}0)$ $(khi0)$ $(hik0)$ $(ikh0)$ $(\bar{k}\bar{h}\bar{i}0)$ $(\bar{h}\bar{i}\bar{k}0)$ $(\bar{i}\bar{k}\bar{h}0)$
6	*c*	*.m.*	Hexagonal pyramid *Hexagon* (*e*)	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(\bar{h}0hl)$ $(h\bar{h}0l)$ $(0h\bar{h}l)$
			Hexagonal prism *Hexagon through origin*	$(10\bar{1}0)$ $(\bar{1}100)$ $(0\bar{1}10)$ $(\bar{1}010)$ $(1\bar{1}00)$ $(01\bar{1}0)$
6	*b*	*..m*	Hexagonal pyramid *Hexagon* (*d*)	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(\bar{h}\bar{h}2hl)$ $(2h\bar{h}\bar{h}l)$ $(\bar{h}2h\bar{h}l)$
			Hexagonal prism *Hexagon through origin*	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ $(\bar{1}\bar{1}20)$ $(2\bar{1}\bar{1}0)$ $(\bar{1}2\bar{1}0)$
1	*a*	$6mm$	Pedion or monohedron *Single point* (*a*)	(0001) or $(000\bar{1})$

Symmetry of special projections

Along [001]	Along [100]	Along [210]
$6mm$	m	m

$\bar{6}m2$ $\quad D_{3h}$



12	*e*	1	Ditrigonal dipyramid *Edge-truncated trigonal prism* (*o*)	$(hkil)$ $(ihkl)$ $(kihl)$ $(hki\bar{l})$ $(ihk\bar{l})$ $(kih\bar{l})$ $(\bar{k}\bar{h}\bar{i}l)$ $(\bar{h}\bar{i}\bar{k}l)$ $(\bar{i}\bar{k}\bar{h}l)$ $(\bar{k}\bar{h}\bar{i}\bar{l})$ $(\bar{h}\bar{i}\bar{k}\bar{l})$ $(\bar{i}\bar{k}\bar{h}\bar{l})$
			Hexagonal dipyramid *Hexagonal prism*	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(hh\overline{2h}\bar{l})$ $(\overline{2h}hh\bar{l})$ $(h\overline{2h}h\bar{l})$ $(\bar{h}\bar{h}2hl)$ $(\bar{h}2h\bar{h}l)$ $(2h\bar{h}\bar{h}l)$ $(\bar{h}\bar{h}2h\bar{l})$ $(\bar{h}2h\bar{h}\bar{l})$ $(2h\bar{h}\bar{h}\bar{l})$
6	*d*	*m..*	Ditrigonal prism *Truncated trigon through origin* (*l*)	$(hki0)$ $(ihk0)$ $(kih0)$ $(\bar{k}\bar{h}\bar{i}0)$ $(\bar{h}\bar{i}\bar{k}0)$ $(\bar{i}\bar{k}\bar{h}0)$
			Hexagonal prism *Hexagon through origin*	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ $(\bar{1}\bar{1}20)$ $(\bar{1}2\bar{1}0)$ $(2\bar{1}\bar{1}0)$
6	*c*	*.m.*	Trigonal dipyramid *Trigonal prism* (*n*)	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(h0\bar{h}\bar{l})$ $(\bar{h}h0\bar{l})$ $(0\bar{h}h\bar{l})$
3	*b*	$mm2$	Trigonal prism *Trigon through origin* (*j*)	$(10\bar{1}0)$ $(\bar{1}100)$ $(0\bar{1}10)$ or $(\bar{1}010)$ $(1\bar{1}00)$ $(01\bar{1}0)$
2	*a*	$3m.$	Pinacoid or parallelohedron *Line segment through origin* (*g*)	(0001) $(000\bar{1})$

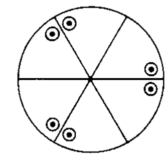
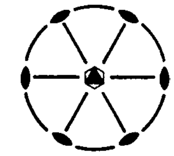
Symmetry of special projections

Along [001]	Along [100]	Along [210]
$3m$	m	$2mm$

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

HEXAGONAL SYSTEM (*cont.*)

$\bar{6}2m$ D_{3h}

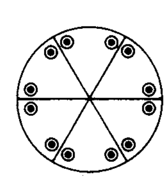
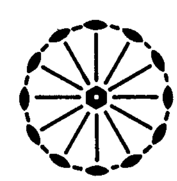
12	*e*	1	Ditrigonal dipyramid *Edge-truncated trigonal prism* (*l*)	$(hkil)$ $(ihkl)$ $(kihl)$ $(hki\bar{l})$ $(ihk\bar{l})$ $(kih\bar{l})$ $(khi\bar{l})$ $(hik\bar{l})$ $(ikh\bar{l})$ $(khil)$ $(hikl)$ $(ikhl)$
			Hexagonal dipyramid *Hexagonal prism*	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(h0\bar{h}\bar{l})$ $(\bar{h}h0\bar{l})$ $(0\bar{h}h\bar{l})$ $(0h\bar{h}\bar{l})$ $(h\bar{h}0\bar{l})$ $(\bar{h}0h\bar{l})$ $(0h\bar{h}l)$ $(h\bar{h}0l)$ $(\bar{h}0hl)$
6	*d*	*m*..	Ditrigonal prism *Truncated trigon through origin* (*j*)	$(hki0)$ $(ihk0)$ $(kih0)$ $(khi0)$ $(hik0)$ $(ikh0)$
			Hexagonal prism *Hexagon through origin*	$(10\bar{1}0)$ $(\bar{1}100)$ $(0\bar{1}10)$ $(01\bar{1}0)$ $(1\bar{1}00)$ $(\bar{1}010)$
6	*c*	..*m*	Trigonal dipyramid *Trigonal prism* (*i*)	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(hh\overline{2h}\bar{l})$ $(\overline{2h}hh\bar{l})$ $(h\overline{2h}h\bar{l})$
3	*b*	*m*2*m*	Trigonal prism *Trigon through origin* (*f*)	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ or $(\bar{1}\bar{1}20)$ $(2\bar{1}\bar{1}0)$ $(\bar{1}2\bar{1}0)$
2	*a*	3.*m*	Pinacoid or parallelohedron *Line segment through origin* (*e*)	(0001) $(000\bar{1})$

Symmetry of special projections

Along [001]	Along [100]	Along [210]
3*m*	2*mm*	*m*

$6/mmm$ D_{6h}

$\frac{6}{m}\frac{2}{m}\frac{2}{m}$

24	*g*	1	Dihexagonal dipyramid *Edge-truncated hexagonal prism* (*r*)	$(hkil)$ $(ihkl)$ $(kihl)$ $(\bar{h}\bar{k}\bar{i}l)$ $(\bar{i}\bar{h}\bar{k}l)$ $(\bar{k}\bar{i}\bar{h}l)$ $(khi\bar{l})$ $(hik\bar{l})$ $(ikh\bar{l})$ $(\bar{k}\bar{h}\bar{i}\bar{l})$ $(\bar{h}\bar{i}\bar{k}\bar{l})$ $(\bar{i}\bar{k}\bar{h}\bar{l})$ $(\bar{h}\bar{k}\bar{i}\bar{l})$ $(\bar{i}\bar{h}\bar{k}\bar{l})$ $(\bar{k}\bar{i}\bar{h}\bar{l})$ $(hki\bar{l})$ $(ihk\bar{l})$ $(kih\bar{l})$ $(\bar{k}\bar{h}\bar{i}l)$ $(\bar{h}\bar{i}\bar{k}l)$ $(\bar{i}\bar{k}\bar{h}l)$ $(khil)$ $(hikl)$ $(ikhl)$
12	*f*	*m*..	Dihexagonal prism *Truncated hexagon through origin* (*p*)	$(hki0)$ $(ihk0)$ $(kih0)$ $(\bar{h}\bar{k}\bar{i}0)$ $(\bar{i}\bar{h}\bar{k}0)$ $(\bar{k}\bar{i}\bar{h}0)$ $(khi0)$ $(hik0)$ $(ikh0)$ $(\bar{k}\bar{h}\bar{i}0)$ $(\bar{h}\bar{i}\bar{k}0)$ $(\bar{i}\bar{k}\bar{h}0)$
12	*e*	.*m*.	Hexagonal dipyramid *Hexagonal prism* (*o*)	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(\bar{h}0hl)$ $(h\bar{h}0l)$ $(0h\bar{h}l)$ $(0h\bar{h}\bar{l})$ $(h\bar{h}0\bar{l})$ $(\bar{h}0h\bar{l})$ $(0\bar{h}h\bar{l})$ $(\bar{h}h0\bar{l})$ $(h0\bar{h}\bar{l})$
12	*d*	..*m*	Hexagonal dipyramid *Hexagonal prism* (*n*)	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(\bar{h}\bar{h}2hl)$ $(2h\bar{h}\bar{h}l)$ $(\bar{h}2h\bar{h}l)$ $(hh\overline{2h}\bar{l})$ $(h\overline{2h}h\bar{l})$ $(\overline{2h}hh\bar{l})$ $(\bar{h}\bar{h}2h\bar{l})$ $(\bar{h}2h\bar{h}\bar{l})$ $(2h\bar{h}\bar{h}\bar{l})$
6	*c*	*mm*2	Hexagonal prism *Hexagon through origin* (*l*)	$(10\bar{1}0)$ $(\bar{1}100)$ $(0\bar{1}10)$ $(\bar{1}010)$ $(1\bar{1}00)$ $(01\bar{1}0)$
6	*b*	*m*2*m*	Hexagonal prism *Hexagon through origin* (*j*)	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ $(\bar{1}\bar{1}20)$ $(2\bar{1}\bar{1}0)$ $(\bar{1}2\bar{1}0)$
2	*a*	6*mm*	Pinacoid or parallelohedron *Line segment through origin* (*e*)	(0001) $(000\bar{1})$

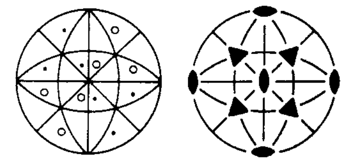
Symmetry of special projections

Along [001]	Along [100]	Along [210]
6*mm*	2*mm*	2*mm*

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

CUBIC SYSTEM

23 *T*



12	*c*	1	Pentagon-tritetrahedron or tetartoid or tetrahedral pentagon-dodecahedron *Snub tetrahedron* (= *pentagon-tritetrahedron* + *two tetrahedra*) (*j*)	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{h}k\bar{l})$ $(h\bar{k}\bar{l})$ (lhk) $(l\bar{h}\bar{k})$ $(\bar{l}\bar{h}k)$ $(\bar{l}h\bar{k})$ (klh) $(\bar{k}l\bar{h})$ $(k\bar{l}\bar{h})$ $(\bar{k}\bar{l}h)$
			{ Trigon-tritetrahedron or tristetrahedron (for $\lvert h\rvert < \lvert l\rvert$) *Tetrahedron truncated by tetrahedron* (*for* $\lvert x\rvert < \lvert z\rvert$) Tetragon-tritetrahedron or deltohedron or deltoid-dodecahedron (for $\lvert h\rvert > \lvert l\rvert$) *Cube* & *two tetrahedra* (*for* $\lvert x\rvert > \lvert z\rvert$) }	(hhl) $(\bar{h}\bar{h}l)$ $(\bar{h}h\bar{l})$ $(h\bar{h}\bar{l})$ (lhh) $(l\bar{h}\bar{h})$ $(\bar{l}\bar{h}h)$ $(\bar{l}h\bar{h})$ (hlh) $(\bar{h}l\bar{h})$ $(h\bar{l}\bar{h})$ $(\bar{h}\bar{l}h)$
			Pentagon-dodecahedron or dihexahedron or pyritohedron *Irregular icosahedron* (= *pentagon-dodecahedron* + *octahedron*)	$(0kl)$ $(0\bar{k}l)$ $(0k\bar{l})$ $(0\bar{k}\bar{l})$ $(l0k)$ $(l0\bar{k})$ $(\bar{l}0k)$ $(\bar{l}0\bar{k})$ $(kl0)$ $(\bar{k}l0)$ $(k\bar{l}0)$ $(\bar{k}\bar{l}0)$
			Rhomb-dodecahedron *Cuboctahedron*	(011) $(0\bar{1}1)$ $(01\bar{1})$ $(0\bar{1}\bar{1})$ (101) $(10\bar{1})$ $(\bar{1}01)$ $(\bar{1}0\bar{1})$ (110) $(\bar{1}10)$ $(1\bar{1}0)$ $(\bar{1}\bar{1}0)$
6	*b*	2..	Cube or hexahedron *Octahedron* (*f*)	(100) $(\bar{1}00)$ (010) $(0\bar{1}0)$ (001) $(00\bar{1})$
4	*a*	.3.	Tetrahedron *Tetrahedron* (*e*)	(111) $(\bar{1}\bar{1}1)$ $(\bar{1}1\bar{1})$ $(1\bar{1}\bar{1})$ or $(\bar{1}\bar{1}\bar{1})$ $(11\bar{1})$ $(1\bar{1}1)$ $(\bar{1}11)$

Symmetry of special projections

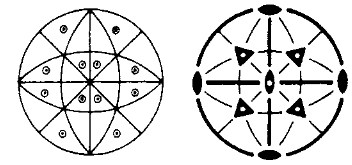
Along [001]	Along [111]	Along [110]
2*mm*	3	*m*

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

CUBIC SYSTEM (*cont.*)

$m\bar{3}$ $\quad T_h$

$\dfrac{2}{m}\bar{3}$



24	*d*	1	Didodecahedron or diploid or dyakisdodecahedron *Cube & octahedron &* *pentagon-dodecahedron* (l)	$(hkl)\ (\bar{h}\bar{k}l)\ (\bar{h}k\bar{l})\ (h\bar{k}\bar{l})$ $(lhk)\ (l\bar{h}\bar{k})\ (\bar{l}\bar{h}k)\ (\bar{l}h\bar{k})$ $(klh)\ (\bar{k}l\bar{h})\ (k\bar{l}\bar{h})\ (\bar{k}\bar{l}h)$ $(\bar{h}\bar{k}\bar{l})\ (hk\bar{l})\ (h\bar{k}l)\ (\bar{h}kl)$ $(\bar{l}\bar{h}\bar{k})\ (\bar{l}hk)\ (lh\bar{k})\ (l\bar{h}k)$ $(\bar{k}\bar{l}\bar{h})\ (k\bar{l}h)\ (\bar{k}lh)\ (kl\bar{h})$
			Tetragon-trioctahedron or trapezohedron or deltoid-icositetrahedron (for $\lvert h\rvert < \lvert l\rvert$) *Cube & octahedron & rhomb-dodecahedron* (*for* $\lvert x\rvert < \lvert z\rvert$) Trigon-trioctahedron or trisoctahedron (for $\lvert h\rvert < \lvert l\rvert$) *Cube truncated by octahedron* (*for* $\lvert x\rvert > \lvert z\rvert$)	$(hhl)\ (\bar{h}\bar{h}l)\ (\bar{h}h\bar{l})\ (h\bar{h}\bar{l})$ $(lhh)\ (l\bar{h}\bar{h})\ (\bar{l}\bar{h}h)\ (\bar{l}h\bar{h})$ $(hlh)\ (\bar{h}l\bar{h})\ (h\bar{l}\bar{h})\ (\bar{h}\bar{l}h)$ $(\bar{h}\bar{h}\bar{l})\ (hh\bar{l})\ (h\bar{h}l)\ (\bar{h}hl)$ $(\bar{l}\bar{h}\bar{h})\ (\bar{l}hh)\ (lh\bar{h})\ (l\bar{h}h)$ $(\bar{h}\bar{l}\bar{h})\ (h\bar{l}h)\ (\bar{h}lh)\ (hl\bar{h})$
12	*c*	*m..*	Pentagon-dodecahedron or dihexahedron or pyritohedron *Irregular icosahedron* (= *pentagon-dodecahedron* + *octahedron*) (j)	$(0kl)\ (0\bar{k}l)\ (0k\bar{l})\ (0\bar{k}\bar{l})$ $(l0k)\ (l0\bar{k})\ (\bar{l}0k)\ (\bar{l}0\bar{k})$ $(kl0)\ (\bar{k}l0)\ (k\bar{l}0)\ (\bar{k}\bar{l}0)$
			Rhomb-dodecahedron *Cuboctahedron*	$(011)\ (0\bar{1}1)\ (01\bar{1})\ (0\bar{1}\bar{1})$ $(101)\ (10\bar{1})\ (\bar{1}01)\ (\bar{1}0\bar{1})$ $(110)\ (\bar{1}10)\ (1\bar{1}0)\ (\bar{1}\bar{1}0)$
8	*b*	.3.	Octahedron *Cube* (i)	$(111)\ (\bar{1}\bar{1}1)\ (\bar{1}1\bar{1})\ (1\bar{1}\bar{1})$ $(\bar{1}\bar{1}\bar{1})\ (11\bar{1})\ (1\bar{1}1)\ (\bar{1}11)$
6	*a*	2*mm..*	Cube or hexahedron *Octahedron* (e)	$(100)\ (\bar{1}00)$ $(010)\ (0\bar{1}0)$ $(001)\ (00\bar{1})$

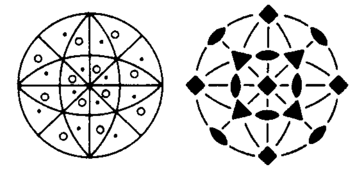
Symmetry of special projections

Along [001]	Along [111]	Along [110]
2*mm*	6	2*mm*

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

CUBIC SYSTEM (*cont.*)

432 *O*



24	*d*	1	Pentagon-trioctahedron or gyroid or pentagon-icositetrahedron *Snub cube(= cube + octahedron + pentagon-trioctahedron) (k)*	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{h}k\bar{l})$ $(h\bar{k}\bar{l})$ $(kh\bar{l})$ $(\bar{k}\bar{h}\bar{l})$ $(k\bar{h}l)$ $(\bar{k}hl)$ (lhk) $(l\bar{h}\bar{k})$ $(\bar{l}\bar{h}k)$ $(\bar{l}h\bar{k})$ $(\bar{l}kh)$ $(\bar{l}\bar{k}\bar{h})$ $(lk\bar{h})$ $(l\bar{k}h)$ (klh) $(\bar{k}l\bar{h})$ $(k\bar{l}\bar{h})$ $(\bar{k}\bar{l}h)$ $(h\bar{l}k)$ $(\bar{h}\bar{l}\bar{k})$ $(\bar{h}lk)$ $(hl\bar{k})$
			Tetragon-trioctahedron or trapezohedron or deltoid-icositetrahedron (for $\lvert h\rvert < \lvert l\rvert$) *Cube & octahedron & rhomb-dodecahedron (for* $\lvert x\rvert < \lvert z\rvert$*)* Trigon-trioctahedron or trisoctahedron (for $\lvert h\rvert > \lvert l\rvert$) *Cube truncated by octahedron (for* $\lvert x\rvert < \lvert z\rvert$*)*	(hhl) $(\bar{h}\bar{h}l)$ $(\bar{h}h\bar{l})$ $(h\bar{h}\bar{l})$ $(hh\bar{l})$ $(\bar{h}\bar{h}\bar{l})$ $(h\bar{h}l)$ $(\bar{h}hl)$ (lhh) $(l\bar{h}\bar{h})$ $(\bar{l}\bar{h}h)$ $(\bar{l}h\bar{h})$ $(\bar{l}hh)$ $(\bar{l}\bar{h}\bar{h})$ $(lh\bar{h})$ $(l\bar{h}h)$ (hlh) $(\bar{h}l\bar{h})$ $(h\bar{l}\bar{h})$ $(\bar{h}\bar{l}h)$ $(h\bar{l}h)$ $(\bar{h}\bar{l}\bar{h})$ $(\bar{h}lh)$ $(hl\bar{h})$
			Tetrahexahedron or tetrakishexahedron *Octahedron truncated by cube*	$(0kl)$ $(0\bar{k}l)$ $(0k\bar{l})$ $(0\bar{k}\bar{l})$ $(k0\bar{l})$ $(\bar{k}0\bar{l})$ $(k0l)$ $(\bar{k}0l)$ $(l0k)$ $(l0\bar{k})$ $(\bar{l}0k)$ $(\bar{l}0\bar{k})$ $(\bar{l}k0)$ $(\bar{l}\bar{k}0)$ $(lk0)$ $(l\bar{k}0)$ $(kl0)$ $(\bar{k}l0)$ $(k\bar{l}0)$ $(\bar{k}\bar{l}0)$ $(0\bar{l}k)$ $(0\bar{l}\bar{k})$ $(0lk)$ $(0l\bar{k})$
12	*c*	..2	Rhomb-dodecahedron *Cuboctahedron (i)*	(011) $(0\bar{1}1)$ $(01\bar{1})$ $(0\bar{1}\bar{1})$ (101) $(10\bar{1})$ $(\bar{1}01)$ $(\bar{1}0\bar{1})$ (110) $(\bar{1}10)$ $(1\bar{1}0)$ $(\bar{1}\bar{1}0)$
8	*b*	.3.	Octahedron *Cube (g)*	(111) $(\bar{1}\bar{1}1)$ $(\bar{1}1\bar{1})$ $(1\bar{1}\bar{1})$ $(\bar{1}\bar{1}\bar{1})$ $(11\bar{1})$ $(1\bar{1}1)$ $(\bar{1}11)$
6	*a*	4..	Cube or hexahedron *Octahedron (e)*	(100) $(\bar{1}00)$ (010) $(0\bar{1}0)$ (001) $(00\bar{1})$

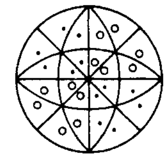
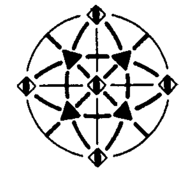
Symmetry of special projections

Along [001]	Along [111]	Along [110]
4*mm*	3*m*	2*mm*

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

CUBIC SYSTEM (*cont.*)

$\bar{4}3m$ $\quad T_d$

24	*d*	1	Hexatetrahedron or hexakistetrahedron *Cube truncated by* *two tetrahedra* (*j*)	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{h}k\bar{l})$ $(h\bar{k}\bar{l})$ (lhk) $(l\bar{h}\bar{k})$ $(\bar{l}\bar{h}k)$ $(\bar{l}h\bar{k})$ (klh) $(\bar{k}l\bar{h})$ $(k\bar{l}\bar{h})$ $(\bar{k}\bar{l}h)$	(khl) $(\bar{k}\bar{h}l)$ $(k\bar{h}\bar{l})$ $(\bar{k}h\bar{l})$ (lkh) $(l\bar{k}\bar{h})$ $(\bar{l}k\bar{h})$ $(\bar{l}\bar{k}h)$ (hlk) $(\bar{h}l\bar{k})$ $(\bar{h}\bar{l}k)$ $(h\bar{l}\bar{k})$
			Tetrahexahedron or tetrakishexahedron *Octahedron truncated by cube*	$(0kl)$ $(0\bar{k}l)$ $(0k\bar{l})$ $(0\bar{k}\bar{l})$ $(l0k)$ $(l0\bar{k})$ $(\bar{l}0k)$ $(\bar{l}0\bar{k})$ $(kl0)$ $(\bar{k}l0)$ $(k\bar{l}0)$ $(\bar{k}\bar{l}0)$	$(k0l)$ $(\bar{k}0l)$ $(k0\bar{l})$ $(\bar{k}0\bar{l})$ $(lk0)$ $(l\bar{k}0)$ $(\bar{l}k0)$ $(\bar{l}\bar{k}0)$ $(0lk)$ $(0l\bar{k})$ $(0\bar{l}k)$ $(0\bar{l}\bar{k})$
12	c	*..m*	Trigon-tritetrahedron or tristetrahedron (for $\|h\| < \|l\|$) *Tetrahedron truncated* *by tetrahedron* (*i*) (*for* $\|x\| < \|z\|$) Tetragon-tritetrahedron or deltohedron or deltoid-dodecahedron (for $\|h\| > \|l\|$) *Cube & two tetrahedra* (*i*) (*for* $\|x\| > \|z\|$)	(hhl) $(\bar{h}\bar{h}l)$ $(\bar{h}h\bar{l})$ $(h\bar{h}\bar{l})$ (lhh) $(l\bar{h}\bar{h})$ $(\bar{l}\bar{h}h)$ $(\bar{l}h\bar{h})$ (hlh) $(\bar{h}l\bar{h})$ $(h\bar{l}\bar{h})$ $(\bar{h}\bar{l}h)$	
			Rhomb-dodecahedron *Cuboctahedron*	(110) $(\bar{1}\bar{1}0)$ $(\bar{1}10)$ $(1\bar{1}0)$ (011) $(0\bar{1}\bar{1})$ $(0\bar{1}1)$ $(01\bar{1})$ (101) $(\bar{1}0\bar{1})$ $(10\bar{1})$ $(\bar{1}01)$	
6	*b*	2.*mm*	Cube or hexahedron *Octahedron* (*f*)	(100) $(\bar{1}00)$ (010) $(0\bar{1}0)$ (001) $(00\bar{1})$	
4	*a*	.3*m*	Tetrahedron *Tetrahedron* (*e*)	(111) $(\bar{1}\bar{1}1)$ $(\bar{1}1\bar{1})$ $(1\bar{1}\bar{1})$ or $(\bar{1}\bar{1}\bar{1})$ $(11\bar{1})$ $(1\bar{1}1)$ $(\bar{1}11)$	

Symmetry of special projections

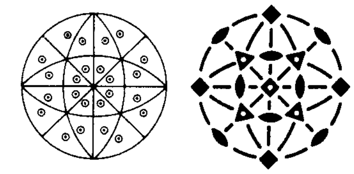
Along [001]	Along [111]	Along [110]
4*mm*	3*m*	*m*

Table 10.1.2.2. *The 32 three-dimensional crystallographic point groups* (*cont.*)

CUBIC SYSTEM (*cont.*)

$m\bar{3}m$ $\quad O_h$

$\dfrac{4}{m}\bar{3}\dfrac{2}{m}$



48	*f*	*l*	Hexaoctahedron or hexakisoctahedron *Cube truncated by octahedron and by rhomb-dodecahedron* (*n*)	(hkl) (lhk) (klh) $(\bar{h}\bar{k}\bar{l})$ $(\bar{l}\bar{h}\bar{k})$ $(\bar{k}\bar{l}\bar{h})$	$(\bar{h}\bar{k}l)$ $(l\bar{h}\bar{k})$ $(\bar{k}l\bar{h})$ $(hk\bar{l})$ $(\bar{l}hk)$ $(k\bar{l}h)$	$(\bar{h}k\bar{l})$ $(\bar{l}\bar{h}k)$ $(k\bar{l}\bar{h})$ $(h\bar{k}l)$ $(lh\bar{k})$ $(\bar{k}lh)$	$(h\bar{k}\bar{l})$ $(\bar{l}h\bar{k})$ $(\bar{k}\bar{l}h)$ $(\bar{h}kl)$ $(l\bar{h}k)$ $(kl\bar{h})$	$(kh\bar{l})$ $(\bar{l}kh)$ $(h\bar{l}k)$ $(\bar{k}\bar{h}l)$ $(l\bar{k}h)$ $(\bar{h}l\bar{k})$	$(\bar{k}\bar{h}\bar{l})$ $(\bar{l}\bar{k}\bar{h})$ $(\bar{h}\bar{l}\bar{k})$ (khl) (lkh) (hlk)	$(k\bar{h}l)$ $(lk\bar{h})$ $(\bar{h}lk)$ $(\bar{k}h\bar{l})$ $(\bar{l}\bar{k}h)$ $(h\bar{l}\bar{k})$	$(\bar{k}hl)$ $(l\bar{k}h)$ $(hl\bar{k})$ $(k\bar{h}\bar{l})$ $(\bar{l}k\bar{h})$ $(\bar{h}\bar{l}k)$
24	*e*	*..m*	Tetragon-trioctahedron or trapezohedron or deltoid-icositetrahedron (for $\|h\| < \|l\|$) *Cube & octahedron & rhomb-dodecahedron* (*m*) (*for* $\|x\| < \|z\|$) Trigon-trioctahedron or trisoctahedron (for $\|h\| > \|l\|$) *Cube truncated by octahedron* (*m*) (*for* $\|x\| < \|z\|$)	(hhl) (lhh) (hlh)	$(\bar{h}\bar{h}l)$ $(l\bar{h}\bar{h})$ $(\bar{h}l\bar{h})$	$(\bar{h}h\bar{l})$ $(\bar{l}\bar{h}h)$ $(h\bar{l}\bar{h})$	$(h\bar{h}\bar{l})$ $(\bar{l}h\bar{h})$ $(\bar{h}\bar{l}h)$	$(hh\bar{l})$ $(\bar{l}hh)$ $(h\bar{l}h)$	$(\bar{h}\bar{h}\bar{l})$ $(\bar{l}\bar{h}\bar{h})$ $(\bar{h}\bar{l}\bar{h})$	$(h\bar{h}l)$ $(lh\bar{h})$ $(\bar{h}lh)$	$(\bar{h}hl)$ $(l\bar{h}h)$ $(hl\bar{h})$
24	*d*	*m..*	Tetrahexahedron or tetrakishexahedron *Octahedron truncated by cube* (*k*)	$(0kl)$ $(l0k)$ $(kl0)$	$(0\bar{k}l)$ $(l0\bar{k})$ $(\bar{k}l0)$	$(0k\bar{l})$ $(\bar{l}0k)$ $(k\bar{l}0)$	$(0\bar{k}\bar{l})$ $(\bar{l}0\bar{k})$ $(\bar{k}\bar{l}0)$	$(k0\bar{l})$ $(\bar{l}k0)$ $(0\bar{l}k)$	$(\bar{k}0\bar{l})$ $(\bar{l}\bar{k}0)$ $(0\bar{l}\bar{k})$	$(k0l)$ $(lk0)$ $(0lk)$	$(\bar{k}0l)$ $(l\bar{k}0)$ $(0l\bar{k})$
12	*c*	*m.m*2	Rhomb-dodecahedron *Cuboctahedron* (*i*)	(011) (101) (110)	$(0\bar{1}1)$ $(10\bar{1})$ $(\bar{1}10)$	$(01\bar{1})$ $(\bar{1}01)$ $(1\bar{1}0)$	$(0\bar{1}\bar{1})$ $(\bar{1}0\bar{1})$ $(\bar{1}\bar{1}0)$				
8	*b*	*.*3*m*	Octahedron *Cube* (*g*)	(111)	$(\bar{1}\bar{1}1)$	$(\bar{1}1\bar{1})$	$(1\bar{1}\bar{1})$	$(11\bar{1})$	$(\bar{1}\bar{1}\bar{1})$	$(1\bar{1}1)$	$(\bar{1}11)$
6	*a*	4*m.m*	Cube or hexahedron *Octahedron* (*e*)	(100) (010) (001)	$(\bar{1}00)$ $(0\bar{1}0)$ $(00\bar{1})$						

Symmetry of special projections

Along [001]	Along [111]	Along [110]
4*mm*	6*mm*	2*mm*

Table 10.1.2.3. *The 47 crystallographic face and point forms, their names, eigensymmetries, and their occurrence in the crystallographic point groups (generating point groups)*

The oriented face (site) symmetries of the forms are given in parentheses after the Hermann–Mauguin symbol (column 6); a symbol such as $mm2(.m., m..)$ indicates that the form occurs in point group $mm2$ twice, with face (site) symmetries $.m.$ and $m..$. Basic (general and special) forms are printed in bold face, limiting (general and special) forms in normal type. The various settings of point groups 32, $3m$, $\bar{3}m$, $\bar{4}2m$ and $\bar{6}m2$ are connected by braces.

No.	Crystal form	Point form	Number of faces or points	*Eigensymmetry*	Generating point groups with oriented face (site) symmetries between parentheses
1	Pedion or monohedron	Single point	1	∞m	$\mathbf{1(1)}$; $\mathbf{2(2)}$; $\boldsymbol{m(m)}$; $\mathbf{3(3)}$; $\mathbf{4(4)}$; $\mathbf{6(6)}$; $\boldsymbol{mm2(mm2)}$; $\boldsymbol{4mm(4mm)}$; $\boldsymbol{3m(3m)}$; $\boldsymbol{6mm(6mm)}$
2	Pinacoid or parallelohedron	Line segment through origin	2	$\frac{\infty}{m}m$	$\bar{\mathbf{1}}(\mathbf{1})$; $2(1)$; $m(1)$; $\boldsymbol{\frac{2}{m}(2.m)}$; $\mathbf{222(2..,.2.,..2)}$; $mm2(.m.,m..)$; $\boldsymbol{mmm(2mm,m2m,mm2)}$; $\bar{\mathbf{4}}\mathbf{(2..)}$; $\boldsymbol{\frac{4}{m}(4..)}$; $\mathbf{422(4..)}$, $\left\{\begin{matrix}\boldsymbol{\bar{4}2m(2.mm)}\\ \boldsymbol{\bar{4}m2(2mm.)}\end{matrix}\right.$; $\boldsymbol{\frac{4}{m}mm(4mm)}$; $\bar{\mathbf{3}}\mathbf{(3..)}$; $\left\{\begin{matrix}\mathbf{321(3..)}\\ \mathbf{312(3..)};\\ \mathbf{32\ (3.)}\end{matrix}\right.$ $\left\{\begin{matrix}\boldsymbol{\bar{3}m1(3m.)}\\ \boldsymbol{\bar{3}1m(3.m)};\\ \boldsymbol{\bar{3}m1(3m)}\end{matrix}\right.$ $\bar{\mathbf{6}}\mathbf{(3..)}$; $\boldsymbol{\frac{6}{m}(6..)}$; $\mathbf{622(6..)}$; $\left\{\begin{matrix}\boldsymbol{\bar{6}m2(3m.)}\\ \boldsymbol{\bar{6}2m(3.m)}\end{matrix}\right.$; $\boldsymbol{\frac{6}{m}mm(6mm)}$
3	Sphenoid, dome, or dihedron	Line segment	2	$mm2$	$\mathbf{2(1)}$; $\boldsymbol{m(1)}$; $\boldsymbol{mm2(.m.,m..)}$
4	Rhombic disphenoid or rhombic tetrahedron	Rhombic tetrahedron	4	222	$\mathbf{222(1)}$
5	Rhombic pyramid	Rectangle	4	$mm2$	$\boldsymbol{mm2(1)}$
6	Rhombic prism	Rectangle through origin	4	mmm	$\boldsymbol{2/m(1)}$; $222(1)$*; $mm2(1)$; $\boldsymbol{mmm(m..,.m.,..m)}$
7	Rhombic dipyramid	Quad	8	mmm	$\boldsymbol{mmm(1)}$
8	Tetragonal pyramid	Square	4	$4mm$	$\mathbf{4(1)}$; $\boldsymbol{4mm(..m,.m.)}$
9	Tetragonal disphenoid or tetragonal tetrahedron	Tetragonal tetrahedron	4	$\bar{4}2m$	$\bar{\mathbf{4}}\mathbf{(1)}$; $\left\{\begin{matrix}\boldsymbol{\bar{4}2m(..m)}\\ \boldsymbol{\bar{4}m2(.m.)}\end{matrix}\right.$
10	Tetragonal prism	Square through origin	4	$\frac{4}{m}mm$	$4(1)$; $\bar{4}(1)$; $\boldsymbol{\frac{4}{m}(m..)}$; $\mathbf{422(..2,.2.)}$; $4mm(..m,.m.)$; $\dagger\left\{\begin{matrix}\boldsymbol{\bar{4}2m(.2.)}\ \&\ \bar{4}2m(..m)\\ \boldsymbol{\bar{4}m2(..2)}\ \&\ \bar{4}m2(.m.)\end{matrix}\right.$; $\boldsymbol{\frac{4}{m}mm(m.m2,m2m.)}$
11	Tetragonal trapezohedron	Twisted tetragonal antiprism	8	422	$\mathbf{422(1)}$
12	Ditetragonal pyramid	Truncated square	8	$4mm$	$\boldsymbol{4mm(1)}$
13	Tetragonal scalenohedron	Tetragonal tetrahedron cut off by pinacoid	8	$\bar{4}2m$	$\left\{\begin{matrix}\boldsymbol{\bar{4}2m(1)}\\ \boldsymbol{\bar{4}m2(1)}\end{matrix}\right.$
14	Tetragonal dipyramid	Tetragonal prism	8	$\frac{4}{m}mm$	$\boldsymbol{\frac{4}{m}(1)}$; $422(1)$*; $\dagger\left\{\begin{matrix}\bar{4}2m(1)\\ \bar{4}m2(1)\end{matrix}\right.$; $\boldsymbol{\frac{4}{m}mm(.m,.m.)}$
15	Ditetragonal prism	Truncated square through origin	8	$\frac{4}{m}mm$	$422(1)$; $4mm(1)$; $\left\{\begin{matrix}\bar{4}2m(1)\\ \bar{4}m2(1)\end{matrix}\right.$; $\boldsymbol{\frac{4}{m}mm(m..)}$
16	Ditetragonal dipyramid	Edge-truncated tetragonal prism	16	$\frac{4}{m}mm$	$\boldsymbol{\frac{4}{m}mm(1)}$

Table 10.1.2.3. *The 47 crystallographic face and point forms, their names, eigensymmetries, and their occurrence in the crystallographic point groups (generating point groups)* (*cont.*)

No.	Crystal form	Point form	Number of faces or points	*Eigensymmetry*	Generating point groups with oriented face (site) symmetries between parentheses
17	Trigonal pyramid	Trigon	3	$3m$	$\boldsymbol{3(1)};\left\{\begin{array}{l}\boldsymbol{3m1(.m.)}\\ \boldsymbol{31m(..m)}\\ \boldsymbol{3m\ \ (.m)}\end{array}\right.$
18	Trigonal prism	Trigon through origin	3	$\bar{6}2m$	$3(1);\left\{\begin{array}{l}\boldsymbol{321(.2.)}\\ \boldsymbol{312(..2)};\\ \boldsymbol{32\ \ (.2)}\end{array}\right.\left\{\begin{array}{l}3m1(.m.)\\ 31m(..m);\\ 3m\ \ (.m)\end{array}\right.$ $\boldsymbol{\bar{6}(m..)};\left\{\begin{array}{l}\boldsymbol{\bar{6}m2(mm2)}\\ \boldsymbol{\bar{6}2m(m2m)}\end{array}\right.$
19	Trigonal trapezohedron	Twisted trigonal antiprism	6	32	$\left\{\begin{array}{l}\boldsymbol{321(1)}\\ \boldsymbol{312(1)}\\ \boldsymbol{32\ \ (1)}\end{array}\right.$
20	Ditrigonal pyramid	Truncated trigon	6	$3m$	$\boldsymbol{3m(1)}$
21	Rhombohedron	Trigonal antiprism	6	$\bar{3}m$	$\boldsymbol{\bar{3}(1)};\left\{\begin{array}{l}321(1)\\ 312(1);\\ 32\ \ (1)\end{array}\right.\left\{\begin{array}{l}\boldsymbol{\bar{3}m1(.m.)}\\ \boldsymbol{\bar{3}1m(..m)}\\ \boldsymbol{\bar{3}m\ \ (.m)}\end{array}\right.$
22	Ditrigonal prism	Truncated trigon through origin	6	$\bar{6}2m$	$\left\{\begin{array}{l}321(1)\\ 312(1);\\ 32\ \ (1)\end{array}\right.\left\{\begin{array}{l}3m1(1)\\ 31m(1);\\ 3m\ \ (1)\end{array}\right.$ $\left\{\begin{array}{l}\boldsymbol{\bar{6}m2(m..)}\\ \boldsymbol{\bar{6}2m(m..)}\end{array}\right.$
23	Hexagonal pyramid	Hexagon	6	$6mm$	$\left\{\begin{array}{l}3m1(1)\\ 31m(1);\\ 3m\ \ (1)\end{array}\right.\boldsymbol{6(1)};\ \boldsymbol{6mm(..m,.m.)}$
24	Trigonal dipyramid	Trigonal prism	6	$\bar{6}2m$	$\left\{\begin{array}{l}321(1)\\ 312(1);\\ 32\ \ (1)\end{array}\right.\boldsymbol{\bar{6}(1)};\left\{\begin{array}{l}\boldsymbol{\bar{6}m2(.m.)}\\ \boldsymbol{\bar{6}2m(..m)}\end{array}\right.$
25	Hexagonal prism	Hexagon through origin	6	$\frac{6}{m}mm$	$\bar{3}(1);\left\{\begin{array}{l}321(1)\\ 312(1);\\ 32\ \ (1)\end{array}\right.\left\{\begin{array}{l}3m1(1)\\ 31m(1)\\ 3m\ \ (1)\end{array}\right.$ $\dagger\left\{\begin{array}{l}\boldsymbol{\bar{3}m1(.2.)}\ \&\ \bar{3}m1(.m.)\\ \boldsymbol{\bar{3}1m(..2)}\ \&\ \bar{3}1m(..m);\\ \boldsymbol{\bar{3}m(.2)}\ \&\ \bar{3}m(.m)\end{array}\right.$ $6(1);\ \boldsymbol{\frac{6}{m}(m..)};\ \boldsymbol{622(.2.,..2)};$ $6mm(..m,.m.);\left\{\begin{array}{l}\bar{6}m2(m..)\\ \bar{6}2m(m..)\end{array}\right.;$ $\boldsymbol{\frac{6}{m}mm(m2m,mm2)}$
26	Ditrigonal scalenohedron or hexagonal scalenohedron	Trigonal antiprism sliced off by pinacoid	12	$\bar{3}m$	$\left\{\begin{array}{l}\boldsymbol{\bar{3}m1(1)}\\ \boldsymbol{\bar{3}1m(1)}\\ \boldsymbol{\bar{3}m\ \ (1)}\end{array}\right.$
27	Hexagonal trapezohedron	Twisted hexagonal antiprism	12	622	$\boldsymbol{622(1)}$
28	Dihexagonal pyramid	Truncated hexagon	12	$6mm$	$\boldsymbol{6mm(1)}$
29	Ditrigonal dipyramid	Edge-truncated trigonal prism	12	$\bar{6}2m$	$\left\{\begin{array}{l}\boldsymbol{\bar{6}m2(1)}\\ \boldsymbol{\bar{6}2m(1)}\end{array}\right.$
30	Dihexagonal prism	Truncated hexagon	12	$\frac{6}{m}mm$	$\left\{\begin{array}{l}\bar{3}m1(1)\\ \bar{3}1m(1);\\ \bar{3}m\ \ (1)\end{array}\right.622(1);\ 6mm(1);$ $\boldsymbol{\frac{6}{m}mm(m..)}$

Table 10.1.2.3. *The 47 crystallographic face and point forms, their names, eigensymmetries, and their occurrence in the crystallographic point groups (generating point groups)* (*cont.*)

No.	Crystal form	Point form	Number of faces or points	*Eigensymmetry*	Generating point groups with oriented face (site) symmetries between parentheses
31	Hexagonal dipyramid	Hexagonal prism	12	$\frac{6}{m}mm$	$\left\{\begin{array}{l}\bar{3}m1(1)\\ \bar{3}1m(1);\\ \bar{3}m\ (1)\end{array}\right.\ \frac{6}{m}(1);\ 622(1)^{*};$ $\left\{\begin{array}{l}\bar{6}m2(1)\\ \bar{6}2m(1)\end{array}\right.;\ \boldsymbol{\frac{6}{m}mm}(\boldsymbol{..m,.m.})$
32	Dihexagonal dipyramid	Edge-truncated hexagonal prism	24	$\frac{6}{m}mm$	$\boldsymbol{\frac{6}{m}mm}(\mathbf{1})$
33	Tetrahedron	Tetrahedron	4	$\bar{4}3m$	$\mathbf{23}(\mathbf{.3.})$; $\boldsymbol{\bar{4}3m}(\boldsymbol{.3m})$
34	Cube or hexahedron	Octahedron	6	$m\bar{3}m$	$\mathbf{23}(\mathbf{2..})$; $\boldsymbol{m\bar{3}}(\boldsymbol{2mm..})$; $\mathbf{432}(\mathbf{4..})$; $\boldsymbol{\bar{4}3m}(\boldsymbol{2.mm})$; $\boldsymbol{m\bar{3}m}(\boldsymbol{4m.m})$
35	Octahedron	Cube	8	$m\bar{3}m$	$\boldsymbol{m\bar{3}}(\mathbf{.3.})$; $\mathbf{432}(\mathbf{.3.})$; $\boldsymbol{m\bar{3}m}(\boldsymbol{.3m})$
36	Pentagon-tritetrahedron or tetartoid or tetrahedral pentagon-dodecahedron	Snub tetrahedron (=pentagon-tritetrahedron + two tetrahedra)	12	23	$\mathbf{23}(\mathbf{1})$
37	Pentagon-dodecahedron or dihexahedron or pyritohedron	Irregular icosahedron (= pentagon-dodecahedron + octahedron)	12	$m\bar{3}$	$23(1)$; $\boldsymbol{m\bar{3}}(\boldsymbol{m..})$
38	Tetragon-tritetrahedron or deltohedron or deltoid-dodecahedron	Cube and two tetrahedra	12	$\bar{4}3m$	$23(1)$; $\boldsymbol{\bar{4}3m}(\boldsymbol{..m})$
39	Trigon-tritetrahedron or tristetrahedron	Tetrahedron truncated by tetrahedron	12	$\bar{4}3m$	$23(1)$; $\boldsymbol{\bar{4}3m}(\boldsymbol{..m})$
40	Rhomb-dodecahedron	Cuboctahedron	12	$m\bar{3}m$	$23(1)$; $m\bar{3}(m..)$; $\mathbf{432}(\mathbf{..2})$; $\bar{4}3m(..m)$; $\boldsymbol{m\bar{3}m}(\boldsymbol{m.m2})$
41	Didodecahedron or diploid or dyakisdodecahedron	Cube & octahedron & pentagon-dodecahedron	24	$m\bar{3}$	$\boldsymbol{m\bar{3}}(\mathbf{1})$
42	Trigon-trioctahedron or trisoctahedron	Cube truncated by octahedron	24	$m\bar{3}m$	$m\bar{3}(1)$; $432(1)$; $\boldsymbol{m\bar{3}m}(\boldsymbol{..m})$
43	Tetragon-trioctahedron or trapezohedron or deltoid-icositetrahedron	Cube & octahedron & rhomb-dodecahedron	24	$m\bar{3}m$	$m\bar{3}(1)$; $432(1)$; $\boldsymbol{m\bar{3}m}(\boldsymbol{..m})$
44	Pentagon-trioctahedron or gyroid	Cube + octahedron + pentagon-trioctahedron	24	432	$\mathbf{432}(\mathbf{1})$
45	Hexatetrahedron or hexakistetrahedron	Cube truncated by two tetrahedra	24	$\bar{4}3m$	$\boldsymbol{\bar{4}3m}(\mathbf{1})$
46	Tetrahexahedron or tetrakishexahedron	Octahedron truncated by cube	24	$m\bar{3}m$	$432(1)$; $\bar{4}3m(1)$; $\boldsymbol{m\bar{3}m}(\boldsymbol{m..})$
47	Hexaoctahedron or hexakisoctahedron	Cube truncated by octahedron and by rhomb-dodecahedron	48	$m\bar{3}m$	$\boldsymbol{m\bar{3}m}(\mathbf{1})$

* These limiting forms occur in three or two non-equivalent orientations (different types of limiting forms); *cf.* Table 10.1.2.2.

† In point groups $\bar{4}2m$ and $\bar{3}m$, the tetragonal prism and the hexagonal prism occur twice, as a 'basic special form' and as a 'limiting special form'. In these cases, the point groups are listed twice, as $\boldsymbol{\bar{4}2m}(\mathbf{.2.})$ & $\bar{4}2m(..m)$ and as $\boldsymbol{\bar{3}m1}(\mathbf{.2.})$ & $\bar{3}m1(.m.)$.

Table 10.1.2.4. *Names and symbols of the 32 crystal classes*

System used in this volume	Point group		Schoenflies symbol	Class names		
	International symbol					
	Short	Full		Groth (1921)	Friedel (1926)	
Triclinic	1	1	C_1	Pedial (asymmetric)	Hemihedry	
	$\bar{1}$	$\bar{1}$	$C_i(S_2)$	Pinacoidal	Holohedry	
Monoclinic	2	2	C_2	Sphenoidal	Holoaxial hemihedry	
	m	m	$C_s(C_{1h})$	Domatic	Antihemihedry	
	$2/m$	$\frac{2}{m}$	C_{2h}	Prismatic	Holohedry	
Orthorhombic	222	222	$D_2(V)$	Disphenoidal	Holoaxial hemihedry	
	$mm2$	$mm2$	C_{2v}	Pyramidal	Antihemihedry	
	mmm	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$D_{2h}(V_h)$	Dipyramidal	Holohedry	
Tetragonal	4	4	C_4	Pyramidal	Tetartohedry with 4-axis	
	$\bar{4}$	$\bar{4}$	S_4	Disphenoidal	Sphenohedral tetartohedry	
	$4/m$	$\frac{4}{m}$	C_{4h}	Dipyramidal	Parahemihedry	
	422	422	D_4	Trapezohedral	Holoaxial hemihedry	
	$4mm$	$4mm$	C_{4v}	Ditetragonal-pyramidal	Antihemihedry with 4-axis	
	$\bar{4}2m$	$\bar{4}2m$	$D_{2d}(V_d)$	Scalenohedral	Sphenohedral antihemihedry	
	$4/mmm$	$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	D_{4h}	Ditetragonal-dipyramidal	Holohedry	
					Hexagonal	*Rhombohedral*
Trigonal	3	3	C_3	Pyramidal	Ogdohedry	Tetartohedry
	$\bar{3}$	$\bar{3}$	$C_{3i}(S_6)$	Rhombohedral	Paratetartohedry	Parahemihedry
	32	32	D_3	Trapezohedral	Holoaxial tetartohedry with 3-axis	Holoaxial hemihedry
	$3m$	$3m$	C_{3v}	Ditrigonal-pyramidal	Hemimorphic antitetartohedry	Antihemihedry
	$\bar{3}m$	$\bar{3}\frac{2}{m}$	D_{3d}	Ditrigonal-scalenohedral	Parahemihedry with 3-axis	Holohedry
Hexagonal	6	6	C_6	Pyramidal	Tetartohedry with 6-axis	
	$\bar{6}$	$\bar{6}$	C_{3h}	Trigonal-dipyramidal	Trigonohedral antitetartohedry	
	$6/m$	$\frac{6}{m}$	C_{6h}	Dipyramidal	Parahemihedry with 6-axis	
	622	622	D_6	Trapezohedral	Holoaxial hemihedry	
	$6mm$	$6mm$	C_{6v}	Dihexagonal-pyramidal	Antihemihedry with 6-axis	
	$\bar{6}2m$	$\bar{6}2m$	D_{3h}	Ditrigonal-dipyramidal	Trigonohedral antihemihedry	
	$6/mmm$	$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	D_{6h}	Dihexagonal-dipyramidal	Holohedry	
Cubic	23	23	T	Tetrahedral-pentagondodecahedral (= tetartoidal)	Tetartohedry	
	$m\bar{3}$	$\frac{2}{m}\bar{3}$	T_h	Disdodecahedral (= diploidal)	Parahemihedry	
	432	432	O	Pentagon-icositetrahedral (= gyroidal)	Holoaxial hemihedry	
	$\bar{4}3m$	$\bar{4}3m$	T_d	Hexakistetrahedral (= hextetrahedral)	Antihemihedry	
	$m\bar{3}m$	$\frac{4}{m}\bar{3}\frac{2}{m}$	O_h	Hexakisoctahedral (= hexoctahedral)	Holohedry	

(2) In point group 32, the general form is a trigonal trapezohedron $\{hkl\}$; this form can be considered as two opposite trigonal pyramids, rotated with respect to each other by an angle χ. The trapezohedron changes into the limiting forms 'trigonal dipyramid' $\{hhl\}$ for $\chi = 0°$ and 'rhombohedron' $\{h0l\}$ for $\chi = 60°$.

(vii) One and the same type of polyhedron can occur as a general, special or limiting form.

Examples

(1) A tetragonal dipyramid is a general form in point group $4/m$, a special form in point group $4/mmm$ and a limiting general form in point groups 422 and $\bar{4}2m$.

(2) A tetragonal prism appears in point group $\bar{4}2m$ both as a basic special form (4*b*) and as a limiting special form (4*c*).

(viii) A peculiarity occurs for the cubic point groups. Here the crystal forms $\{hhl\}$ are realized as two topologically different kinds of polyhedra with the same face symmetry, multiplicity and, in addition, the same *eigensymmetry*. The realization of one or other of these forms depends upon whether the Miller indices obey the conditions $|h| > |l|$ or $|h| < |l|$, *i.e.* whether, in the stereographic projection, a face pole is located between the directions [110] and [111] or between the directions [111] and [001]. These two kinds of polyhedra have to be considered as two *realizations* of *one type* of crystal form because their face poles are located on the same set of conjugate symmetry elements. Similar considerations apply to the point forms x, x, z.

In the point groups $m\bar{3}m$ and $\bar{4}3m$, the two kinds of polyhedra represent two realizations of one *special* 'Wyckoff position'; hence, they have the same Wyckoff letter. In the groups 23, $m\bar{3}$ and 432, they represent two realizations of the same type of limiting *general* forms. In the tables of the cubic point groups, the two entries are always connected by braces.

The same kind of peculiarity occurs for the two icosahedral point groups, as mentioned in Section 10.1.4 and listed in Table 10.1.4.3.

10.1.2.5. *Names and symbols of the crystal classes*

Several different sets of names have been devised for the 32 crystal classes. Their use, however, has greatly declined since the introduction of the international point-group symbols. As examples, two sets (both translated into English) that are frequently found in the literature are given in Table 10.1.2.4. To the name of the class the name of the system has to be added: *e.g.* 'tetragonal pyramidal' or 'tetragonal tetartohedry'.

Note that Friedel (1926) based his nomenclature on the point symmetry of the lattice. Hence, two names are given for the five trigonal point groups, depending whether the lattice is hexagonal or rhombohedral: *e.g.* 'hexagonal ogdohedry' and 'rhombohedral tetartohedry'.

10.1.3. Subgroups and supergroups of the crystallographic point groups

In this section, the sub- and supergroup relations between the crystallographic point groups are presented in the form of a 'family tree'.* Figs. 10.1.3.1 and 10.1.3.2 apply to two and three dimensions. The sub- and supergroup relations between two groups are represented by solid or dashed lines. For a given point group $\mathcal{P}$ of order k_P the lines to groups of lower order connect $\mathcal{P}$ with all its *maximal subgroups* $\mathcal{H}$ with orders k_H; the index [*i*] of each subgroup is given by the ratio of the orders k_P/k_H. The lines to groups of higher order connect $\mathcal{P}$ with all its *minimal supergroups* $\mathcal{S}$ with orders k_S; the index [*i*] of each supergroup is given by the ratio k_S/k_P. In other words: if the diagram is read downwards, subgroup relations are displayed; if it is read upwards, supergroup relations are revealed. The index is always an integer (theorem of Lagrange) and can be easily obtained from the group orders given on the left of the diagrams. The highest index of a maximal subgroup is [3] for two dimensions and [4] for three dimensions.

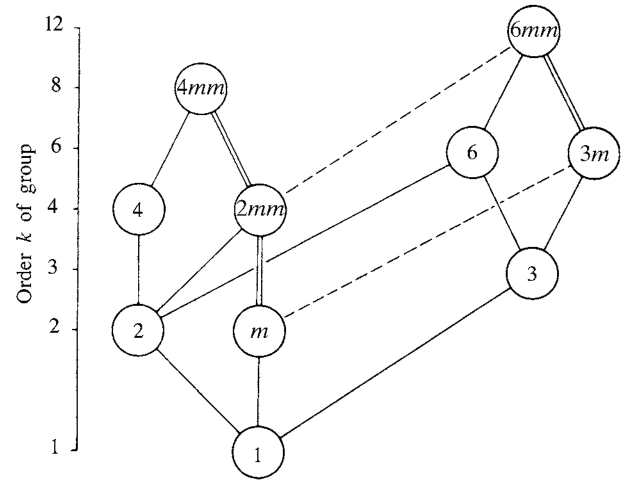


Fig. 10.1.3.1. Maximal subgroups and minimal supergroups of the two-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. The group orders are given on the left.

Two important kinds of subgroups, namely sets of conjugate subgroups and normal subgroups, are distinguished by dashed and solid lines. They are characterized as follows:

The subgroups $\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_n$ of a group $\mathcal{P}$ are *conjugate* subgroups if $\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_n$ are symmetrically equivalent in $\mathcal{P}$, *i.e.* if for every pair $\mathcal{H}_i, \mathcal{H}_j$ at least one symmetry operation W of $\mathcal{P}$ exists which maps $\mathcal{H}_i$ onto $\mathcal{H}_j : \mathsf{W}^{-1}\mathcal{H}_i\mathsf{W} = \mathcal{H}_j$; *cf.* Section 8.3.6.

Examples

(1) Point group $3m$ has three different mirror planes which are equivalent due to the threefold axis. In each of the three maximal subgroups of type m, one of these mirror planes is retained. Hence, the three subgroups m are conjugate in $3m$. This set of conjugate subgroups is represented by *one* dashed line in Figs. 10.1.3.1 and 10.1.3.2.

(2) Similarly, group 432 has three maximal conjugate subgroups of type 422 and four maximal conjugate subgroups of type 32.

The subgroup $\mathcal{H}$ of a group $\mathcal{P}$ is a *normal* (or invariant) subgroup if *no* subgroup $\mathcal{H}'$ of $\mathcal{P}$ exists that is conjugate to $\mathcal{H}$ in $\mathcal{P}$. Note that this does not imply that $\mathcal{H}$ is also a normal subgroup of any supergroup of $\mathcal{P}$. Subgroups of index [2] are always normal and maximal. (The role of normal subgroups for the structure of space groups is discussed in Section 8.1.6.)

Examples

(1) Fig. 10.1.3.2 shows two solid lines between point groups 422 and 222, indicating that 422 has two maximal normal subgroups 222 of index [2]. The symmetry elements of one subgroup are rotated by 45° around the *c* axis with respect to those of the other subgroup. Thus, in one subgroup the symmetry elements of the two secondary, in the other those of the two tertiary tetragonal symmetry directions (*cf.* Table 2.2.4.1) are retained, whereas the primary twofold axis is the same for both subgroups. There exists no symmetry operation of 422 that maps one subgroup onto the other. This is illustrated by the stereograms below. The two normal subgroups can be indicated by the 'oriented

* This type of diagram was first used in *IT* (1935): in *IT* (1952) a somewhat different approach was employed.

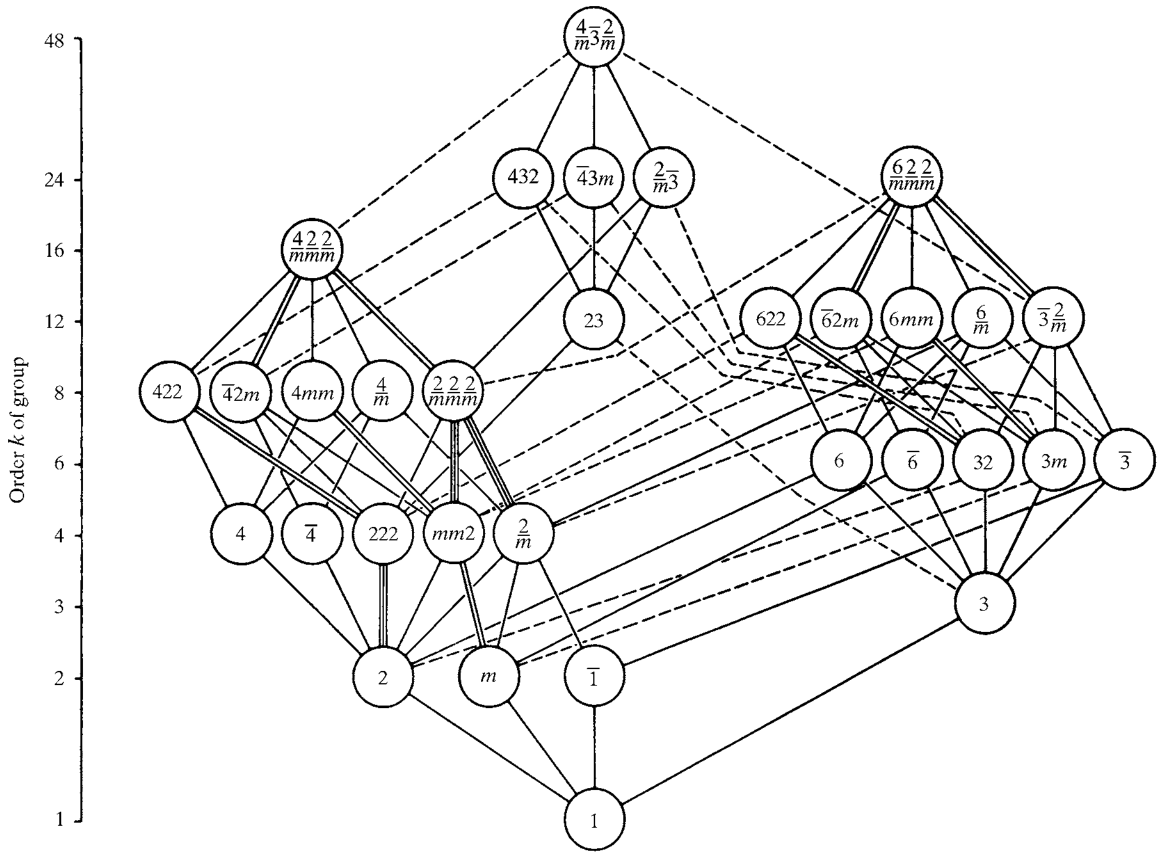
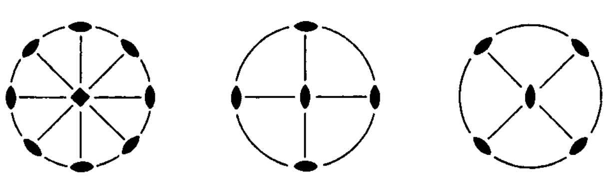


Fig. 10.1.3.2. Maximal subgroups and minimal supergroups of the three-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double or triple solid lines mean that there are two or three maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. The group orders are given on the left. Full Hermann–Mauguin symbols are used.

symbols' 222. and 2.22.



422 222. 2.22

(2) Similarly, group 432 has one maximal normal subgroup, 23.

Figs. 10.1.3.1 and 10.1.3.2 show that there exist two 'summits' in both two and three dimensions from which all other point groups can be derived by 'chains' of maximal subgroups. These summits are formed by the square and the hexagonal holohedry in two dimensions and by the cubic and the hexagonal holohedry in three dimensions.

The sub- and supergroups of the point groups are useful both in their own right and as basis of the *translationengleiche* or *t* subgroups and supergroups of space groups; this is set out in Section 2.2.15. Tables of the sub- and supergroups of the plane groups and space groups are contained in Parts 6 and 7. A general discussion of sub- and supergroups of crystallographic groups, together with further explanations and examples, is given in Section 8.3.3.

10.1.4. Noncrystallographic point groups

10.1.4.1. *Description of general point groups*

In Sections 10.1.2 and 10.1.3, only the 32 *crystallographic* point groups (crystal classes) are considered. In addition, infinitely many *noncrystallographic* point groups exist that are of interest as possible symmetries of molecules and of quasicrystals and as approximate local site symmetries in crystals. Crystallographic *and* noncrystallographic point groups are collected here under the name *general point groups.* They are reviewed in this section and listed in Tables 10.1.4.1 to 10.1.4.3.

Because of the infinite number of these groups only *classes of general point groups* (*general classes*)* can be listed. They are grouped into *general systems*, which are similar to the crystal systems. The 'general classes' are of two kinds: in the cubic, icosahedral, circular, cylindrical and spherical system, each general class contains *one* point group only, whereas in the $4N$-gonal, $(2N+1)$-gonal and $(4N+2)$-gonal system, each general class contains *infinitely* many point groups, which differ in their principal n-fold symmetry axis, with $n = 4, 8, 12, \ldots$ for the $4N$-gonal system, $n = 1, 3, 5, \ldots$ for the $(2N+1)$-gonal system and $n = 2, 6, 10, \ldots$ for the $(4N+2)$-gonal system.

Furthermore, some general point groups are of order infinity because they contain symmetry axes (rotation or rotoinversion axes) of order infinity† (∞-fold axes). These point groups occur in the

* The 'classes of general point groups' are not the same as the commonly used 'crystal classes' because some of them contain point groups of *different orders.* All these orders, however, follow a common scheme. In this sense, the 'general classes' are an extension of the concept of (geometric) crystal classes. For example, the general class *nmm* of the $4N$-gonal system contains the point groups $4mm$ (tetragonal), $8mm$ (octagonal), $12mm$ (dodecagonal), $16mm$ *etc.*

† The axes of order infinity, as considered here, do not correspond to cyclic groups (as do the axes of finite order) because there is no smallest rotation from which all other rotations can be derived as higher powers, *i.e.* by successive application. Instead, rotations of all possible angles exist. Nevertheless, it is customary to symbolize these axes as ∞ or C_∞; note that the Hermann–Mauguin symbols ∞/m and $\overline{\infty}$ are equivalent, and so are the Schoenflies symbols $C_{\infty h}, S_\infty$ and $C_{\infty i}$. (There exist also axes of order infinity that do correspond to cyclic groups, namely axes based upon smallest rotations with irrational values of the rotation angle.)

circular system (two dimensions) and in the cylindrical and spherical systems (three dimensions).

The Hermann–Mauguin and Schoenflies symbols for the general point groups follow the rules of the crystallographic point groups (*cf.* Section 2.2.4 and Chapter 12.1). This extends also to the infinite groups where symbols like ∞m or $C_{\infty v}$ are immediately obvious.

In *two dimensions* (Table 10.1.4.1), the eight general classes are collected into three systems. Two of these, the 4*N*-gonal and the $(4N+2)$-gonal systems, contain only point groups of finite order with one *n*-fold rotation point each. These systems are generalizations of the square and hexagonal crystal systems. The circular system consists of two infinite point groups, with one ∞-fold rotation point each.

In *three dimensions* (Table 10.1.4.2), the 28 general classes are collected into seven systems. Three of these, the 4*N*-gonal, the $(2N+1)$-gonal and the $(4N+2)$-gonal systems,* contain only point groups of finite order with one principal *n*-fold symmetry axis each. These systems are generalizations of the tetragonal, trigonal, and hexagonal crystal systems (*cf.* Table 10.1.1.2). The five cubic groups are well known as crystallographic groups. The two icosahedral groups of orders 60 and 120, characterized by special combinations of twofold, threefold and fivefold symmetry axes, are discussed in more detail below. The groups of the cylindrical and the spherical systems are all of order infinity; they describe the symmetries of cylinders, cones, rotation ellipsoids, spheres *etc.*

It is possible to define the three-dimensional point groups on the basis of either rotoinversion axes $\overline{n}$ or rotoreflection axes $\tilde{n}$. The equivalence between these two descriptions is apparent from the following examples:

$$\begin{array}{lllll} n=4N & : \overline{4}=\tilde{4} & \overline{8}=\tilde{8} & \ldots & \overline{n}=\tilde{n} \\ n=2N+1 & : \overline{1}=\tilde{2} & \overline{3}=\tilde{6}=3\times\overline{1} & \ldots & \overline{n}=\widetilde{2n}=n\times\overline{1} \\ n=4N+2 & : \overline{2}=\tilde{1}=m & \overline{6}=\tilde{3}=3/m & \ldots & \overline{n}=\widetilde{\tfrac{1}{2}n}=\tfrac{1}{2}n/m. \end{array}$$

In the present tables, the standard convention of using rotoinversion axes is followed.

Tables 10.1.4.1 and 10.1.4.2 contain for each class its general Hermann–Mauguin and Schoenflies symbols, the group order and the names of the general face form and its dual, the general point form.† Special and limiting forms are not given, nor are 'Miller indices' (*hkl*) and point coordinates *x*, *y*, *z*. They can be derived easily from Tables 10.1.2.1 and 10.1.2.2 for the crystallographic groups.‡

10.1.4.2. *The two icosahedral groups*

The two point groups 235 and $m\overline{3}\overline{5}$ of the icosahedral system (orders 60 and 120) are of particular interest among the noncrystallographic groups because of the occurrence of fivefold axes and their increasing importance as symmetries of molecules (viruses), of quasicrystals, and as approximate local site symmetries in crystals (alloys, B_{12} icosahedron). Furthermore, they contain as special forms the two noncrystallographic *platonic solids*, the regular icosahedron (20 faces, 12 vertices) and its dual, the regular pentagon-dodecahedron (12 faces, 20 vertices).

The icosahedral groups (*cf.* diagrams in Table 10.1.4.3) are characterized by six fivefold axes that include angles of 63.43°. Each fivefold axis is surrounded by five threefold and five twofold axes, with angular distances of 37.38° between a fivefold and a threefold axis and of 31.72° between a fivefold and a twofold axis. The angles between neighbouring threefold axes are 41.81°, between neighbouring twofold axes 36°. The smallest angle between a threefold and a twofold axis is 20.90°.

Each of the six fivefold axes is perpendicular to five twofold axes; there are thus six maximal conjugate pentagonal subgroups of types 52 (for 235) and $\overline{5}m$ (for $m\overline{3}\overline{5}$) with index [6]. Each of the ten threefold axes is perpendicular to three twofold axes, leading to ten maximal conjugate trigonal subgroups of types 32 (for 235) and $\overline{3}m$ (for $m\overline{3}\overline{5}$) with index [10]. There occur, furthermore, five maximal conjugate cubic subgroups of types 23 (for 235) and $m\overline{3}$ (for $m\overline{3}\overline{5}$) with index [5].

The two icosahedral groups are listed in Table 10.1.4.3, in a form similar to the cubic point groups in Table 10.1.2.2. Each group is illustrated by stereographic projections of the symmetry elements and the general face poles (general points); the complete sets of symmetry elements are listed below the stereograms. Both groups are referred to a cubic coordinate system, with the coordinate axes along three twofold rotation axes and with four threefold axes along the body diagonals. This relation is well brought out by symbolizing these groups as 235 and $m\overline{3}\overline{5}$ instead of the customary symbols 532 and $\overline{5}\overline{3}m$.

The table contains also the multiplicities, the Wyckoff letters and the names of the general and special face forms and their duals, the point forms, as well as the oriented face- and site-symmetry symbols. In the icosahedral 'holohedry' $m\overline{3}\overline{5}$, the *special* 'Wyckoff position' 60*d* occurs in three realizations, *i.e.* with three types of polyhedra. In 235, however, these three types of polyhedra are different realizations of the limiting *general* forms, which depend on the location of the poles with respect to the axes 2, 3 and 5. For this reason, the three entries are connected by braces; *cf.* Section 10.1.2.4, *Notes on crystal and point forms*, item (viii).

Not included are the sets of equivalent Miller indices and point coordinates. Instead, only the 'initial' triplets (*hkl*) and *x*, *y*, *z* for each type of form are listed. The complete sets of indices and coordinates can be obtained in two steps§ as follows:

(i) For the face forms the cubic point groups 23 and $m\overline{3}$ (Table 10.1.2.2), and for the point forms the cubic space groups *P*23 (195) and $Pm\overline{3}$ (200) have to be considered. For each 'initial' triplet (*hkl*), the set of Miller indices of the (general or special) crystal form with the same face symmetry in 23 (for group 235) or $m\overline{3}$ (for $m\overline{3}\overline{5}$) is taken. For each 'initial' triplet *x*, *y*, *z*, the coordinate triplets of the (general or special) position with the same site symmetry in *P*23 or $Pm\overline{3}$ are taken; this procedure is similar to that described in Section 10.1.2.3 for the crystallographic point forms.

(ii) To obtain the complete set of icosahedral Miller indices and point coordinates, the 'cubic' (*hkl*) triplets (as rows) and *x*, *y*, *z* triplets (as columns) have to be multiplied with the identity matrix and with

(*a*) the matrices Y, Y^2, Y^3 and Y^4 for the Miller indices;

* Here, the $(2N+1)$-gonal and the $(4N+2)$-gonal systems are distinguished in order to bring out the analogy with the trigonal and the hexagonal crystal systems. They could equally well be combined into one, in correspondence with the hexagonal 'crystal family' (*cf.* Chapter 2.1).

† The noncrystallographic face and point forms are extensions of the corresponding crystallographic forms: *cf.* Section 10.1.2.4, *Notes on crystal and point forms*. The name *streptohedron* applies to the general face forms of point groups $\overline{n}$ with $n=4N$ and $n=2N+1$; it is thus a generalization of the tetragonal disphenoid or tetragonal tetrahedron ($\overline{4}$) and the rhombohedron ($\overline{3}$).

‡ The term 'Miller indices' is used here also for the noncrystallographic point groups. Note that these indices do not have to be integers or rational numbers, as for the crystallographic point groups. Irrational indices, however, can always be closely approximated by integers, quite often even by small integers.

§ A one-step procedure applies to the icosahedral 'Wyckoff position' 12*a*, the face poles and points of which are located on the fivefold axes. Here, step (ii) is redundant and can be omitted. The forms $\{01\tau\}$ and $0, y, \tau y$ are contained in the cubic point groups 23 and $m\overline{3}$ and in the cubic space groups *P*23 and $Pm\overline{3}$ as limiting cases of Wyckoff positions $\{0kl\}$ and 0, *y*, *z* with specialized (irrational) values of the indices and coordinates. In geometric terms, the regular pentagon-dodecahedron is a noncrystallographic 'limiting polyhedron' of the 'crystallographic' pentagon-dodecahedron and the regular icosahedron is a 'limiting polyhedron' of the 'irregular' icosahedron (*cf.* Section 10.1.2.2, *Crystal and point forms*).

Table 10.1.4.1. *Classes of general point groups in two dimensions* ($N = integer \geq 0$)

General Hermann–Mauguin symbol	Order of group	General edge form	General point form	Crystallographic groups
$4N$-gonal system (n-fold rotation point with $n = 4N$)				
n	n	Regular n-gon	Regular n-gon	4
nmm	$2n$	Semiregular di-n-gon	Truncated n-gon	$4mm$
$(4N+2)$-gonal system (n-fold or $\frac{1}{2}n$-fold rotation point with $n = 4N+2$)				
$\frac{1}{2}n$	$\frac{1}{2}n$	Regular $\frac{1}{2}n$-gon	Regular $\frac{1}{2}n$-gon	1, 3
$\frac{1}{2}nm$	n	Semiregular di-$\frac{1}{2}n$-gon	Truncated $\frac{1}{2}n$-gon	m, $3m$
n	n	Regular n-gon	Regular n-gon	2, 6
nmm	$2n$	Semiregular di-n-gon	Truncated n-gon	$2mm$, $6mm$
Circular system *				
∞	∞	Rotating circle	Rotating circle	–
∞m	∞	Stationary circle	Stationary circle	–

* A rotating circle has no mirror lines; there exist two enantiomorphic circles with opposite senses of rotation. A stationary circle has infinitely many mirror lines through its centre.

Table 10.1.4.2. *Classes of general point groups in three dimensions* ($N = integer \geq 0$)

Short general Hermann–Mauguin symbol, followed by full symbol where different	Schoenflies symbol	Order of group	General face form	General point form	Crystallographic groups
$4N$-gonal system (single n-fold symmetry axis with $n = 4N$)					
n	C_n	n	n-gonal pyramid	Regular n-gon	4
$\bar{n}$	S_n	n	$\frac{1}{2}n$-gonal streptohedron	$\frac{1}{2}n$-gonal antiprism	$\bar{4}$
n/m	C_{nh}	$2n$	n-gonal dipyramid	n-gonal prism	$4/m$
$n22$	D_n	$2n$	n-gonal trapezohedron	Twisted n-gonal antiprism	422
nmm	C_{nv}	$2n$	Di-n-gonal pyramid	Truncated n-gon	$4mm$
$\bar{n}2m$	$D_{\frac{1}{2}nd}$	$2n$	n-gonal scalenohedron	$\frac{1}{2}n$-gonal antiprism sliced off by pinacoid	$\bar{4}2m$
n/mmm, $\frac{n}{m}\frac{2}{m}\frac{2}{m}$	D_{nh}	$4n$	Di-n-gonal dipyramid	Edge-truncated n-gonal prism	$4/mmm$
$(2N+1)$-gonal system (single n-fold symmetry axis with $n = 2N+1$)					
n	C_n	n	n-gonal pyramid	Regular n-gon	1, 3
$\bar{n} = n \times \bar{1}$	C_{ni}	$2n$	n-gonal streptohedron	n-gonal antiprism	$\bar{1}$, $\bar{3} = 3 \times \bar{1}$
$n2$	D_n	$2n$	n-gonal trapezohedron	Twisted n-gonal antiprism	32
nm	C_{nv}	$2n$	Di-n-gonal pyramid	Truncated n-gon	$3m$
$\bar{n}m$, $\bar{n}\frac{2}{m}$	D_{nd}	$4n$	Di-n-gonal scalenohedron	n-gonal antiprism sliced off by pinacoid	$\bar{3}m$
$(4N+2)$-gonal system (single n-fold symmetry axis with $n = 4N+2$)					
n	C_n	n	n-gonal pyramid	Regular n-gon	2, 6
$\bar{n} = \frac{1}{2}n/m$	$C_{\frac{1}{2}nh}$	n	$\frac{1}{2}n$-gonal dipyramid	$\frac{1}{2}n$-gonal prism	$\bar{2} \equiv m$, $\bar{6} \equiv 3/m$
n/m	C_{nh}	$2n$	n-gonal dipyramid	n-gonal prism	$2/m$, $6/m$
$n22$	D_n	$2n$	n-gonal trapezohedron	Twisted n-gonal antiprism	222, 622
nmm	C_{nv}	$2n$	Di-n-gonal pyramid	Truncated n-gon	$mm2$, $6mm$
$\bar{n}2m = \frac{1}{2}n/m2m$	$D_{\frac{1}{2}nh}$	$2n$	Di-$\frac{1}{2}n$-gonal dipyramid	Truncated $\frac{1}{2}n$-gonal prism	$\bar{6}2m$
n/mmm, $\frac{n}{m}\frac{2}{m}\frac{2}{m}$	D_{nh}	$4n$	Di-n-gonal dipyramid	Edge-truncated n-gonal prism	mmm, $6/mmm$

Table 10.1.4.2. *Classes of general point groups in three dimensions* ($N = integer \geq 0$) (*cont.*)

Short general Hermann–Mauguin symbol, followed by full symbol where different	Schoenflies symbol	Order of group	General face form	General point form	Crystallographic groups
Cubic system (for details see Table 10.1.2.2)					
23	T	12	Pentagon-tritetrahedron	Snub tetrahedron	23
$m\bar{3}$, $\frac{2}{m}\bar{3}$	T_h	24	Didodecahedron	Cube & octahedron & pentagon-dodecahedron	$m\bar{3}$
432	O	24	Pentagon-trioctahedron	Snub cube	432
$\bar{4}3m$	T_d	24	Hexatetrahedron	Cube truncated by two tetrahedra	$\bar{4}3m$
$m\bar{3}m$, $\frac{4}{m}\bar{3}\frac{2}{m}$	O_h	48	Hexaoctahedron	Cube truncated by octahedron and by rhomb-dodecahedron	$m\bar{3}m$
Icosahedral system* (for details see Table 10.1.4.3)					
235	I	60	Pentagon-hexecontahedron	Snub pentagon-dodecahedron	–
$m\bar{3}\bar{5}$, $\frac{2}{m}\bar{3}\bar{5}$	I_h	120	Hecatonicosahedron	Pentagon-dodecahedron truncated by icosahedron and by rhomb-triacontahedron	–
Cylindrical system†					
∞	C_∞	∞	Rotating cone	Rotating circle	–
$\infty/m \equiv \overline{\infty}$	$C_{\infty h} \equiv S_\infty \equiv C_{\infty i}$	∞	Rotating double cone	Rotating finite cylinder	–
$\infty 2$	D_∞	∞	'Anti-rotating' double cone	'Anti-rotating' finite cylinder	–
∞m	$C_{\infty v}$	∞	Stationary cone	Stationary circle	–
$\infty/mm \equiv \overline{\infty}m$, $\frac{\infty}{m}\frac{2}{m} \equiv \overline{\infty}\frac{2}{m}$	$D_{\infty h} \equiv D_{\infty d}$	∞	Stationary double cone	Stationary finite cylinder	–
Spherical system‡					
2∞	K	∞	Rotating sphere	Rotating sphere	–
$m\overline{\infty}$, $\frac{2}{m}\overline{\infty}$	K_h	∞	Stationary sphere	Stationary sphere	–

* The Hermann–Mauguin symbols of the two icosahedral point groups are often written as 532 and $\bar{5}\bar{3}m$ (see text).

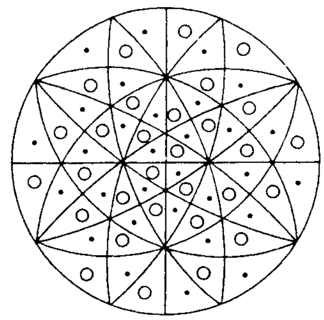
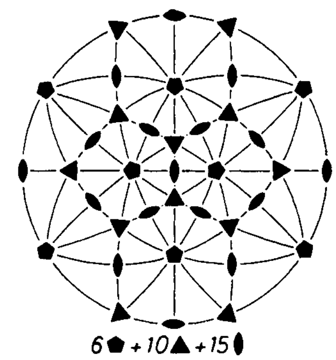
† Rotating and 'anti-rotating' forms in the cylindrical system have no 'vertical' mirror planes, whereas stationary forms have infinitely many vertical mirror planes. In classes ∞ and $\infty 2$, enantiomorphism occurs, *i.e.* forms with opposite senses of rotation. Class $\infty/m \equiv \overline{\infty}$ exhibits no enantiomorphism due to the centre of symmetry, even though the double cone is rotating in one direction. This can be understood as follows: One single rotating cone can be regarded as a right-handed or left-handed screw, depending on the sense of rotation with respect to the axial direction from the base to the tip of the cone. Thus, the rotating double cone consists of two cones with opposite handedness and opposite orientations related by the (single) horizontal mirror plane. In contrast, the 'anti-rotating' double cone in class $\infty 2$ consists of two cones of equal handedness and opposite orientations, which are related by the (infinitely many) twofold axes. The term 'anti-rotating' means that upper and lower halves of the forms rotate in opposite directions.

‡ The spheres in class 2∞ of the spherical system must rotate around an axis with at least two different orientations, in order to suppress all mirror planes. This class exhibits enantiomorphism, *i.e.* it contains spheres with either right-handed or left-handed senses of rotation around the axes (*cf.* Section 10.2.4, *Optical properties*). The stationary spheres in class $m\overline{\infty}$ contain infinitely many mirror planes through the centres of the spheres.

Group 2∞ is sometimes symbolized by $\infty\infty$; group $m\overline{\infty}$ by $\overline{\infty}\,\overline{\infty}$ or $\infty\infty m$. The symbols used here indicate the minimal symmetry necessary to generate the groups; they show, furthermore, the relation to the cubic groups. The Schoenflies symbol K is derived from the German name *Kugelgruppe*.

Table 10.1.4.3. *The two icosahedral point groups*

General, special and limiting face forms and point forms, oriented face- and site-symmetry symbols, and 'initial' values of (*hkl*) and *x*, *y*, *z* (see text).

235	*I*			
60	*d*	1	Pentagon-hexecontahedron *Snub pentagon-dodecahedron* (= *pentagon-dodecahedron* + *icosahedron* + *pentagon-hexecontahedron*)	(*hkl*) *x*, *y*, *z*
			Trisicosahedron *Pentagon-dodecahedron truncated by icosahedron* (poles between axes 2 and 3)	$(0kl)$ with $\lvert l\rvert < 0.382\lvert k\rvert$ $0, y, z$ *with* $\lvert z\rvert < 0.382\lvert y\rvert$
			Deltoid-hexecontahedron *Rhomb-triacontahedron* & *pentagon-dodecahedron* & *icosahedron* (poles between axes 3 and 5)	$(0kl)$ with $0.382\lvert k\rvert < \lvert l\rvert < 1.618\lvert k\rvert$ $0, y, z$ *with* $0.382\lvert y\rvert < \lvert z\rvert < 1.618\lvert y\rvert$
			Pentakisdodecahedron *Icosahedron truncated by pentagon-dodecahedron* (poles between axes 5 and 2)	$(0kl)$ with $\lvert l\rvert > 1.618\lvert k\rvert$ $0, y, z$ *with* $\lvert z\rvert > 1.618\lvert y\rvert$
30	*c*	2..	Rhomb-triacontahedron *Icosadodecahedron* (= *pentagon-dodecahedron* & *icosahedron*)	(100) $x, 0, 0$
20	*b*	.3.	Regular icosahedron *Regular pentagon-dodecahedron*	(111) *x*, *x*, *x*
12	*a*	..5	Regular pentagon-dodecahedron *Regular icosahedron*	(01τ), $0, y, \tau y$ } with $\tau = \frac{1}{2}(\sqrt{5}+1) = 1.618$

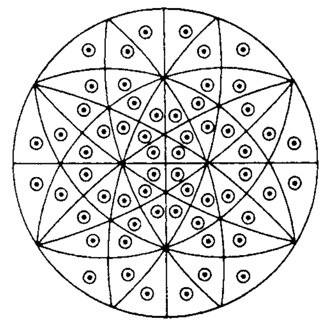
Symmetry of special projections

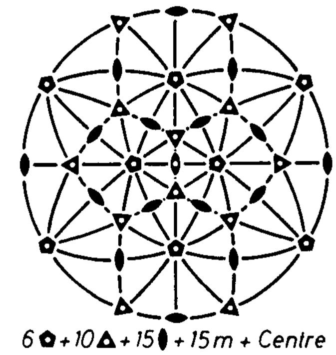
Along [001]	Along [111]	Along $[1\tau0]$
2*mm*	3*m*	5*m*

Table 10.1.4.3. *The two icosahedral point groups* (*cont.*)

$m\bar{3}\bar{5}$ I_h

$\frac{2}{m}\bar{3}\bar{5}$





120	*e*	1	Hecatonicosahedron or hexaicosahedron *Pentagon-dodecahedron truncated by icosahedron and by rhomb-triacontahedron*	(hkl) x, y, z
60	*d*	*m..*	Trisicosahedron *Pentagon-dodecahedron truncated by icosahedron* (poles between axes 2 and $\bar{3}$)	($0kl$) with $\lvert l\rvert < 0.382\lvert k\rvert$ $0, y, z$ *with* $\lvert z\rvert < 0.382\lvert y\rvert$
			Deltoid-hexecontahedron *Rhomb-triacontahedron & pentagon-dodecahedron & icosahedron* (poles between axes $\bar{3}$ and $\bar{5}$)	($0kl$) with $0.382\lvert k\rvert < \lvert l\rvert < 1.618\lvert k\rvert$ $0, y, z$ *with* $0.382\lvert y\rvert < \lvert z\rvert < 1.618\lvert y\rvert$
			Pentakisdodecahedron *Icosahedron truncated by pentagon-dodecahedron* (poles between axes $\bar{5}$ and 2)	($0kl$) with $\lvert l\rvert > 1.618\lvert k\rvert$ $0, y, z$ *with* $\lvert z\rvert > 1.618\lvert y\rvert$
30	*c*	*2mm..*	Rhomb-triacontahedron *Icosadodecahedron* (= *pentagon-dodecahedron* & *icosahedron*)	(100) $x, 0, 0$
20	*b*	$3m$ ($m3.$)	Regular icosahedron *Regular pentagon-dodecahedron*	(111) x, x, x
12	*a*	$5m$ ($m.5$)	Regular pentagon-dodecahedron *Regular icosahedron*	$\left.\begin{matrix}(01\tau)\\ 0, y, \tau y\end{matrix}\right\}$ with $\tau = \frac{1}{2}(\sqrt{5}+1) = 1.618$

Symmetry of special projections

Along [001]	Along [111]	Along [1τ0]
$2mm$	$6mm$	$10mm$

(*b*) the matrices Y^{-1}, Y^{-2}, Y^{-3} and Y^{-4} for the point coordinates.

This sequence of matrices ensures the same correspondence between the Miller indices and the point coordinates as for the crystallographic point groups in Table 10.1.2.2.

The matrices* are

$$Y = Y^{-4} = \begin{pmatrix} \frac{1}{2} & g & G \\ g & G & -\frac{1}{2} \\ -G & \frac{1}{2} & g \end{pmatrix}, \quad Y^2 = Y^{-3} = \begin{pmatrix} -g & G & \frac{1}{2} \\ G & \frac{1}{2} & -g \\ -\frac{1}{2} & g & -G \end{pmatrix},$$

$$Y^3 = Y^{-2} = \begin{pmatrix} -g & G & -\frac{1}{2} \\ G & \frac{1}{2} & g \\ \frac{1}{2} & -g & -G \end{pmatrix}, \quad Y^4 = Y^{-1} = \begin{pmatrix} \frac{1}{2} & g & -G \\ g & G & \frac{1}{2} \\ G & -\frac{1}{2} & g \end{pmatrix},$$

with†

$$G = \frac{\sqrt{5}+1}{4} = \frac{\tau}{2} = \cos 36^\circ = 0.80902 \simeq \frac{72}{89}$$

$$g = \frac{\sqrt{5}-1}{4} = \frac{\tau - 1}{2} = \cos 72^\circ = 0.30902 \simeq \frac{17}{55}.$$

These matrices correspond to counter-clockwise rotations of 72, 144, 216 and 288° around a fivefold axis parallel to $[1\tau 0]$.

The resulting indices h, k, l and coordinates x, y, z are irrational but can be approximated closely by rational (or integral) numbers. This explains the occurrence of almost regular icosahedra or pentagon-dodecahedra as crystal forms (for instance pyrite) or atomic groups (for instance B_{12} icosahedron).

Further descriptions (including diagrams) of noncrystallographic groups are contained in papers by Nowacki (1933) and A. Niggli (1963) and in the textbooks by P. Niggli (1941, pp. 78–80, 96), Shubnikov & Koptsik (1974) and Vainshtein (1994). For the geometry of polyhedra, the well known books by H. S. M. Coxeter (especially Coxeter, 1973) are recommended.

10.1.4.3. *Sub- and supergroups of the general point groups*

In Figs. 10.1.4.1 to 10.1.4.3, the subgroup and supergroup relations between the two-dimensional and three-dimensional general point groups are illustrated. It should be remembered that the index of a group–subgroup relation between two groups of order infinity may be finite or infinite. For the two spherical groups, for instance, the index is [2]; the cylindrical groups, on the other hand, are subgroups of index [∞] of the spherical groups.

Fig. 10.1.4.1 for *two dimensions* shows that the two circular groups ∞m and ∞ have subgroups of types nmm and n, respectively, each of index [∞]. The order of the rotation point may be $n = 4N, n = 4N+2$ or $n = 2N+1$. In the first case, the subgroups belong to the $4N$-gonal system, in the latter two cases, they belong to the $(4N+2)$-gonal system. [In the diagram of the $(4N+2)$-gonal system, the $(2N+1)$-gonal groups appear with the symbols $\frac{1}{2}nm$ and $\frac{1}{2}n$.] The subgroups of the circular groups are not maximal because for any given value of N there exists a group with $N' = 2N$ which is both a subgroup of the circular group and a supergroup of the initial group.

The subgroup relations, for a specified value of N, within the $4N$-gonal and the $(4N+2)$-gonal system, are shown in the lower part of the figure. They correspond to those of the crystallographic groups. A finite number of further maximal subgroups is obtained for lower values of N, until the crystallographic groups (Fig. 10.1.3.1) are reached. This is illustrated for the case $N = 4$ in Fig. 10.1.4.2.

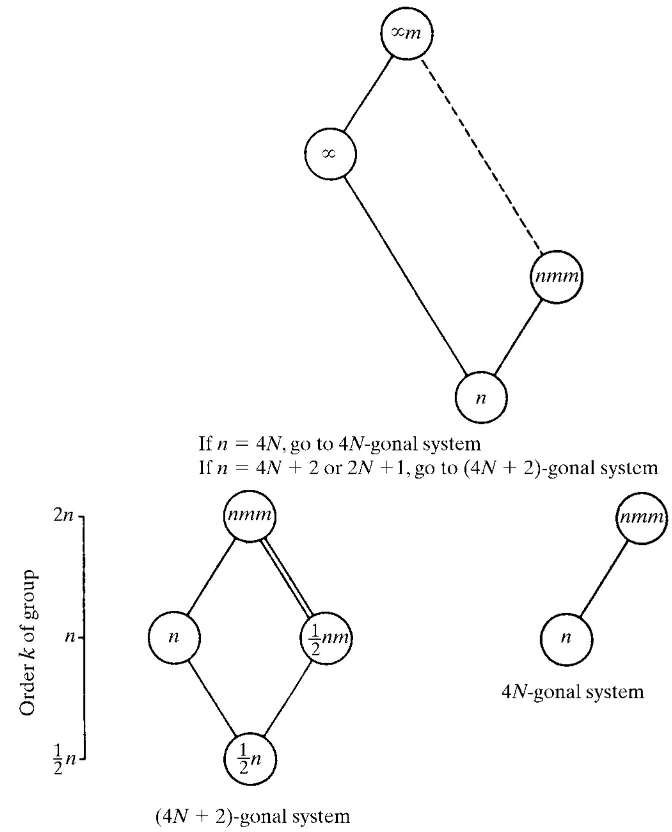


Fig. 10.1.4.1. Subgroups and supergroups of the two-dimensional general point groups. Solid lines indicate maximal normal subgroups, double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. For the finite groups, the orders are given on the left. Note that the subgroups of the two circular groups are not maximal and the diagram applies only to a specified value of N (see text). For complete examples see Fig. 10.1.4.2.

Fig. 10.1.4.3 for *three dimensions* illustrates that the two spherical groups $2/m\overline{\infty}$ and 2∞ each have one infinite set of cylindrical maximal conjugate subgroups, as well as one infinite set

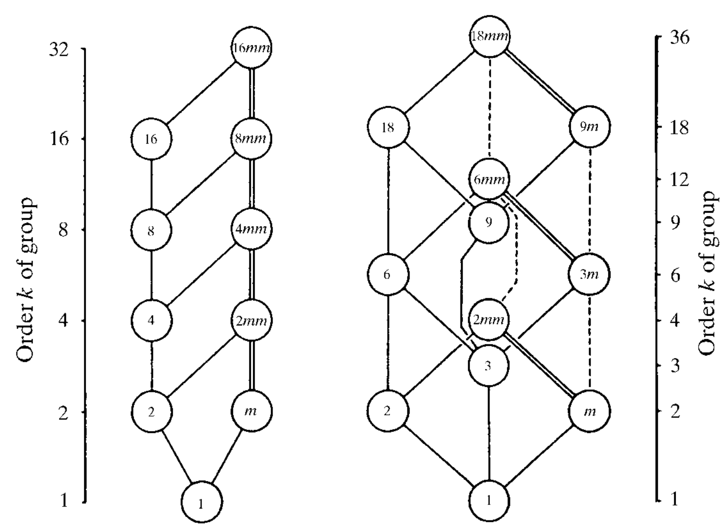


Fig. 10.1.4.2. The subgroups of the two-dimensional general point groups $16mm$ ($4N$-gonal system) and $18mm$ [$(4N+2)$-gonal system, including the $(2N+1)$-gonal groups]. Compare with Fig. 10.1.4.1 which applies only to one value of N.

* Note that for orthogonal matrices $Y^{-1} = Y^t$ (t = transposed).

† The number $\tau = 2G = 2g + 1 = 1.618034$ (Fibonacci number) is the characteristic value of the *golden section* $(\tau + 1) : \tau = \tau : 1$, *i.e.* $\tau(\tau - 1) = 1$. Furthermore, τ is the distance between alternating vertices of a regular pentagon of unit edge length and the distance from centre to vertex of a regular decagon of unit edge length.

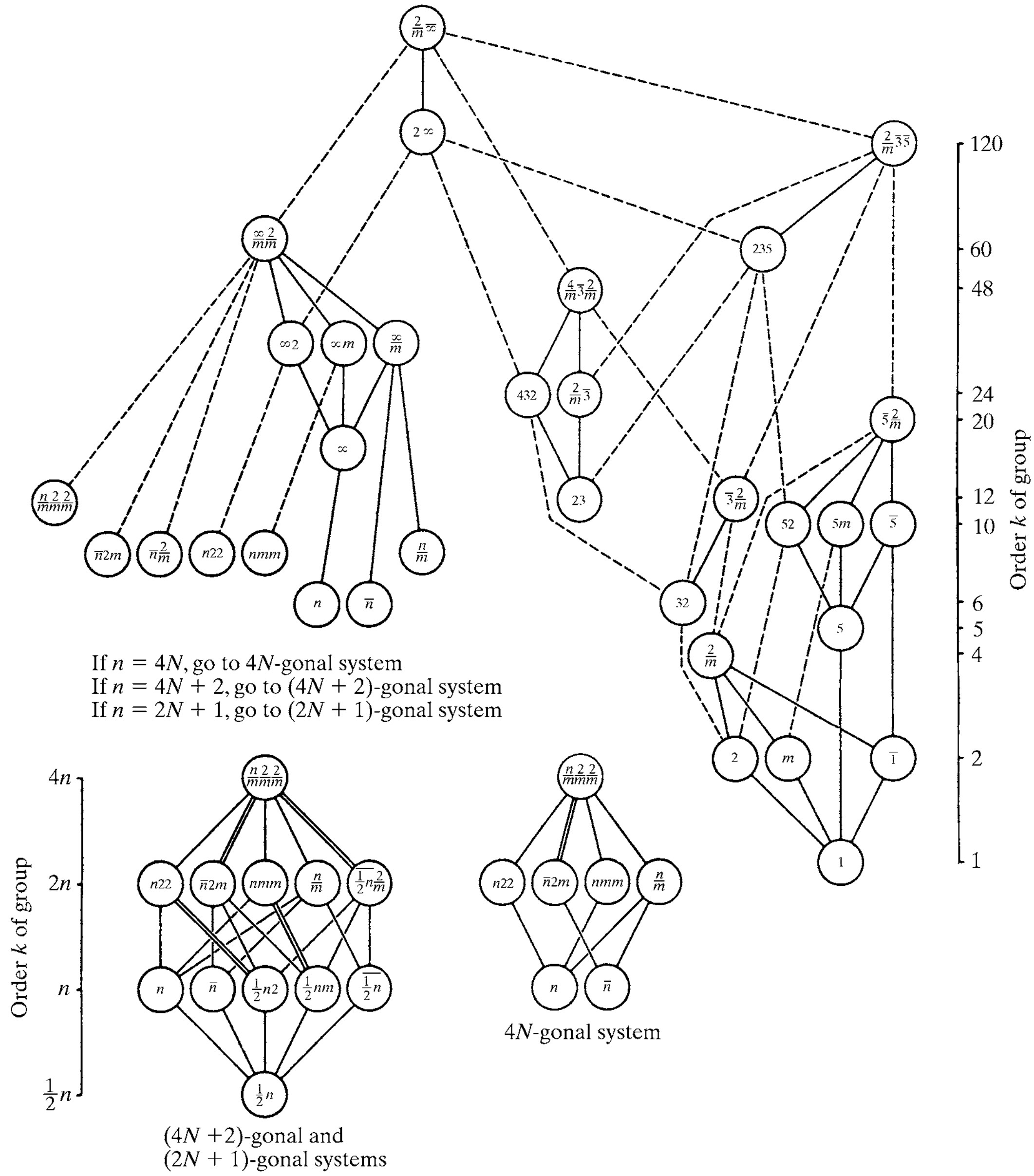


Fig. 10.1.4.3. Subgroups and supergroups of the three-dimensional general point groups. Solid lines indicate maximal normal subgroups, double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. For the finite groups, the orders are given on the left and on the right. Note that the subgroups of the five cylindrical groups are not maximal and that the diagram applies only to a specified value of N (see text). Only those crystallographic point groups are included that are maximal subgroups of noncrystallographic point groups. Full Hermann–Mauguin symbols are used.

of cubic and one infinite set of icosahedral maximal finite conjugate subgroups, all of index $[\infty]$.

Each of the two icosahedral groups 235 and $2/m\bar{3}\bar{5}$ has one set of five cubic, one set of six pentagonal and one set of ten trigonal maximal conjugate subgroups of indices [5], [6] and [10], respectively (*cf.* Section 10.1.4.2, *The two icosahedral groups*); they are listed on the right of Fig. 10.1.4.3. For crystallographic groups, Fig. 10.1.3.2 applies. The subgroup types of the five cylindrical point groups are shown on the left of Fig. 10.1.4.3. As explained above for two dimensions, these subgroups are *not maximal* and of index $[\infty]$. Depending upon whether the main symmetry axis has the multiplicity $4N$, $4N + 2$ or $2N + 1$, the subgroups belong to the $4N$-gonal, $(4N + 2)$-gonal or $(2N + 1)$-gonal system.

The subgroup and supergroup relations within these three systems are displayed in the lower left part of Fig 10.1.4.3. They are analogous to the crystallographic groups. To facilitate the use of the diagrams, the $(4N + 2)$-gonal and the $(2N + 1)$-gonal systems are combined, with the consequence that the five classes of the $(2N + 1)$-gonal system now appear with the symbols $\overline{\frac{1}{2}n}\frac{2}{m}$, $\frac{1}{2}n2$, $\frac{1}{2}nm$, $\overline{\frac{1}{2}n}$ and $\frac{1}{2}n$. Again, the diagrams apply to a specified value of N. A finite number of further maximal subgroups is obtained for lower values of N, until the crystallographic groups (Fig. 10.1.3.2) are reached (*cf.* the two-dimensional examples in Fig. 10.1.4.2).

Acknowledgements

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10.2. Point-group symmetry and physical properties of crystals

BY H. KLAPPER AND TH. HAHN

10.2.1. General restrictions on physical properties imposed by symmetry

The point group of a crystal is the symmetry that is common to all of its macroscopic properties. In other words, the point group of a crystal is a (not necessarily proper) subgroup of the symmetry group of any of its physical properties. It follows that the symmetry group of any property of a crystal must include the symmetry operations of the crystal point group. This is the so-called 'Neumann's principle', which can be used to derive information about the symmetry of a crystal from its physical properties.

Certain interesting physical properties occur only in noncentrosymmetric crystals; *cf.* Table 10.2.1.1. These are mainly properties represented by polar tensors of odd rank (*e.g.* pyroelectricity, piezoelectricity) or axial tensors of second rank (*e.g.* optical activity); see textbooks of tensor physics, *e.g.* Nye (1957). These properties are, as a rule, the most important ones, not only for physical applications but also for structure determination, because they allow a proof of the absence of a symmetry centre. For the description of noncentrosymmetric crystals and their specific properties, certain notions are of importance and these are explained below. Further detailed treatments of tensor properties are presented in *International Tables for Crystallography* Vol. D (2003).

10.2.1.1. *Enantiomorphism, enantiomerism, chirality, dissymmetry*

These terms refer to the same symmetry restriction, the absence of improper rotations (rotoinversions, rotoreflections) in a crystal or in a molecule. This implies in particular the absence of a centre of symmetry, $\bar{1}$, and of a mirror plane, $m = \bar{2}$, but also of a $\bar{4}$ axis. As a consequence, such *chiral* crystals or molecules can occur in two different forms, which are related as a right and a left hand; hence, they are called right-handed and left-handed forms. These two forms of a molecule or a crystal are mirror-related and not superimposable (not congruent). Thus, the only symmetry operations that are allowed for *chiral* objects are proper rotations. Such objects are also called *dissymmetric*, in contrast to *asymmetric* objects, which have no symmetry.

The terms *enantiomerism* and *chirality* are mainly used in chemistry and applied to molecules, whereas the term *enantiomorphism* is preferred in crystallography if reference is made to crystals.

Enantiomorphic crystals, as well as solutions or melts containing chiral molecules of one handedness, exhibit optical activity (*cf.* Section 10.2.4.2). Crystals and molecules of the other handedness show optical activity with the opposite sense of rotation. For this reason, two molecules of opposite chirality are also called *optical isomers*.

Chiral molecules form enantiomorphic crystals of the corresponding handedness. The crystals belong, therefore, to one of the 11 crystal classes allowing enantiomorphism (Table 10.2.1.1). Racemic mixtures (containing equal amounts of molecules of each chirality), however, may crystallize in non-enantiomorphic or even centrosymmetric crystal classes. Racemization (*i.e.* the switching of molecules from one chirality to the other) of an optically active melt or solution can occur in some cases during crystallization, leading to non-enantiomorphic crystals.

Enantiomorphic crystals can also be built up from achiral molecules or atom groups. In these cases, the achiral molecules or atom groups form chiral configurations in the structure. The best known examples are quartz and $NaClO_3$. For details, reference should be made to Rogers (1975).

10.2.1.2. *Polar directions, polar axes, polar point groups*

A *direction* is called *polar* if its two directional senses are geometrically or physically different. A *polar symmetry direction* of a crystal is called a *polar axis*. Only proper rotation or screw axes can be polar. The polar and nonpolar directions in the 21 noncentrosymmetric point groups are listed in Table 10.2.1.2.

The terms *polar point group* or *polar crystal class* are used in two different meanings. In crystal physics, a crystal class is considered as polar if it allows the existence of a permanent dipole moment, *i.e.* if it is capable of pyroelectricity (*cf.* Section 10.2.5). In crystallography, however, the term *polar crystal class* is frequently used synonymously with *noncentrosymmetric crystal class*. The synonymous use of polar and acentric, however, can be misleading, as is shown by the following example. Consider an optically active liquid. Its symmetry can be represented as a right-handed or a left-handed sphere (*cf.* Sections 10.1.4 and 10.2.4). The optical activity is isotropic, *i.e.* magnitude and rotation sense are the same in any direction and its counterdirection. Thus, no polar direction exists, although the liquid is noncentrosymmetric with respect to optical activity.

According to Neumann's principle, information about the point group of a crystal may be obtained by the observation of physical effects. Here, the term 'physical properties' includes crystal morphology and etch figures. The use of any of the techniques described below does not necessarily result in the complete determination of symmetry but, when used in conjunction with other methods, much information may be obtained. It is important to realize that the evidence from these methods is often negative, *i.e.* that symmetry conclusions drawn from such evidence must be considered as only provisional.

In the following sections, the physical properties suitable for the determination of symmetry are outlined briefly. For more details, reference should be made to the monographs by Bhagavantam (1966), Nye (1957) and Wooster (1973).

10.2.2. Morphology

If a crystal shows well developed faces, information on its symmetry may be derived from the external form of the crystal. By means of the optical goniometer, faces related by symmetry can be determined even for crystals far below 1 mm in diameter. By this procedure, however, only the *eigensymmetry* (*cf.* Section 10.1.2.2) of the crystal morphology (which may consist of a single form or a combination of forms) can be established. The determination of the point group is unique in all cases where the observed *eigensymmetry* group is compatible with only one generating group.

Column 6 in Table 10.1.2.3 lists all point groups for which a given crystal form (characterized by its name and *eigensymmetry*) can occur. In 19 cases, the point group can be uniquely determined because only one entry appears in column 6. These crystal forms are always characteristic general forms, for which *eigensymmetry* and generating point-group symmetry are identical. They belong to the 19 point groups with more than one symmetry direction.

If a crystal exhibits a combination of forms which by themselves do not permit unambiguous determination of the point group, those generating point groups are possible that are common to all crystal forms of the combination. The mutual orientation of the forms, if variable, has to be taken into account, too.

Example

Two tetragonal pyramids, each of *eigensymmetry* $4mm$, rotated with respect to each other by an angle $\neq 45°$, determine the point

Table 10.2.1.1. *Laue classes, noncentrosymmetric crystal classes, and the occurrence* (+) *of specific physical effects*

For pyroelectricity, the direction of the pyroelectric vector is given (with unique axis *b* for the monoclinic system).

Crystal system	Laue class	Noncentrosymmetric crystal classes	Enantiomorphism	Optical activity	Pyroelectricity; piezoelectricity under hydrostatic pressure	Piezoelectricity; second-harmonic generation
Triclinic	$\bar{1}$	1	+	+	+ [uvw]	+
Monoclinic	$\frac{2}{m}$	2	+	+	+ [010]	+
		m	–	+	+ [$u0w$]	+
Orthorhombic	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	222	+	+	–	+
		$mm2$	–	+	+ [001]	+
Tetragonal	$\frac{4}{m}$	4	+	+	+ [001]	+
		$\bar{4}$	–	+	–	+
	$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	422	+	+	–	+
		$4mm$	–	–	+ [001]	+
		$\bar{4}2m$	–	+	–	+
Trigonal	$\bar{3}$	3	+	+	+ [001]	+
	$\bar{3}\frac{2}{m}$	32	+	+	–	+
		$3m$	–	–	+ [001]	+
Hexagonal	$\frac{6}{m}$	6	+	+	+ [001]	+
		$\bar{6}$	–	–	–	+
	$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	622	+	+	–	+
		$6mm$	–	–	+ [001]	+
		$\bar{6}2m$	–	–	–	+
Cubic	$\frac{2}{m}\bar{3}$	23	+	+	–	+
	$\frac{4}{m}\bar{3}\frac{2}{m}$	432	+	+	–	–
		$\bar{4}3m$	–	–	–	+

group 4 uniquely because the *eigensymmetry* of the *combination* is only 4.

In practice, however, unequal or incomplete development of the faces of a form often simulates a symmetry that is lower than the actual crystal symmetry. In such cases, or when the morphological analysis is ambiguous, the crystallization of a small amount of the compound on a seed crystal, ground to a sphere, is useful. By this procedure, faces of additional forms (and often of the characteristic general form) appear as small facets on the sphere and their interfacial angles can be measured.

In favourable cases, even the space group can be derived from the morphology of a crystal: this is based on the so-called *Bravais–Donnay–Harker principle* (*cf*. Section 3.1.3). A textbook description is given by Phillips (1971).

Furthermore, measurements of the interfacial angles by means of the optical goniometer permit the determination of the relative dimensions of a 'morphological unit cell' with good accuracy. Thus, for instance, the interaxial angles α, β, γ and the axial ratio a:b:c of a triclinic crystal may be derived. The ratio a:b:c, however, may contain an uncertainty by an integral factor with respect to the actual cell edges of the crystal. This means that any one unit length may have to be multiplied by an integer in order to obtain correspondence to the 'structural' unit cell.

10.2.3. Etch figures

Additional information on the point group of a crystal can be gained from the face symmetry, which is usually determined by observation of etch figures, striations and other face markings. Etch pits are produced by heating the crystal in vacuum (evaporation from the surface) or by attacking it with an appropriate reagent, which should not be optically active. The etch pits generally appear at the end points of dislocation lines on the face. They exhibit the symmetry of one of the ten two-dimensional point groups which, in general,* corresponds to the symmetry of the crystal face under investigation.

* It should be noted, however, that asymmetric etch figures may occur that are due, for example, to an inclination of dislocation lines against the surface.

Table 10.2.1.2. *Polar axes and nonpolar directions in the 21 noncentrosymmetric crystal classes*

All directions normal to an evenfold rotation axis and along rotoinversion axes are nonpolar. All directions other than those in the column 'Nonpolar directions' are polar. A symbol like [$u0w$] refers to the set of directions obtained for all possible values of u and w, in this case to all directions normal to the b axis, *i.e.* parallel to the plane (010). Symmetrically equivalent sets of nonpolar directions are placed between semicolons; the sequence of these sets follows the sequence of the symmetry directions in Table 2.2.4.1

System	Class	Polar (symmetry) axes	Nonpolar directions
Triclinic	1	None	None
Monoclinic	2	[010]	[$u0w$]
Unique axis b	m	None	[010]
Monoclinic	2	[001]	[$uv0$]
Unique axis c	m	None	[001]
Orthorhombic	222	None	[$0vw$]; [$u0w$]; [$uv0$]
	$mm2$	[001]	[$uv0$]
Tetragonal	4	[001]	[$uv0$]
	$\bar{4}$	None	[001]; [$uv0$]
	422	None	[$uv0$]; [$0vw$] [$u0w$];
			[uuw] [$u\bar{u}w$]
	$4mm$	[001]	[$uv0$]
	$\bar{4}2m$	None	[$uv0$]; [$0vw$] [$u0w$]
	$\bar{4}m2$	None	[$uv0$]; [uuw] [$u\bar{u}w$]
Trigonal (Hexagonal axes)	3	[001]	None
	321	[100], [010], [$\bar{1}\bar{1}0$]	[$u2uw$] [$\overline{2u}\bar{u}w$] [$u\bar{u}w$]
	312	[$1\bar{1}0$], [120], [$\bar{2}\bar{1}0$]	[uuw] [$\bar{u}0w$] [$0\bar{v}w$]
	$3m1$	[001]	[100] [010] [$\bar{1}\bar{1}0$]
	$31m$	[001]	[$1\bar{1}0$] [120] [$\bar{2}\bar{1}0$]
Trigonal (Rhombohedral axes)	3	[111]	None
	32	[$1\bar{1}0$], [$01\bar{1}$], [$\bar{1}01$]	[uuw] [uvv] [uvu]
	$3m$	[111]	[$1\bar{1}0$] [$01\bar{1}$] [$\bar{1}01$]
Hexagonal	6	[001]	[$uv0$]
	$\bar{6}$	None	[001]
	622	None	[$u2uw$] [$\overline{2u}\bar{u}w$] [$u\bar{u}w$]
			[uuw] [$\bar{u}0w$] [$0\bar{v}w$]
	$6mm$	[001]	[$uv0$]
	$\bar{6}m2$	[$1\bar{1}0$], [120], [$\bar{2}\bar{1}0$]	[uuw] [$\bar{u}0w$] [$0\bar{v}w$]
	$\bar{6}2m$	[100], [010], [$\bar{1}\bar{1}0$]	[$u2uw$] [$\overline{2u}\bar{u}w$] [$u\bar{u}w$]
Cubic	23	Four threefold axes along ⟨111⟩	[$0vw$] [$u0w$] [$uv0$]
	$\bar{4}3m$		[$0vw$] [$u0w$] [$uv0$]
	432	None	[$0vw$] [$u0w$] [$uv0$]; [uuw] [uvv] [uvu]; [$u\bar{u}w$] [$uv\bar{v}$] [$\bar{u}vu$]

The observation of etch figures is important when the morphological analysis is ambiguous (*cf.* Section 10.2.2). For instance, a tetragonal pyramid, which is compatible with point groups 4 and $4mm$, can be uniquely attributed to point group 4 if its face symmetry is found to be 1. For face symmetry m, group $4mm$ would result. The (oriented) face symmetries of the 47 crystal forms in the various point groups are listed in column 6 of Table 10.1.2.3 and in column 3 of Table 10.1.2.2.

In noncentrosymmetric crystals, the etch pits on parallel but opposite faces, even though they have the same symmetry, may be of different size or shape, thus proving the absence of a symmetry centre. Note that the orientation of etch pits with respect to the edges of the face is significant (*cf.* Buerger, 1956), as well as the mutual arrangement of etch pits on opposite faces. Thus, for a pinacoid with face symmetry 1, the possible point groups $\bar{1}$, 2 and m of the crystal can be distinguished by the mutual orientation of etch pits on the two faces. Moreover, twinning by merohedry and the true symmetry of the two (or more) twin partners ('twin domains') may be detected.

The method of etching can be applied not only to growth faces but also to cleavage faces or arbitrarily cut faces.

Table 10.2.4.1. *Categories of crystal systems distinguished according to the different forms of the indicatrix*

Crystal system	Shape of indicatrix	Optical character
Cubic	Sphere	Isotropic (not doubly refracting)
Tetragonal, Trigonal, Hexagonal	Rotation ellipsoid	Uniaxial — Anisotropic (doubly refracting)
Orthorhombic, Monoclinic, Triclinic	General ellipsoid	Biaxial — Anisotropic (doubly refracting)

10.2.4. Optical properties

Optical studies provide good facilities to determine the symmetry of transparent crystals. The following optical properties may be used.

10.2.4.1. *Refraction*

The dependence of the *refractive index* on the vibration direction of a plane-polarized light wave travelling through the crystal can be obtained from the optical indicatrix. This surface is an ellipsoid which can degenerate into a rotation ellipsoid or even into a sphere. Thus, the lowest symmetry of the property 'refraction' is $2/m\ 2/m\ 2/m$, the point group of the general ellipsoid. According to the three different forms of the indicatrix three categories of crystal systems have to be distinguished (Table 10.2.4.1).

The orientation of the indicatrix is related to the symmetry directions of the crystal. In tetragonal, trigonal and hexagonal crystals, the rotation axis of the indicatrix (which is the unique optic axis) is parallel to the main symmetry axis. For orthorhombic crystals, the three principal axes of the indicatrix are oriented parallel to the three symmetry directions. In the monoclinic system, one of the axes of the indicatrix coincides with the monoclinic symmetry direction, whereas, in the triclinic case, the indicatrix can, in principle, have any orientation relative to a chosen reference system. Thus, in triclinic and, with restrictions, in monoclinic crystals, the *orientation* of the indicatrix can change with wavelength λ and temperature T (orientation dispersion). In any system, the *size* of the indicatrix and, in all but the cubic system, its *shape* can also vary with λ and T.

When studying the symmetry of a crystal by optical means, note that strain can lower the apparent symmetry owing to the high sensitivity of optical properties to strain.

10.2.4.2. *Optical activity*

The symmetry information obtained from *optical activity* is quite different from that given by optical refraction. Optical activity is in principle confined to the 21 noncentrosymmetric classes but it can occur in only 15 of them (Table 10.2.1.1). In the 11 enantiomorphism classes, a single crystal is either right- or left-handed. In the four non-enantiomorphous classes m, $mm2$, $\bar{4}$ and $\bar{4}2m$, optical activity may also occur; here directions of both right- and left-handed rotations of the plane of polarization exist in the same crystal. In the other six noncentrosymmetric classes, $3m$, $4mm$, $\bar{6}$, $6mm$, $\bar{6}2m$, $\bar{4}3m$, optical activity is not possible.

In the two cubic enantiomorphous classes 23 and 432, the optical activity is isotropic and can be observed along any direction.* For the other optically active crystals, the rotation of the plane of polarization can, in practice, be detected only in directions parallel (or approximately parallel) to the optic axes. This is because of the dominating effect of double refraction. No optical activity, however, is present along an inversion axis or along a direction parallel or perpendicular to a mirror plane. Thus, no activity occurs along the optic axis in crystal classes $\bar{4}$ and $\bar{4}2m$. In classes m and $mm2$, no activity can be present along the two optic axes, if these axes lie in m. If they are not parallel to m, they show optical rotation(s) of opposite sense.

10.2.4.3. *Second-harmonic generation (SHG)*

Light waves passing through a noncentrosymmetric crystal induce new waves of twice the incident frequency. This second-harmonic generation is due to the nonlinear optical susceptibility. The *second-harmonic coefficients* form a third-rank tensor, which is subject to the same symmetry constraints as the piezoelectric tensor (see Section 10.2.6). Thus, only noncentrosymmetric crystals, except those of class 432, can show the second-harmonic effect; *cf.* Table 10.2.1.1.

Second-harmonic generation is a powerful method of testing crystalline materials for the absence of a symmetry centre. With an appropriate experimental device, very small amounts (less than 10 mg) of powder are sufficient to detect the second-harmonic signals, even for crystals with small deviations from centrosymmetry (Dougherty & Kurtz, 1976).

10.2.5. Pyroelectricity and ferroelectricity

In principle, *pyroelectricity* can only exist in crystals with a permanent electric dipole moment. This moment is changed by heating and cooling, thus giving rise to electric charges on certain crystal faces, which can be detected by simple experimental procedures.

An electric dipole moment can be present only along a polar direction which has no symmetrically equivalent directions.† Such polar directions occur in the following ten classes: $6mm$, $4mm$, and their subgroups 6, 4, $3m$, 3, $mm2$, 2, m, 1 (*cf.* Table 10.2.1.1). In point groups with a rotation axis, the electric moment is along this axis. In class m, the electric moment is parallel to the mirror plane (direction $[u0w]$). In class 1, any direction $[uvw]$ is possible. In point groups 1 and m, besides a change in magnitude, a directional variation of the electric moment can also occur during heating or cooling.

In practice, it is difficult to prevent strains from developing throughout the crystal as a result of temperature gradients in the sample. This gives rise to piezoelectrically induced charges superposed on the true pyroelectric effect. Consequently, when the development of electric charges by a change in temperature is observed, the only safe deduction is that the specimen must lack a centre of symmetry. Failure to detect pyroelectricity may be due to extreme weakness of the effect, although modern methods are very sensitive.

A crystal is *ferroelectric* if the direction of the permanent electric dipole moment can be changed by an electric field. Thus, ferroelectricity can only occur in the ten pyroelectric crystal classes, mentioned above.

10.2.6. Piezoelectricity

In piezoelectric crystals, an electric dipole moment can be induced by compressional and torsional stress. For a uniaxial compression, the induced moment may be parallel, normal or inclined to the compression axis. These cases are called longitudinal, transverse or mixed compressional piezoeffect, respectively. Correspondingly, for torsional stress, the electric moment may be parallel, normal or inclined to the torsion axis.

The *piezoelectricity* is described by a third-rank tensor, the moduli of which vanish for all centrosymmetric point groups. Additionally, in class 432, all piezoelectric moduli are zero owing to the high symmetry. Thus, piezoelectricity can only occur in 20 noncentrosymmetric crystal classes (Table 10.2.1.1).

The piezoelectric point groups 422 and 622 show the following peculiarity: there is no direction for which a longitudinal component of the electric moment is induced under uniaxial compression. Thus, no longitudinal or mixed compressional effects occur. The moment is always normal to the compression axis (pure transverse compressional effect). This means that, with the compression pistons as electrodes, no electric charges can be found, since only transverse compressional or torsional piezoeffects occur. In all other piezoelectric classes, there exist directions in which both longitudinal and transverse components of the electric dipole moment are induced under uniaxial compression.

An electric moment can also develop under hydrostatic pressure. This kind of piezoelectricity, like pyroelectricity, can be represented by a first-rank tensor (vector), whereby the hydrostatic pressure is regarded as a scalar. Thus, piezoelectricity under hydrostatic pressure is subject to the same symmetry constraints as pyroelectricity.

Like ‘second-harmonic generation’ (Section 10.2.4.3), the piezoelectric effect is very useful to test crystals for the absence of a symmetry centre. There exist powerful methods for testing powder samples or even small single crystals. In the old technique of Giebe & Scheibe (*cf.* Wooster & Brenton, 1970), the absorption and emission of radio-frequency energy by electromechanical oscillations of piezoelectric particles are detected. In the more modern method of observing ‘polarization echoes’, radio-frequency pulses are applied to powder samples. By this procedure, electromechanical vibration pulses are induced in piezoelectric particles, the echoes of which can be detected (*cf.* Melcher & Shiren, 1976).

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* This property can be represented by enantiomorphic spheres of point group 2∞, *cf.* Table 10.1.4.2.

† In the literature, the requirement for pyroelectricity is frequently expressed as ‘a unique (or singular) polar axis’. This term, however, is misleading for point groups 1 and m.

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11.1. Point coordinates, symmetry operations and their symbols

BY W. FISCHER AND E. KOCH

11.1.1. Coordinate triplets and symmetry operations

The coordinate triplets of a general position, as given in the space-group tables, can be taken as a shorthand notation for the symmetry operations of the space group. Each coordinate triplet $\tilde{x}, \tilde{y}, \tilde{z}$ corresponds to the symmetry operation that maps a point with coordinates x, y, z onto a point with coordinates $\tilde{x}, \tilde{y}, \tilde{z}$. The mapping of x, y, z onto $\tilde{x}, \tilde{y}, \tilde{z}$ is given by the equations:

$$\begin{aligned}\tilde{x} &= W_{11}x + W_{12}y + W_{13}z + w_1\\ \tilde{y} &= W_{21}x + W_{22}y + W_{23}z + w_2\\ \tilde{z} &= W_{31}x + W_{32}y + W_{33}z + w_3.\end{aligned}$$

If, as usual, the symmetry operation is represented by a matrix pair, consisting of a (3×3) matrix $\boldsymbol{W}$ and a (3×1) column matrix $\boldsymbol{w}$, the equations read

$$\tilde{\boldsymbol{x}} = (\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$$

with

$$\boldsymbol{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \qquad \tilde{\boldsymbol{x}} = \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix},$$

$$\boldsymbol{w} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}, \quad \boldsymbol{W} = \begin{pmatrix} W_{11} & W_{12} & W_{13} \\ W_{21} & W_{22} & W_{23} \\ W_{31} & W_{32} & W_{33} \end{pmatrix}.$$

$\boldsymbol{W}$ is called the rotation part and $\boldsymbol{w} = \boldsymbol{w}_g + \boldsymbol{w}_l$ the translation part; $\boldsymbol{w}$ is the sum of the intrinsic translation part $\boldsymbol{w}_g$ (glide part or screw part) and the location part $\boldsymbol{w}_l$ (due to the location of the symmetry element) of the symmetry operation.

Example

The coordinate triplet $-x + y, y, -z + \frac{1}{2}$ stands for the symmetry operation with rotation part

$$\boldsymbol{W} = \begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$$

and with translation part

$$\boldsymbol{w} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}.$$

Matrix multiplication yields

$$\begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix} = \begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix} = \begin{pmatrix} -x + y \\ y \\ -z + \frac{1}{2} \end{pmatrix}.$$

Using the above relation, the assignment of coordinate triplets to symmetry operations given as pairs $(\boldsymbol{W}, \boldsymbol{w})$ is straightforward.

11.1.2. Symbols for symmetry operations

The information required to describe a symmetry operation by a unique notation depends on the type of the operation (Table 11.1.2.1). The symbols explained below are based on the Hermann–Mauguin symbols (see Chapter 12.2), modified and supplemented where necessary. Note that a change of the coordinate basis generally alters the symbol of a given symmetry operation.

(i) A *translation* is symbolized by the letter *t*, followed by the components of the translation vector between parentheses.

Example

$t(\frac{1}{2}, \frac{1}{2}, 0)$ stands for a translation by the vector $\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$, *i.e.* a C centring.

(ii) A *rotation* is symbolized by a number $n = 2$, 3, 4 or 6 (according to the rotation angle $360°/n$) and a superscript, $+$ or $-$, which specifies the sense of rotation (not needed for $n = 2$). This is followed by the location of the rotation axis. Since the definition of the positive sense of a pure rotation is arbitrary, the following convention has been adopted: The sense of a rotation is symbolized by $+$ if the rotation appears to be in the mathematically positive sense (*i.e.* counter-clockwise) when viewed along the rotation axis in the direction of decreasing values of the parameter describing that axis. This convention leads to a particular symbol for each rotation and avoids describing some rotations by powers of other rotations. It corresponds to looking at the usual tetragonal or hexagonal space-group diagrams.

Example

$4^+\ 0, y, 0$ indicates a rotation of 90° about the line $0y0$ that brings point 001 onto point 100, a rotation that is seen in the mathematically positive sense if viewed from point 010 to point 000.

(iii) A *screw rotation* is symbolized in the same way as a pure rotation, but with the screw part added between parentheses.

Example

$3^-\ (0, 0, \frac{1}{3})\ \frac{1}{3}, \frac{1}{3}, z$ indicates a rotation of 120° around the line $\frac{1}{3}\frac{1}{3}z$ in the mathematically negative sense if viewed from the point $\frac{1}{3}\frac{1}{3}1$ towards $\frac{1}{3}\frac{1}{3}0$, combined with a translation of $\frac{1}{3}\mathbf{c}$.

Thus, with respect to the coordinate basis chosen, each screw rotation is designated uniquely. This could not have been achieved by deriving the screw-rotation symbols from the Hermann–Mauguin screw-axis symbols.

Table 11.1.2.1. *Information necessary to describe symmetry operations*

Type of symmetry operation	Necessary information
Translation	Translation vector
Rotation	Location of the rotation axis, angle and sense of rotation
Screw rotation	As for rotation, plus screw vector
Reflection	Location of the mirror plane
Glide reflection	As for reflection, plus glide vector
Inversion	Location of the inversion centre
Rotoinversion	As for rotation, plus location of the inversion point

Example

The symmetry operation represented by $-y, z+\frac{1}{2}, -x+\frac{1}{2}$ occurs in space group $P2_13$ as well as in $I2_13$ and is labelled (10) in the space-group tables (see Section 2.2.9) both times. The corresponding symmetry element, however, is a 3_1 axis in $P2_13$, but a 3_2 axis in $I2_13$, because the subscript refers to the shortest translation parallel to the axis.

(iv) A *reflection* is symbolized by the letter m, followed by the location of the mirror plane.

(v) A *glide reflection* in general is symbolized by the letter g, with the glide part given between parentheses, followed by the location of the glide plane. These specifications characterize every glide reflection uniquely. Exceptions are the traditional symbols a, b, c, n and d that are used instead of g. In the case of a glide plane a, b or c, the explicit statement of the glide vector is omitted if it is $\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$ or $\frac{1}{2}\mathbf{c}$, respectively.

Example

$a\ x, y, \frac{1}{4}$ means a glide reflection with glide part $\frac{1}{2}\mathbf{a}$ and the glide plane a at $x\,y\,\frac{1}{4}$; $d(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})\ x, x-\frac{1}{4}, z$ denotes a glide reflection with glide part $(\frac{1}{4}\frac{1}{4}\frac{3}{4})$ and the glide plane d at $x, x-\frac{1}{4}, z$.

The letter g is kept for those glide reflections that cannot be described with one of the symbols a, b, c, n, d without additional conventions.

Example

$g(-\frac{1}{6}, \frac{1}{6}, \frac{1}{6})\ x+\frac{1}{2}, -x, z$ implies a glide reflection with glide part $(-\frac{1}{6}, \frac{1}{6}, \frac{1}{6})$ and the glide plane at $x+\frac{1}{2}, -x, z$.

(vi) An *inversion* is symbolized by $\bar{1}$, followed by the location of the symmetry centre.

(vii) A *rotoinversion* is symbolized, in analogy to a rotation, by $\bar{3}, \bar{4}$ or $\bar{6}$ and the superscript $+$ or $-$, again followed by the location of the (rotoinversion) axis. Note that angle and sense of rotation refer to the pure rotation and not to the combination of rotation and inversion. In addition, the location of the inversion point is given by the appropriate coordinate triplet after a semicolon.

Example

$\bar{4}^+\ 0, \frac{1}{2}, z;\ 0, \frac{1}{2}, \frac{1}{4}$ means a 90° rotoinversion with axis at $0\frac{1}{2}z$ and inversion point at $0\frac{1}{2}\frac{1}{4}$. The rotation is performed in the mathematically positive sense, when viewed from $0\frac{1}{2}1$ towards $0\frac{1}{2}0$. Therefore, the rotoinversion maps point 000 onto point $-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$.

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11.2. Derivation of symbols and coordinate triplets

By W. Fischer and E. Koch
with Tables 11.2.2.1 and 11.2.2.2 by H. Arnold

11.2.1. Derivation of symbols for symmetry operations from coordinate triplets or matrix pairs

In the space-group tables, all symmetry operations with $0 \le w < 1$ are listed explicitly. As a consequence, the number of entries under the heading *Symmetry operations* equals the multiplicity of the general position. For space groups with centred unit cells, $w \ge 1$ may result if the centring translations are applied to the explicitly listed coordinate triplets. In those cases, all w values have been reduced modulo 1 for the derivation of the corresponding symmetry operations (see Section 2.2.9). In addition to the tabulated symmetry operations, each space group contains an infinite number of further operations obtained by application of integral lattice translations. In many cases, it is not trivial to obtain the additional symmetry operations (*cf.* Part 4) from the ones listed. Therefore, a general procedure is described below by which symbols for symmetry operations as described in Section 11.1.2 may be derived from coordinate triplets or, more specifically, from the corresponding matrix pairs $(\boldsymbol{W}, \boldsymbol{w})$. [For a similar treatment of this topic, see Wondratschek & Neubüser (1967).] This procedure may also be applied to cases where space groups are given in descriptions not contained in *International Tables.* In practice, two cases may be distinguished:

(i) The matrix $\boldsymbol{W}$ is the unit matrix:

$$\boldsymbol{W} = \boldsymbol{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

In this case, the symmetry operation is a *translation* with translation vector $\boldsymbol{w}$.

Example

$$x+\tfrac{1}{2}, y+\tfrac{1}{2}, z \;\Rightarrow\; \boldsymbol{W} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \boldsymbol{I}, \quad \boldsymbol{w} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$$

$\Rightarrow$ translation with translation vector $\mathbf{w} = \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$ (C centring).

(ii) The matrix $\boldsymbol{W}$ is not the unit matrix: $\boldsymbol{W} \ne \boldsymbol{I}$. In this case, one calculates the trace, $\mathrm{tr}(\boldsymbol{W}) = W_{11} + W_{22} + W_{33}$, and the determinant, $\det(\boldsymbol{W})$, and identifies the type of the rotation part of the symmetry operation from Table 11.2.1.1.

One has to distinguish three subcases:

(*a*) $\boldsymbol{W}$ corresponds to a *rotoinversion*. The inversion point X is obtained by solving the equation $(\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x} = \boldsymbol{x}$. For a rotoinversion other than $\bar{1}$, the location of the axis follows from the equation $(\boldsymbol{W}, \boldsymbol{w})^2\boldsymbol{x} = (\boldsymbol{W}^2, \boldsymbol{W}\boldsymbol{w} + \boldsymbol{w})\boldsymbol{x} = \boldsymbol{x}$. The rotation sense may be found either by geometrical inspection of a pair of points related by the symmetry operation or by the algebraic procedure described below.

Table 11.2.1.1. *Identification of the type of the rotation part of the symmetry operation*

det($\boldsymbol{W}$) \ tr($\boldsymbol{W}$)	−3	−2	−1	0	1	2	3
1			2	3	4	6	1
−1	$\bar{1}$	$\bar{6}$	$\bar{4}$	$\bar{3}$	m		

Example

$$z, -y+\tfrac{1}{2}, -x+\tfrac{1}{2} \;\Rightarrow\; \boldsymbol{W} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}, \quad \boldsymbol{w} = \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

$\Rightarrow \mathrm{tr}(\boldsymbol{W}) = -1, \quad \det(\boldsymbol{W}) = -1$

$\Rightarrow$ fourfold rotoinversion;

$$(\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x} = \boldsymbol{x} \;\Rightarrow\; \begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$\Rightarrow x = y = z = \frac{1}{4}$

$\Rightarrow$ inversion point at $\frac{1}{4}\frac{1}{4}\frac{1}{4}$;

$(\boldsymbol{W}^2, \boldsymbol{W}\boldsymbol{w} + \boldsymbol{w})\boldsymbol{x} = \boldsymbol{x}$

$$\Rightarrow \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$\Rightarrow x = z = \frac{1}{4},\; y$ undetermined

$\Rightarrow$ rotoinversion axis at $\frac{1}{4}\,y\,\frac{1}{4}$;

$$(\boldsymbol{W}, \boldsymbol{w}) \begin{pmatrix} \frac{1}{4} \\ \frac{1}{4} \\ z \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{4} \\ \frac{1}{4} \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} = \begin{pmatrix} z \\ \frac{1}{4} \\ \frac{1}{4} \end{pmatrix}$$

$\Rightarrow$ the rotation sense is negative as verified by geometrical inspection.

$\Rightarrow \bar{4}^-\; \frac{1}{4}, y, \frac{1}{4};\; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}.$

(*b*) $\boldsymbol{W}$ corresponds to an n-fold *rotation*. $(\boldsymbol{W}, \boldsymbol{w})$ is thus either a rotation or a screw rotation. To distinguish between these alternatives, $(\boldsymbol{W}, \boldsymbol{w})^n = (\boldsymbol{I}, \boldsymbol{t})$ has to be calculated. For $\boldsymbol{t} = \boldsymbol{o}$, $(\boldsymbol{W}, \boldsymbol{w})$ describes a pure rotation, the rotation axis of which is found by solving $(\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x} = \boldsymbol{x}$. For $\boldsymbol{t} \ne \boldsymbol{o}$, $(\boldsymbol{W}, \boldsymbol{w})$ describes a screw rotation with screw part $\boldsymbol{w}_g = (1/n)\boldsymbol{t}$. The location of the screw axis is found as the set of fixed points for the corresponding pure rotation $(\boldsymbol{W}, \boldsymbol{w}_l)$ with $\boldsymbol{w}_l = \boldsymbol{w} - \boldsymbol{w}_g$, *i.e.* by solving $(\boldsymbol{W}, \boldsymbol{w}_l)\boldsymbol{x} = \boldsymbol{x}$. The sense of the rotation may be found either by geometrical inspection or by the algebraic procedure described below.

Example

$$-z, -x+\tfrac{1}{2}, y \;\Rightarrow\; \boldsymbol{W} = \begin{pmatrix} 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad \boldsymbol{w} = \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \end{pmatrix}$$

$\Rightarrow \mathrm{tr}(\boldsymbol{W}) = 0, \quad \det(\boldsymbol{W}) = 1$

$\Rightarrow$ threefold rotation or screw rotation;

$(\boldsymbol{W}, \boldsymbol{w})^3 = (\boldsymbol{W}^3, \boldsymbol{W}^2\boldsymbol{w} + \boldsymbol{W}\boldsymbol{w} + \boldsymbol{w})$

and

$$\boldsymbol{W}^2\boldsymbol{w} + \boldsymbol{W}\boldsymbol{w} + \boldsymbol{w} = \boldsymbol{t} = \begin{pmatrix} -\frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

$\Rightarrow$ threefold screw rotation with screw part

$$\boldsymbol{w}_g = \tfrac{1}{3}\boldsymbol{t} = \begin{pmatrix} -\frac{1}{6} \\ \frac{1}{6} \\ \frac{1}{6} \end{pmatrix};$$

$$(\boldsymbol{W}, \boldsymbol{w}_l)\boldsymbol{x} = \boldsymbol{x}$$

$$\Rightarrow \begin{pmatrix} 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} \frac{1}{6} \\ \frac{1}{3} \\ -\frac{1}{6} \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$\Rightarrow y = \frac{1}{3} - x;\quad z = \frac{1}{6} - x;\quad x$ undetermined

$\Rightarrow$ screw axis at $x, \frac{1}{3} - x, \frac{1}{6} - x$

(for the sense of rotation see example below).

(*c*) $\boldsymbol{W}$ corresponds to a (glide) *reflection*. The glide character is now found by means of the equation $(\boldsymbol{W}, \boldsymbol{w})^2 = (\boldsymbol{I}, \boldsymbol{W}\boldsymbol{w} + \boldsymbol{w}) = (\boldsymbol{I}, \boldsymbol{t})$. For $\boldsymbol{t} = \boldsymbol{o}$, $(\boldsymbol{W}, \boldsymbol{w})$ describes a pure reflection and the location of the mirror plane follows from $(\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x} = \boldsymbol{x}$. For $\boldsymbol{t} \neq \boldsymbol{o}$, $(\boldsymbol{W}, \boldsymbol{w})$ corresponds to a glide reflection with glide part $\boldsymbol{w}_g = \frac{1}{2}\boldsymbol{t}$. The location of the glide plane is the set of fixed points for the corresponding pure reflection $(\boldsymbol{W}, \boldsymbol{w}_l) = (\boldsymbol{W}, \boldsymbol{w} - \frac{1}{2}\boldsymbol{t})$ and is thus calculated by solving $(\boldsymbol{W}, \boldsymbol{w}_l)\boldsymbol{x} = \boldsymbol{x}$.

Example

$$-y + \tfrac{1}{2},\ -x, z + \tfrac{3}{4} \ \Rightarrow\ \boldsymbol{W} = \begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{w} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{3}{4} \end{pmatrix}$$

$\Rightarrow \mathrm{tr}(\boldsymbol{W}) = 1, \quad \det(\boldsymbol{W}) = -1$

$\Rightarrow$ reflection or glide reflection;

$$(\boldsymbol{W}, \boldsymbol{w})^2 = (\boldsymbol{W}^2, \boldsymbol{W}\boldsymbol{w} + \boldsymbol{w}), \quad \boldsymbol{W}\boldsymbol{w} + \boldsymbol{w} = \boldsymbol{t} = \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ \frac{3}{2} \end{pmatrix}$$

$\Rightarrow$ glide reflection with glide part

$$\boldsymbol{w}_g = \tfrac{1}{2}\boldsymbol{t} = \begin{pmatrix} \frac{1}{4} \\ -\frac{1}{4} \\ \frac{3}{4} \end{pmatrix};$$

$$(\boldsymbol{W}, \boldsymbol{w}_l)\boldsymbol{x} = \boldsymbol{x} \ \Rightarrow\ \begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} \frac{1}{4} \\ \frac{1}{4} \\ 0 \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$\Rightarrow y = -x + \frac{1}{4};\ x, z$ undetermined

$\Rightarrow$ glide plane d at $x, -x + \frac{1}{4}, z$

$\Rightarrow d(\frac{1}{4}, -\frac{1}{4}, \frac{3}{4})\quad x, -x + \frac{1}{4}, z.$

The sense of a pure or screw rotation or of a rotoinversion may be calculated as follows: One takes two arbitrary points P_0 and P_1 on the rotation axis, P_0 having the lower value for the free parameter of the axis. One takes a point P_2 not lying on the axis and generates P_3 from P_2 by the symmetry operation under consideration. One calculates the determinant d of the matrix $(\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3)$ composed of the components of vectors $\boldsymbol{v}_1 = \overrightarrow{P_0P_1}, \boldsymbol{v}_2 = \overrightarrow{P_0P_2}$ and $\boldsymbol{v}_3 = \overrightarrow{P_0P_3}$. For rotations or screw rotations, the sense is positive for $d > 0$ and negative for $d < 0$. For rotoinversions, the sense is positive for $d < 0$ and negative for $d > 0$.

Example

According to example in (*b*) above, the triplet $-z, -x + \frac{1}{2}, y$ represents a threefold screw rotation with screw part $\begin{pmatrix} -\frac{1}{6} \\ \frac{1}{6} \\ \frac{1}{6} \end{pmatrix}$ and screw axis at $x, \frac{1}{3} - x, \frac{1}{6} - x$. To obtain the sense of the rotation, the points $0\frac{1}{3}\frac{1}{6}$ and $\frac{1}{6}\frac{1}{6}0$ are used as P_0 and P_1 on the axis and the points 000 and $0\frac{1}{2}0$ as P_2 and P_3 outside the axis. The resulting vectors are

$$\boldsymbol{v}_1 = \begin{pmatrix} \frac{1}{6} \\ -\frac{1}{6} \\ -\frac{1}{6} \end{pmatrix}, \quad \boldsymbol{v}_2 = \begin{pmatrix} 0 \\ -\frac{1}{3} \\ -\frac{1}{6} \end{pmatrix}, \quad \boldsymbol{v}_3 = \begin{pmatrix} 0 \\ \frac{1}{6} \\ -\frac{1}{6} \end{pmatrix}$$

$$\Rightarrow d = \begin{vmatrix} \frac{1}{6} & 0 & 0 \\ -\frac{1}{6} & -\frac{1}{3} & \frac{1}{6} \\ -\frac{1}{6} & -\frac{1}{6} & -\frac{1}{6} \end{vmatrix} = \frac{1}{72} > 0$$

$\Rightarrow$ the sense of the rotation is positive

$\Rightarrow 3^+(-\frac{1}{6}, \frac{1}{6}, \frac{1}{6})\quad x, \frac{1}{3} - x, \frac{1}{6} - x.$

11.2.2. Derivation of coordinate triplets from symbols for symmetry operations

A particular symmetry operation is uniquely described by its symbol, as introduced in Section 11.1.2, and the coordinate system to which it refers. In the examples of the previous section, the symbols have been derived from the coordinate triplets representing the respective symmetry operations. Inversely, the pair $(\boldsymbol{W}, \boldsymbol{w})$ of the symmetry operation and the coordinate triplet of the image point can be deduced from the symbol.

(i) For all symmetry operations of space groups, the *rotation parts* $\boldsymbol{W}$ referring to conventional coordinate systems are listed in Tables 11.2.2.1 and 11.2.2.2 as matrices for point-group symmetry operations. For rotoinversions, the position of the inversion point at 0, 0, 0 is not explicitly given.

(ii) The *location part* $\boldsymbol{w}_l$ of $\boldsymbol{w}$ may easily be derived from

$$(\boldsymbol{W}, \boldsymbol{w}_l)\begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix} = \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix}, \quad \textit{i.e.}\ \boldsymbol{w}_l = (\boldsymbol{I} - \boldsymbol{W})\begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix}$$

with x_0, y_0, z_0 being the coordinate triplet of the inversion point of a rotoinversion or the coordinate triplet of an arbitrary fixed point of any other symmetry operation. The *intrinsic translation part* $\boldsymbol{w}_g$ of $\boldsymbol{w}$ is given explicitly in the symbol of the symmetry operation, so that the translation part $\boldsymbol{w}$ is obtained as

$$\boldsymbol{w} = \boldsymbol{w}_g + \boldsymbol{w}_l = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}.$$

(iii) The coordinate triplet $\tilde{x}, \tilde{y}, \tilde{z}$ corresponding to the symmetry operation is now given by

$$\tilde{x} = W_{11}x + W_{12}y + W_{13}z + w_1$$
$$\tilde{y} = W_{21}x + W_{22}y + W_{23}z + w_2$$
$$\tilde{z} = W_{31}x + W_{32}y + W_{33}z + w_3.$$

Example

$4^-(0,0,\frac{3}{4})\ \frac{1}{4},-\frac{1}{4},z$ tetragonal system

$$4^-\ 0,0,z \ \Rightarrow\ \boldsymbol{W} = \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ from Table 11.2.2.1.}$$

$x_0 = \frac{1}{4}, y_0 = -\frac{1}{4}, z_0 = 0$ is a fixed point of $4^-\ \frac{1}{4}, -\frac{1}{4}, z$, *i.e.* a point on the screw axis.

$$\boldsymbol{w}_l = (\boldsymbol{I} - \boldsymbol{W})\begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix}$$

$$\Rightarrow \boldsymbol{w}_l = \begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \frac{1}{4} \\ -\frac{1}{4} \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \end{pmatrix};$$

$\boldsymbol{w} = \boldsymbol{w}_g + \boldsymbol{w}_l$

$$\Rightarrow \boldsymbol{w} = \begin{pmatrix} 0 \\ 0 \\ \frac{3}{4} \end{pmatrix} + \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{3}{4} \end{pmatrix}$$

$$\Rightarrow \tilde{x} = y + \tfrac{1}{2}, \quad \tilde{y} = -x, \quad \tilde{z} = z + \tfrac{3}{4}.$$

References

Wondratschek, H. & Neubüser, J. (1967). *Determination of the symmetry elements of a space group from the 'general positions' listed in International Tables for X-ray Crystallography, Vol. I. Acta Cryst.* **23**, 349–352.

Table 11.2.2.1. *Matrices for point-group symmetry operations and orientation of corresponding symmetry elements, referred to a cubic, tetragonal, orthorhombic, monoclinic, triclinic or rhombohedral coordinate system (cf. Table 2.1.2.1)*

Symbol of symmetry operation and orientation of symmetry element	Transformed coordinates $\tilde{x},\tilde{y},\tilde{z}$	Matrix $\boldsymbol{W}$	Symbol of symmetry operation and orientation of symmetry element	Transformed coordinates $\tilde{x},\tilde{y},\tilde{z}$	Matrix $\boldsymbol{W}$	Symbol of symmetry operation and orientation of symmetry element	Transformed coordinates $\tilde{x},\tilde{y},\tilde{z}$	Matrix $\boldsymbol{W}$	Symbol of symmetry operation and orientation of symmetry element	Transformed coordinates $\tilde{x},\tilde{y},\tilde{z}$	Matrix $\boldsymbol{W}$
1	x,y,z	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	2 $0,0,z$ $[001]$	$\bar{x},\bar{y},z$	$\begin{pmatrix}\bar{1}&0&0\\0&\bar{1}&0\\0&0&1\end{pmatrix}$	2 $0,y,0$ $[010]$	$\bar{x},y,\bar{z}$	$\begin{pmatrix}\bar{1}&0&0\\0&1&0\\0&0&\bar{1}\end{pmatrix}$	2 $x,0,0$ $[100]$	$x,\bar{y},\bar{z}$	$\begin{pmatrix}1&0&0\\0&\bar{1}&0\\0&0&\bar{1}\end{pmatrix}$
3^+ x,x,x $[111]$	z,x,y	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$	3^+ $x,\bar{x},\bar{x}$ $[1\bar{1}\bar{1}]$	$\bar{z},\bar{x},y$	$\begin{pmatrix}0&0&\bar{1}\\\bar{1}&0&0\\0&1&0\end{pmatrix}$	3^+ $\bar{x},x,\bar{x}$ $[\bar{1}1\bar{1}]$	$z,\bar{x},\bar{y}$	$\begin{pmatrix}0&0&1\\\bar{1}&0&0\\0&\bar{1}&0\end{pmatrix}$	3^+ $\bar{x},\bar{x},x$ $[\bar{1}\bar{1}1]$	$\bar{z},x,\bar{y}$	$\begin{pmatrix}0&0&\bar{1}\\1&0&0\\0&\bar{1}&0\end{pmatrix}$
3^- x,x,x $[111]$	y,z,x	$\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}$	3^- $x,\bar{x},\bar{x}$ $[1\bar{1}\bar{1}]$	$\bar{y},z,\bar{x}$	$\begin{pmatrix}0&\bar{1}&0\\0&0&1\\\bar{1}&0&0\end{pmatrix}$	3^- $\bar{x},x,\bar{x}$ $[\bar{1}1\bar{1}]$	$\bar{y},\bar{z},x$	$\begin{pmatrix}0&\bar{1}&0\\0&0&\bar{1}\\1&0&0\end{pmatrix}$	3^- $\bar{x},\bar{x},x$ $[\bar{1}\bar{1}1]$	$y,\bar{z},\bar{x}$	$\begin{pmatrix}0&1&0\\0&0&\bar{1}\\\bar{1}&0&0\end{pmatrix}$
			2 $x,x,0$ $[110]$	$y,x,\bar{z}$	$\begin{pmatrix}0&1&0\\1&0&0\\0&0&\bar{1}\end{pmatrix}$	2 $x,0,x$ $[101]$	$z,\bar{y},x$	$\begin{pmatrix}0&0&1\\0&\bar{1}&0\\1&0&0\end{pmatrix}$	2 $0,y,y$ $[011]$	$\bar{x},z,y$	$\begin{pmatrix}\bar{1}&0&0\\0&0&1\\0&1&0\end{pmatrix}$
			2 $x,\bar{x},0$ $[1\bar{1}0]$	$\bar{y},\bar{x},\bar{z}$	$\begin{pmatrix}0&\bar{1}&0\\\bar{1}&0&0\\0&0&\bar{1}\end{pmatrix}$	2 $\bar{x},0,x$ $[\bar{1}01]$	$\bar{z},\bar{y},\bar{x}$	$\begin{pmatrix}0&0&\bar{1}\\0&\bar{1}&0\\\bar{1}&0&0\end{pmatrix}$	2 $0,y,\bar{y}$ $[01\bar{1}]$	$\bar{x},\bar{z},\bar{y}$	$\begin{pmatrix}\bar{1}&0&0\\0&0&\bar{1}\\0&\bar{1}&0\end{pmatrix}$
			4^+ $0,0,z$ $[001]$	$\bar{y},x,z$	$\begin{pmatrix}0&\bar{1}&0\\1&0&0\\0&0&1\end{pmatrix}$	4^+ $0,y,0$ $[010]$	$z,y,\bar{x}$	$\begin{pmatrix}0&0&1\\0&1&0\\\bar{1}&0&0\end{pmatrix}$	4^+ $x,0,0$ $[100]$	$x,\bar{z},y$	$\begin{pmatrix}1&0&0\\0&0&\bar{1}\\0&1&0\end{pmatrix}$
			4^- $0,0,z$ $[001]$	$y,\bar{x},z$	$\begin{pmatrix}0&1&0\\\bar{1}&0&0\\0&0&1\end{pmatrix}$	4^- $0,y,0$ $[010]$	$\bar{z},y,x$	$\begin{pmatrix}0&0&\bar{1}\\0&1&0\\1&0&0\end{pmatrix}$	4^- $x,0,0$ $[100]$	$x,z,\bar{y}$	$\begin{pmatrix}1&0&0\\0&0&1\\0&\bar{1}&0\end{pmatrix}$
$\bar{1}$ $0,0,0$	$\bar{x},\bar{y},\bar{z}$	$\begin{pmatrix}\bar{1}&0&0\\0&\bar{1}&0\\0&0&\bar{1}\end{pmatrix}$	m $x,y,0$ $[001]$	$x,y,\bar{z}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&\bar{1}\end{pmatrix}$	m $x,0,z$ $[010]$	$x,\bar{y},z$	$\begin{pmatrix}1&0&0\\0&\bar{1}&0\\0&0&1\end{pmatrix}$	m $0,y,z$ $[100]$	$\bar{x},y,z$	$\begin{pmatrix}\bar{1}&0&0\\0&1&0\\0&0&1\end{pmatrix}$
$\bar{3}^+$ x,x,x $[111]$	$\bar{z},\bar{x},\bar{y}$	$\begin{pmatrix}0&0&\bar{1}\\\bar{1}&0&0\\0&\bar{1}&0\end{pmatrix}$	$\bar{3}^+$ $x,\bar{x},\bar{x}$ $[1\bar{1}\bar{1}]$	$z,x,\bar{y}$	$\begin{pmatrix}0&0&1\\1&0&0\\0&\bar{1}&0\end{pmatrix}$	$\bar{3}^+$ $\bar{x},x,\bar{x}$ $[\bar{1}1\bar{1}]$	$\bar{z},x,y$	$\begin{pmatrix}0&0&\bar{1}\\1&0&0\\0&1&0\end{pmatrix}$	$\bar{3}^+$ $\bar{x},\bar{x},x$ $[\bar{1}\bar{1}1]$	$z,\bar{x},y$	$\begin{pmatrix}0&0&1\\\bar{1}&0&0\\0&1&0\end{pmatrix}$
$\bar{3}^-$ x,x,x $[111]$	$\bar{y},\bar{z},\bar{x}$	$\begin{pmatrix}0&\bar{1}&0\\0&0&\bar{1}\\\bar{1}&0&0\end{pmatrix}$	$\bar{3}^-$ $x,\bar{x},\bar{x}$ $[1\bar{1}\bar{1}]$	$y,\bar{z},x$	$\begin{pmatrix}0&1&0\\0&0&\bar{1}\\1&0&0\end{pmatrix}$	$\bar{3}^-$ $\bar{x},x,\bar{x}$ $[\bar{1}1\bar{1}]$	$y,z,\bar{x}$	$\begin{pmatrix}0&1&0\\0&0&1\\\bar{1}&0&0\end{pmatrix}$	$\bar{3}^-$ $\bar{x},\bar{x},x$ $[\bar{1}\bar{1}1]$	$\bar{y},z,x$	$\begin{pmatrix}0&\bar{1}&0\\0&0&1\\1&0&0\end{pmatrix}$
			m $x,\bar{x},z$ $[110]$	$\bar{y},\bar{x},z$	$\begin{pmatrix}0&\bar{1}&0\\\bar{1}&0&0\\0&0&1\end{pmatrix}$	m $\bar{x},y,x$ $[101]$	$\bar{z},y,\bar{x}$	$\begin{pmatrix}0&0&\bar{1}\\0&1&0\\\bar{1}&0&0\end{pmatrix}$	m $x,y,\bar{y}$ $[011]$	$x,\bar{z},\bar{y}$	$\begin{pmatrix}1&0&0\\0&0&\bar{1}\\0&\bar{1}&0\end{pmatrix}$
			m x,x,z $[1\bar{1}0]$	y,x,z	$\begin{pmatrix}0&1&0\\1&0&0\\0&0&1\end{pmatrix}$	m x,y,x $[\bar{1}01]$	z,y,x	$\begin{pmatrix}0&0&1\\0&1&0\\1&0&0\end{pmatrix}$	m x,y,y $[01\bar{1}]$	x,z,y	$\begin{pmatrix}1&0&0\\0&0&1\\0&1&0\end{pmatrix}$
			$\bar{4}^+$ $0,0,z$ $[001]$	$y,\bar{x},\bar{z}$	$\begin{pmatrix}0&1&0\\\bar{1}&0&0\\0&0&\bar{1}\end{pmatrix}$	$\bar{4}^+$ $0,y,0$ $[010]$	$\bar{z},\bar{y},x$	$\begin{pmatrix}0&0&\bar{1}\\0&\bar{1}&0\\1&0&0\end{pmatrix}$	$\bar{4}^+$ $x,0,0$ $[100]$	$\bar{x},z,\bar{y}$	$\begin{pmatrix}\bar{1}&0&0\\0&0&1\\0&\bar{1}&0\end{pmatrix}$
			$\bar{4}^-$ $0,0,z$ $[001]$	$\bar{y},x,\bar{z}$	$\begin{pmatrix}0&\bar{1}&0\\1&0&0\\0&0&\bar{1}\end{pmatrix}$	$\bar{4}^-$ $0,y,0$ $[010]$	$z,\bar{y},\bar{x}$	$\begin{pmatrix}0&0&1\\0&\bar{1}&0\\\bar{1}&0&0\end{pmatrix}$	$\bar{4}^-$ $x,0,0$ $[100]$	$\bar{x},\bar{z},y$	$\begin{pmatrix}\bar{1}&0&0\\0&0&\bar{1}\\0&1&0\end{pmatrix}$

Table 11.2.2.2. *Matrices for point-group symmetry operations and orientation of corresponding symmetry elements, referred to a hexagonal coordinate system (cf. Table 2.1.2.1)*

Symbol of symmetry operation and orientation of symmetry element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$	Symbol of symmetry operation and orientation of symmetry element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$	Symbol of symmetry operation and orientation of symmetry element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$
1	x, y, z	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	3^{+} $0, 0, z$ [001]	$\bar{y}, x-y, z$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	3^{-} $0, 0, z$ [001]	$y-x, \bar{x}, z$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
2 $0, 0, z$ [001]	$\bar{x}, \bar{y}, z$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	6^{+} $0, 0, z$ [001]	$x-y, x, z$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	6^{-} $0, 0, z$ [001]	$y, y-x, z$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
2 $x, x, 0$ [110]	$y, x, \bar{z}$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $x, 0, 0$ [100]	$x-y, \bar{y}, \bar{z}$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $0, y, 0$ [010]	$\bar{x}, y-x, \bar{z}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
2 $x, \bar{x}, 0$ [1$\bar{1}$0]	$\bar{y}, \bar{x}, \bar{z}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $x, 2x, 0$ [120]	$y-x, y, \bar{z}$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $2x, x, 0$ [210]	$x, x-y, \bar{z}$	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
$\bar{1}$ $0, 0, 0$	$\bar{x}, \bar{y}, \bar{z}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{3}^{+}$ $0, 0, z$ [001]	$y, y-x, \bar{z}$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{3}^{-}$ $0, 0, z$ [001]	$x-y, x, \bar{z}$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
m $x, y, 0$ [001]	$x, y, \bar{z}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{6}^{+}$ $0, 0, z$ [001]	$y-x, \bar{x}, \bar{z}$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{6}^{-}$ $0, 0, z$ [001]	$\bar{y}, x-y, \bar{z}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
m $x, \bar{x}, z$ [110]	$\bar{y}, \bar{x}, z$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $x, 2x, z$ [100]	$y-x, y, z$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $2x, x, z$ [010]	$x, x-y, z$	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$
m x, x, z [1$\bar{1}$0]	y, x, z	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $x, 0, z$ [120]	$x-y, \bar{y}, z$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $0, y, z$ [210]	$\bar{x}, y-x, z$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

references

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12.1. Point-group symbols

BY H. BURZLAFF AND H. ZIMMERMANN

12.1.1. Introduction

For symbolizing space groups, or more correctly types of space groups, different notations have been proposed. The following three are the main ones in use today:

(i) the notation of Schoenflies (1891, 1923);

(ii) the notation of Shubnikov (Shubnikov & Koptsik, 1972), which is frequently used in the Russian literature;

(iii) the international notation of Hermann (1928) and Mauguin (1931). It was used in *IT* (1935) and was somewhat modified in *IT* (1952).

In all three notations, the space-group symbol is a modification of a point-group symbol.

Symmetry elements occur in lattices, and thus in crystals, only in distinct directions. Point-group symbols make use of these discrete directions and their mutual relations.

12.1.2. Schoenflies symbols

Most Schoenflies symbols (Table 12.1.4.2, column 1) consist of the basic parts C_n, D_n,* T or O, designating cyclic, dihedral, tetrahedral and octahedral rotation groups, respectively, with $n = 1, 2, 3, 4, 6$. The remaining point groups are described by additional symbols for mirror planes, if present. The subscripts h and v indicate mirror planes perpendicular and parallel to a main axis taken as vertical. For T, the three mutually perpendicular twofold axes and, for O, the three fourfold axes are considered to be the main axes. The index d is used for mirror planes that bisect the angle between two consecutive equivalent rotation axes, *i.e.* which are diagonal with respect to these axes. For the rotoinversion axes $\bar{1}, \bar{2} \equiv m, \bar{3}$ and $\bar{4}$, which do not fit into the general Schoenflies concept of symbols, other symbols C_i, C_s, C_{3i} and S_4 are in use. The rotoinversion axis $\bar{6}$ is equivalent to $3/m$ and thus designated as C_{3h}.

12.1.3. Shubnikov symbols

The Shubnikov symbol is constructed from a minimal set of generators of a point group (for exceptions, see below). Thus, strictly speaking, the symbols represent types of symmetry operations. Since each symmetry operation is related to a symmetry element, the symbols also have a geometrical meaning. The Shubnikov symbols for symmetry operations differ slightly from the international symbols (Table 12.1.3.1). Note that Shubnikov, like Schoenflies, regards symmetry operations of the second kind as rotoreflections rather than as rotoinversions.

If more than one generator is required, it is not sufficient to give only the types of the symmetry elements; their mutual orientations must be symbolized too. In the Shubnikov symbol, a colon (:), a dot (·) or a slash (/) is used to designate perpendicular, parallel or oblique arrangement of the symmetry elements. For a reflection, the orientation of the actual mirror plane is considered, not that of its normal. The exception mentioned above is the use of $3 : m$ instead of $\tilde{3}$ in the description of point groups.

12.1.4. Hermann–Mauguin symbols

12.1.4.1. *Symmetry directions*

The Hermann–Mauguin symbols for finite point groups make use of the fact that the symmetry elements, *i.e.* proper and improper rotation axes, have definite mutual orientations. If for each point group the symmetry directions are grouped into classes of symmetrical equivalence, at most three classes are obtained. These classes were called *Blickrichtungssysteme* (Heesch, 1929). If a class contains more than one direction, one of them is chosen as representative.

The Hermann–Mauguin symbols for the crystallographic point groups refer to the symmetry directions of the lattice point groups (holohedries, *cf.* Part 9) and use other representatives than chosen by Heesch [*IT* (1935), p. 13]. For instance, in the hexagonal case, the primary set of lattice symmetry directions consists of $\{[001], [00\bar{1}]\}$, representative is [001]; the secondary set of lattice symmetry directions consists of [100], [010], $[\bar{1}\bar{1}0]$ and their counter-directions, representative is [100]; the tertiary set of lattice symmetry directions consists of $[1\bar{1}0], [120], [\bar{2}\bar{1}0]$ and their counter-directions, representative is $[1\bar{1}0]$. The representatives for the sets of lattice symmetry directions for all lattice point groups are listed in Table 12.1.4.1. The directions are related to the conventional crystallographic basis of each lattice point group (*cf.* Part 9).

The relation between the concept of lattice symmetry directions and group theory is evident. The maximal cyclic subgroups of the maximal rotation group contained in a lattice point group can be divided into, at most, three sets of conjugate subgroups. Each of these sets corresponds to one set of lattice symmetry directions.

12.1.4.2. *Full Hermann–Mauguin symbols*

After the classification of the directions of rotation axes, the description of the seven maximal rotation subgroups of the lattice point groups is rather simple. For each representative direction, the rotational symmetry element is symbolized by an integer n for an n-fold axis, resulting in the symbols of the maximal rotation subgroups 1, 2, 222, 32, 422, 622, 432. The symbol 1 is used for the triclinic case. The complete lattice point group is constructed by multiplying the rotation group by the inversion $\bar{1}$. For the even-fold axes, 2, 4 and 6, this multiplication results in a mirror plane perpendicular to the rotation axis yielding the symbols $2n/m$ $(n = 1, 2, 3)$. For the odd-fold axes 1 and 3, this product leads to the rotoinversion axes $\bar{1}$ and $\bar{3}$. Thus, for each representative of a set of lattice symmetry directions, the symmetry forms a point

Table 12.1.3.1. *International (Hermann–Mauguin) and Shubnikov symbols for symmetry elements*

The first power of a symmetry operation is often designated by the symmetry-element symbol without exponent 1, the other powers of the operation carry the appropriate exponent.

	Symmetry elements	
	of the first kind	of the second kind
Hermann–Mauguin	1 2 3 4 6	$\bar{1}$ m $\bar{3}$ $\bar{4}$ $\bar{6}$
Shubnikov*	1 2 3 4 6	$\tilde{2}$ m $\tilde{6}$ $\tilde{4}$ $\tilde{3}$

* According to a private communication from J. D. H. Donnay, the symbols for elements of the second kind were proposed by M. J. Buerger. Koptsik (1966) used them for the Shubnikov method.

* Instead of D_2, in older papers V (from *Vierergruppe*) is used.

Table 12.1.4.1. *Representatives for the sets of lattice symmetry directions in the various crystal families*

	Crystal family	Anorthic (triclinic)	Monoclinic	Orthorhombic	Tetragonal	Hexagonal		Cubic
Lattice point group	Schoenflies	C_i	C_{2h}	D_{2h}	D_{4h}	D_{6h}	D_{3d}	O_h
	Hermann–Mauguin	$\bar{1}$	$\frac{2}{m}$	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	$\bar{3}\frac{2}{m}$ *	$\frac{4}{m}\bar{3}\frac{2}{m}$
Set of lattice symmetry directions	Primary	–	[010] **b** unique [001] **c** unique	[100]	[001]	[001]	[001]	[001]
	Secondary	–	–	[010]	[100]	[100]	[100]	[111]
	Tertiary	–	–	[001]	[1$\bar{1}$0]	[1$\bar{1}$0]	–	[1$\bar{1}$0] [110] †

* In this table, the directions refer to the hexagonal description. The use of the primitive rhombohedral cell brings out the relations between cubic and rhombohedral groups: the primary set is represented by [111] and the secondary by [1$\bar{1}$0].
† Only for $\bar{4}3m$ and 432 [for reasons see text].

Table 12.1.4.2. *Point-group symbols*

Schoenflies	Shubnikov	*International Tables*, short symbol	*International Tables*, full symbol
C_1	1	1	1
C_i	$\tilde{2}$	$\bar{1}$	$\bar{1}$
C_2	2	2	2
C_s	m	m	m
C_{2h}	$2:m$	$2/m$	$2/m$
D_2	$2:2$	222	222
C_{2v}	$2\cdot m$	$mm2$	$mm2$
D_{2h}	$m\cdot 2:m$	mmm	$2/m\ 2/m\ 2/m$
C_4	4	4	4
S_4	$\tilde{4}$	$\bar{4}$	$\bar{4}$
C_{4h}	$4:m$	$4/m$	$4/m$
D_4	$4:2$	422	422
C_{4v}	$4\cdot m$	$4mm$	$4mm$
D_{2d}	$\tilde{4}:2$	$\bar{4}2m$ or $\bar{4}m2$	$\bar{4}2m$ or $\bar{4}m2$
D_{4h}	$m\cdot 4:m$	$4/mmm$	$4/m\ 2/m\ 2/m$
C_3	3	3	3
C_{3i}	$\tilde{6}$	$\bar{3}$	$\bar{3}$
D_3	$3:2$	32 or 321 or 312	32 or 321 or 312
C_{3v}	$3\cdot m$	$3m$ or $3m1$ or $31m$	$3m$ or $3m1$ or $31m$
D_{3d}	$\tilde{6}\cdot m$	$\bar{3}m$ or $\bar{3}m1$ or $\bar{3}1m$	$\bar{3}\ 2/m$ or $\bar{3}\ 2/m1$ or $\bar{3}12/m$
C_6	6	6	6
C_{3h}	$3:m$	$\bar{6}$	$\bar{6}$
C_{6h}	$6:m$	$6/m$	$6/m$
D_6	$6:2$	622	622
C_{6v}	$6\cdot m$	$6mm$	$6mm$
D_{3h}	$m\cdot 3:m$	$\bar{6}m2$ or $\bar{6}2m$	$\bar{6}m2$ or $\bar{6}2m$
D_{6h}	$m\cdot 6:m$	$6/mmm$	$6/m\ 2/m\ 2/m$
T	$3/2$	23	23
T_h	$\tilde{6}/2$	$m\bar{3}$	$2/m\bar{3}$
O	$3/4$	432	432
T_d	$3/\tilde{4}$	$\bar{4}3m$	$\bar{4}3m$
O_h	$\tilde{6}/4$	$m\bar{3}m$	$4/m\ \bar{3}\ 2/m$

group that can be generated by one, or at most two, symmetry operations. The resulting symbols are called *full Hermann–Mauguin (or international) symbols*. For the lattice point groups they are shown in Table 12.1.4.1.

For the description of a point group of a crystal, we use its lattice symmetry directions. For the representative of each set of lattice symmetry directions, the remaining subgroup is symbolized; if only the primary symmetry direction contains symmetry higher than 1, the symbols '1' for the secondary and tertiary set (if present) can be omitted. For the cubic point groups T and T_h, the representative of the tertiary set would be '1', which is omitted. For the rotoinversion groups $\bar{1}$ and $\bar{3}$, the remaining subgroups can only be 1 and 3. If the supergroup is $2n/\underline{m}$, five different types of subgroups can be derived: n/m, $2n$, $\overline{2n}$, n and m. In the cubic system, for instance, $4/m$, $2/m$, $\bar{4}$, 4 or 2 may occur in the primary set. In this case, the symbol m can only occur in the combinations $2/m$ or $4/m$ as can be seen from Table 12.1.4.2.

12.1.4.3. *Short symbols and generators*

If the symbols are not only used for the identification of a group but also for its construction, the symbol must contain a list of generating operations and additional relations, if necessary. Following this aspect, the Hermann–Mauguin symbols can be shortened. The choice of generators is not unique; two proposals were presented by Mauguin (1931). In the first proposal, in almost all cases the generators are the same as those of the Shubnikov symbols. In the second proposal, which, apart from some exceptions (see Chapter 12.4), is used for the international symbols, Mauguin selected a set of generators and thus a list of short symbols in which reflections have priority (Table 12.1.4.2, column 3). This selection makes the transition from the short point-group symbols to the space-group symbols fairly simple. These short symbols contain two kinds of notation components:

(i) components that represent the type of the generating operation, which are called *generators*;

(ii) components that are not used as generators but that serve to fix the directions of other symmetry elements (Hermann, 1931), and which are called *indicators*.

The generating matrices are uniquely defined by (i) and (ii), if it is assumed that they describe motions with counterclockwise rotational sense about the representative direction looked at end on by the observer. The symbols 2, 4, $\bar{4}$, 6 and $\bar{6}$ referring to direction [001] are indicators when the point-group symbol uses three sets of lattice symmetry directions. For instance, in 4*mm* the indicator 4 fixes the directions of the mirrors normal to [100] and [1$\bar{1}$0].

Note

The generation of (*a*) point group 432 by a rotation 3 around [111] and a rotation 2 and (*b*) point group $\bar{4}3m$ by 3 around [111] and a reflection *m* is only possible if the representative direction of the tertiary set is changed from [1$\bar{1}$0] to [$\bar{1}$10]; otherwise only the subgroup 32 or 3*m* of 432 or $\bar{4}3m$ will be generated.

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12.2. Space-group symbols

BY H. BURZLAFF AND H. ZIMMERMANN

12.2.1. Introduction

Each space group is related to a crystallographic point group. Space-group symbols, therefore, can be obtained by a modification of point-group symbols. The simplest modification which merely gives an enumeration of the space-group types (*cf.* Section 8.2.2) has been used by Schoenflies. The Shubnikov and Hermann–Mauguin symbols, however, reveal the glide or screw components of the symmetry operations and are designed in such a way that the nature of the symmetry elements and their relative locations can be deduced from the symbol.

12.2.2. Schoenflies symbols

Space groups related to one point group are distinguished by adding a numerical superscript to the point-group symbol. Thus, the space groups related to the point group C_2 are called C_2^1, C_2^2, C_2^3.

12.2.3. The role of translation parts in the Shubnikov and Hermann–Mauguin symbols

A crystallographic symmetry operation $\mathbf{W}$ (*cf.* Part 11) is described by a pair of matrices

$$(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{I}, \boldsymbol{w})(\boldsymbol{W}, \boldsymbol{o}).$$

$\boldsymbol{W}$ is called the *rotation part*, $\boldsymbol{w}$ describes the *translation part* and determines the translation vector $\mathbf{w}$ of the operation. $\boldsymbol{w}$ can be decomposed into a *glide/screw part* $\boldsymbol{w}_g$ and a *location part* $\boldsymbol{w}_l : \boldsymbol{w} = \boldsymbol{w}_g + \boldsymbol{w}_l$; here, $\boldsymbol{w}_l$ determines the location of the corresponding symmetry element with respect to the origin. The glide/screw part $\boldsymbol{w}_g$ may be derived by projecting $\boldsymbol{w}$ on the space invariant under $\boldsymbol{W}$, *i.e.* for rotations and reflections $\boldsymbol{w}$ is projected on the corresponding rotation axis or mirror plane. With matrix notation, $\boldsymbol{w}_g$ is determined by $(\boldsymbol{W}, \boldsymbol{w})^k = (\boldsymbol{I}, \boldsymbol{t})$ and $\boldsymbol{w}_g = (1/k)\boldsymbol{t}$, where k is the order of the operation $\boldsymbol{W}$. If $\boldsymbol{w}_g$ is not a symmetry translation, the space group contains sets of screw axes or glide planes instead of the rotation axis or the mirror plane of the related point group. A screw rotation is symbolized by n_m, where $\boldsymbol{w}_g = (m/n)\boldsymbol{t}$, with $\boldsymbol{t}$ the shortest lattice vector in the direction of the rotation axis. The Shubnikov notation and the international notation use the same symbols for screw rotations. The symbols for glide reflections in both notations are listed in Table 12.2.3.1.

If the point-group symbol contains only one generator, the related space group is described completely by the Bravais lattice and a symbol corresponding to that of the point group in which rotations and reflections are replaced by screw rotations or glide reflections, if necessary. If, however, two or more operations generate the point group, it is necessary to have information on the mutual orientations and locations of the corresponding space-group symmetry elements, *i.e.* information on the location components $\boldsymbol{w}$. This is described in the following sections.

12.2.4. Shubnikov symbols

For the description of the mutual orientation of symmetry elements, the same symbols as for point groups are applied. In space groups, however, the symmetry elements need not intersect. In this case, the orientational symbols · (dot), : (colon), / (slash) are modified to $\odot$, $\circ\!\!\!\!:$, //. The space-group symbol starts with a description of the lattice defined by the basis **a**, **b**, **c**. For centred cells, the vectors to the centring points are given first. The same letters are used for basis vectors related by symmetry. The relative orientations of the vectors are denoted by the orientational symbols introduced above. The description of the lattice given in parentheses is followed by symbols of the generating elements of the related point group. If necessary, the symbols of the symmetry operations are modified to indicate their glide/screw parts. The first generator is separated from the lattice description by an orientation symbol. If this generator represents a mirror or glide plane, the dot connects the plane with the last two vectors whereas the colon refers only to the last vector. If the generator represents a rotation or a rotoreflection, the colon orients the related axis perpendicular to the plane given by the last two vectors whereas the dot refers only to the last vector. Two generators are separated by the symbols mentioned above to denote their relative orientations and sites. To make this description unique for space groups related to point group $O_h \equiv \tilde{6}/4$ with Bravais lattices cP and cF, it is necessary to use three generators instead of two: $4/\tilde{6} \cdot m$. For the sake of unification, this kind of description is extended to the remaining two space groups having Bravais lattice cI.

Example: *Shubnikov symbol for the space group with Schoenflies symbol* D_{2h}^{26} (72).

The Bravais lattice is oI (orthorhombic, body-centred). Therefore, the symbol for the lattice basis is

$$\left(\frac{a+b+c}{2} \Big/ c : (a : b)\right),$$

indicating that there is a centring vector $1/2(\mathbf{a}+\mathbf{b}+\mathbf{c})$ relative to the conventional orthorhombic cell. This vector is oblique with respect to the basis vector **c**, which is orthogonal to the perpendicular pair **a** and **b**. The basis vectors have independent lengths and are thus indicated by different letters a, b and c in arbitrary sequence.

To complete the symbol of the space group, we consider the point group D_{2h}. Its Shubnikov symbol is $m : 2 \cdot m$. Parallel to the (**a**, **b**) plane, there is a glide plane $\widetilde{ab}$ and a mirror plane m. The latter is chosen as generator. From the screw axis 2_1 and the rotation axis 2, both parallel to **c**, the latter is chosen as generator. The third generator can be a glide plane c perpendicular to **b**. Thus the Shubnikov symbol of D_{2h}^{26} is

$$\left(\frac{a+b+c}{2} \Big/ c : (a : b)\right) \cdot m : 2 \cdot \tilde{c}.$$

Table 12.2.3.1. *Symbols of glide planes in the Shubnikov and Hermann–Mauguin space-group symbols*

Glide plane perpendicular to	Glide vector	Shubnikov symbol	Hermann–Mauguin symbol
b or **c**	$\frac{1}{2}\mathbf{a}$	$\tilde{a}$	a
a or **c**	$\frac{1}{2}\mathbf{b}$	$\tilde{b}$	b
a or **b** or **a** − **b**	$\frac{1}{2}\mathbf{c}$	$\tilde{c}$	c
c	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$	$\widetilde{ab}$	n
a	$\frac{1}{2}(\mathbf{b}+\mathbf{c})$	$\widetilde{bc}$	n
b	$\frac{1}{2}(\mathbf{c}+\mathbf{a})$	$\widetilde{ac}$	n
a − **b**	$\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\widetilde{abc}$	n
c	$\frac{1}{4}(\mathbf{a}+\mathbf{b})$	$\frac{1}{2}\widetilde{ab}$	d
a	$\frac{1}{4}(\mathbf{b}+\mathbf{c})$	$\frac{1}{2}\widetilde{bc}$	d
b	$\frac{1}{4}(\mathbf{c}+\mathbf{a})$	$\frac{1}{2}\widetilde{ac}$	d
a − **b**	$\frac{1}{4}(\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\frac{1}{2}\widetilde{abc}$	d
a + **b**	$\frac{1}{4}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$		d

The list of all Shubnikov symbols is given in column 3 of Table 12.3.4.1.

12.2.5. International short symbols

The international symbol of a space group consists of two parts, just like the Shubnikov symbol. The first part is a capital letter that describes the type of centring of the conventional cell. It is followed by a modified point-group symbol that refers to the lattice symmetry directions. Centring type and point-group symbol determine the Bravais type of the translation group (*cf.* Chapter 9.1) and thus the point group of the lattice and the appropriate lattice symmetry directions. To derive the short international symbol of a given space group, the short symbol of the related point group must be modified in such a way that not only the rotation parts of the generating operations but also their translation parts can be constructed. This can be done by the following procedure:

(i) The glide/screw parts of generators and indicators are symbolized by applying the symbols for glide planes in Table 12.2.3.1 and the appropriate rules for screw rotations.

(ii) The generators are chosen in such a way that the related symmetry elements do intersect as far as possible. Exceptions may occur for space groups related to the pure rotation point groups 222, 422, 622, 23 and 432. In these cases, the axes of the generators may or may not intersect.

(iii) Subgroups of lattice point groups may have lattice symmetry directions with which no symmetry elements are associated. Such symmetry directions are symbolized by '1'. This symbol can only be omitted if no ambiguity arises, *e.g.* $P4/m11$ is reduced to $P4/m$. $P31m$ and $P3m1$, however, cannot be reduced. The use of the symbol '1' is discussed by Buerger (1967) and Donnay (1969, 1977).

Example

Again consider space group D_{2h}^{26} (72). The space group contains glide planes c and b perpendicular to the primary set, c and a normal to the secondary set of symmetry directions and m and n perpendicular to the tertiary set. To determine the short symbol, one generator must be chosen from each pair. The standardization rules (see following chapter) lead to the symbol *Ibam*.

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12.3. Properties of the international symbols

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12.3.1. Derivation of the space group from the short symbol

Because the short international symbol contains a set of generators, it is possible to deduce the space group from it. With the same distinction between generators and indicators as for point groups, the modified point-group symbol directly gives the rotation parts $\boldsymbol{W}$ of the generating operations $(\boldsymbol{W}, \boldsymbol{w})$.

The modified symbols of the generators determine the glide/screw parts $\boldsymbol{w}_g$ of $\boldsymbol{w}$. To find the location parts $\boldsymbol{w}_l$ of $\boldsymbol{w}$, it is necessary to inspect the product relations of the group. The deduction of the set of complete generating operations can be summarized in the following rules:

(i) The integral translations are included in the set of generators. If the unit cell has centring points, the centring operations are generators.

(ii) The location parts of the generators can be set to zero except for the two cases noted under (iii) and (iv).

(iii) For non-cubic rotation groups with indicators in the symbol, the location part of the first generator can be set to zero. The location part of the second generator is $\boldsymbol{w}_l = (0, 0, -m/n)$; the intersection parameter $-m/n$ is derived from the indicator n_m in the [001] direction [*cf.* example (3) below].

(iv) For cubic rotation groups, the location part of the threefold rotation can be set to zero. For space groups related to the point group 23, the location part of the twofold rotation is $\boldsymbol{w}_l = (-m/n, 0, 0)$ derived from the symbol n_m of the twofold operation itself. For space groups related to the point group 432, the location part of the twofold generating rotation is $w_l = (-m/n, m/n, m/n)$ derived from the indicator n_m in the [001] direction [*cf.* examples (4) and (5) below].

The origin that is selected by these rules is called 'origin of the symbol' (Burzlaff & Zimmermann, 1980). It is evident that the reference to the origin of the symbol allows a very short and unique notation of all desirable origins by appending a matrix $\boldsymbol{q} = \langle q^1, q^2, q^3\rangle$ to the short space-group symbol. The shift of origin can be performed easily, for only the translation parts have to be changed. The new matrix of the translation part can be obtained by

$$\boldsymbol{w}' = \boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I}) \cdot \boldsymbol{q}.$$

Applications can be found in Burzlaff & Zimmermann (2002).

Examples: *Deduction of the generating operations from the short symbol*

Some examples for the use of these rules are now described in detail. It is convenient to describe the symmetry operation ($\boldsymbol{W}$, $\boldsymbol{w}$) by a pair of row matrices. The first one consists of the coordinates of a point in general position after the application of $\boldsymbol{W}$ on $\begin{pmatrix} x \\ y \\ z \end{pmatrix}$; the second represents the translation part $\begin{pmatrix} w^1 \\ w^2 \\ w^3 \end{pmatrix}$. In the following, both are written as a row. The sum of both matrices is tabulated as *general position* in the space-group tables (in some cases a shift of origin is necessary). If preference is given to full matrix notation, Table 11.2.2.1 may be used. The following examples contain, besides the description of the symmetry operations, references to the numbering of the general positions in the space-group tables of this volume; *cf.* Sections 2.2.9 and 2.2.11. Centring translations are written after the numbers, if necessary.

(1) $Pccm = D_{2h}^3$ (49)

Besides the integral translations, the generators, as given in the symbol, are according to rule (ii):

$$\begin{array}{lll} \text{glide reflection} & c_{[100]} & : (\bar{x}yz, 00\tfrac{1}{2}) \quad (8) \\ \text{glide reflection} & c_{[010]} & : (x\bar{y}z, 00\tfrac{1}{2}) \quad (7) \\ \text{reflection} & m_{[001]} & : (xy\bar{z}, 000) \quad (6). \end{array}$$

No shift of origin is necessary. The extended symbol is $Pccm\langle 000\rangle$.

(2) $Ibam = D_{2h}^{26}$ (72)

According to rule (i), the I centring is an additional generating translation. Thus, the generators are:

$$\begin{array}{lll} I \text{ centring} & : (xyz, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}) & (1) + (\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}) \\ \text{glide reflection } b_{[100]} & : (\bar{x}yz, 0\tfrac{1}{2}0) & (8) \\ \text{glide reflection } a_{[010]} & : (x\bar{y}z, \tfrac{1}{2}00) & (7) \\ \text{reflection} \quad m_{[001]} & : (xy\bar{z}, 000) & (6). \end{array}$$

To obtain the tabulated general position, a shift of origin by $(-\tfrac{1}{4}, -\tfrac{1}{4}, 0)$ is necessary, the extended symbol is $Ibam\langle -\tfrac{1}{4} -\tfrac{1}{4} 0\rangle$.

(3) $P4_12_12 = D_4^4$ (92)

Apart from the translations, the generating elements are:

$$\begin{array}{ll} \text{screw rotation } 2_1 \text{ in } [100] : (x\bar{y}\bar{z}, \tfrac{1}{2}00) & (6) \\ \text{rotation} \qquad 2 \;\text{ in } [1\bar{1}0] : (\bar{y}\bar{x}\bar{z}, 00\tfrac{1}{4}) & (8). \end{array}$$

According to rule (iii), the location part of the first generator, referring to the secondary set of symmetry direction, is equal to zero. For the second generator, the screw part is equal to zero. The location part is $(0, 0, -\tfrac{1}{4})$.

The extended symbol $P4_12_12\langle\tfrac{1}{4} - \tfrac{1}{4} - \tfrac{3}{8}\rangle$ gives the tabulated setting.

(4) $P2_13 = T^4$ (198)

According to rule (iv), the generators are

$$\begin{array}{ll} \text{rotation 3 in } [111] \qquad : (zxy, 000) & (5) \\ \text{screw rotation } 2_1 \text{ in } [001] : (\bar{x}\bar{y}z, \tfrac{1}{2}0\tfrac{1}{2}) & (2). \end{array}$$

Following rule (iv), the location part of the threefold axis must be set to zero. The screw part of the twofold axis in [001] is $(0, 0, \tfrac{1}{2})$, the location part $\boldsymbol{w}_l$ is $(-\tfrac{1}{2}, 0, 0) \equiv (\tfrac{1}{2}, 0, 0)$. No origin shift is necessary. The extended symbol is $P2_13\langle 000\rangle$.

(5) $P4_132 = O^7$ (213)

Besides the integral translations, the generators given by the symbol are:

$$\begin{array}{ll} \text{rotation 3 in } [111] : (zxy, 000) & (5) \\ \text{rotation 2 in } [110] : (yx\bar{z}, -\tfrac{1}{4}\tfrac{1}{4}\tfrac{1}{4}) & (13). \end{array}$$

The screw part of the twofold axis is zero. According to rule (iv), the location part $\boldsymbol{w}_l$ is $(-\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4})$. No origin shift is necessary. The extended symbol is $P4_132\langle 000\rangle$.

12.3.2. Derivation of the full symbol from the short symbol

If the geometrical point of view is again considered, it is possible to derive the full international symbol for a space group. This full symbol can be interpreted as consisting of symmetry elements. It can be generated from the short symbol with the aid of products

Table 12.3.4.1. *Standard space-group symbols*

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*				Comments*†
			1935 Edition		Present Edition		
			Short	Full	Short	Full	
1	C_1^1	$(a/b/c) \cdot 1$	$P1$	$P1$	$P1$	$P1$	
2	C_i^1	$(a/b/c) \cdot \tilde{2}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$(a/b/c) \cdot \bar{1}$ (Sh–K)
3	C_2^1	$(b:(c/a)):2$	$P2$	$P2$	$P2$	$P121$	
		$(c:(a/b)):2$				$P112$	
4	C_2^2	$(b:(c/a)):2_1$	$P2_1$	$P2_1$	$P2_1$	$P12_11$	
		$(c:(a/b)):2_1$				$P112_1$	
5	C_2^3	$\left(\frac{a+b}{2}\Big/ b:(c/a)\right):2$	$C2$	$C2$	$C2$	$C121$	$B2$, $B112$ (*IT*, 1952)
		$\left(\frac{b+c}{2}\Big/ c:(b/a)\right):2$				$A112$	$\left(\frac{a+c}{2}\Big/ c:(a/b)\right):2$ (Sh–K)
6	C_s^1	$(b:(c/a)) \cdot m$	Pm	Pm	Pm	$P1m1$	
		$(c:(a/b)) \cdot m$				$P11m$	
7	C_s^2	$(b:(c/a)) \cdot \tilde{c}$	Pc	Pc	Pc	$P1c1$	Pb, $P11b$ (*IT*, 1952)
		$(c:(b/a)) \cdot \tilde{a}$				$P11a$	$(c:(a/b)) \cdot \tilde{b}$ (Sh–K)
8	C_s^3	$\left(\frac{a+b}{2}\Big/ b:(c/a)\right) \cdot m$	Cm	Cm	Cm	$C1m1$	Bm, $B11m$ (*IT*, 1952)
		$\left(\frac{b+c}{2}\Big/ c:(b/a)\right) \cdot m$				$A11m$	$\left(\frac{a+c}{2}\Big/ c:(a/b)\right) \cdot m$ (Sh–K)
9	C_s^4	$\left(\frac{a+b}{2}\Big/ b:(c/a)\right) \cdot \tilde{c}$	Cc	Cc	Cc	$C1c1$	Bb, $B11b$ (*IT*, 1952)
		$\left(\frac{b+c}{2}\Big/ c:(b/a)\right) \cdot \tilde{a}$				$A11a$	$\left(\frac{a+c}{2}\Big/ c:(a/b)\right) \cdot \tilde{b}$ (Sh–K)
10	C_{2h}^1	$(b:(c/a)) \cdot m:2$	$P2/m$	$P2/m$	$P2/m$	$P1\ 2/m\ 1$	
		$(c:(a/b)) \cdot m:2$				$P11\ 2/m$	
11	C_{2h}^2	$(b:(c/a)) \cdot m:2_1$	$P2_1/m$	$P2_1/m$	$P2_1/m$	$P1\ 2_1/m\ 1$	
		$(c:(a/b)) \cdot m:2_1$				$P11\ 2_1/m$	
12	C_{2h}^3	$\left(\frac{a+b}{2}\Big/ b:(c/a)\right) \cdot m:2$	$C2/m$	$C2/m$	$C2/m$	$C1\ 2/m\ 1$	$B2/m$, $B11\ 2/m$ (*IT*, 1952)
		$\left(\frac{b+c}{2}\Big/ c:(b/a)\right) \cdot m:2$				$A11\ 2/m$	$\left(\frac{a+c}{2}\Big/ c:(a/b)\right) \cdot m:2$ (Sh–K)
13	C_{2h}^4	$(b:(c/a)) \cdot \tilde{c}:2$	$P2/c$	$P2/c$	$P2/c$	$P1\ 2/c\ 1$	$P2/b$, $P11\ 2/b$ (*IT*, 1952)
		$(c:(a/b)) \cdot \tilde{a}:2$				$P11\ 2/a$	$(c:(a/b)) \cdot \tilde{b}:2$ (Sh–K)
14	C_{2h}^5	$(b:(c/a)) \cdot \tilde{c}:2_1$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P1\ 2_1/c\ 1$	$P2_1/b, P11\ 2_1/b$ (*IT*, 1952)
		$(c:(a/b)) \cdot \tilde{a}:2_1$				$P11\ 2_1/a$	$(c:(a/b)) \cdot \tilde{b}:2_1$ (Sh–K)
15	C_{2h}^6	$\left(\frac{a+b}{2}\Big/ b:(c/a)\right) \cdot \tilde{c}:2$	$C2/c$	$C2/c$	$C2/c$	$C1\ 2/c\ 1$	$B2/b$, $B11\ 2/b$ (*IT*, 1952)
		$\left(\frac{b+c}{2}\Big/ c:(b/a)\right) \cdot \tilde{a}:2$				$A11\ 2/a$	$\left(\frac{a+c}{2}\Big/ c:(a/b)\right) \cdot \tilde{b}:2$ (Sh–K)
16	D_2^1	$(c:(a:b)):2:2$	$P222$	$P222$	$P222$	$P222$	
17	D_2^2	$(c:(a:b)):2_1:2$	$P222_1$	$P222_1$	$P222_1$	$P222_1$	
18	D_2^3	$(c:(a:b)):2 \odot 2_1$	$P2_12_12$	$P2_12_12$	$P2_12_12$	$P2_12_12$	
19	D_2^4	$(c:(a:b)):2_1 \odot 2_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	
20	D_2^5	$\left(\frac{a+b}{2}:c:(a:b)\right):2_1:2$	$C222_1$	$C222_1$	$C222_1$	$C222_1$	
21	D_2^6	$\left(\frac{a+b}{2}:c:(a:b)\right):2:2$	$C222$	$C222$	$C222$	$C222$	
22	D_2^7	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:c:(a:b)\right):2:2$	$F222$	$F222$	$F222$	$F222$	
23	D_2^8	$\left(\frac{a+b+c}{2}\Big/ c:(a:b)\right):2:2$	$I222$	$I222$	$I222$	$I222$	
24	D_2^9	$\left(\frac{a+b+c}{2}\Big/ c:(a:b)\right):2:2_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	

Table 12.3.4.1. *Standard space-group symbols* (*cont.*)

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*: 1935 Edition, Short	1935 Edition, Full	Present Edition, Short	Present Edition, Full	Comments*†
25	C_{2v}^1	$(c:(a:b)):m\cdot 2$	*Pmm*	*Pmm*2	*Pmm*2	*Pmm*2	
26	C_{2v}^2	$(c:(a:b)):\tilde{c}\cdot 2_1$	*Pmc*	$Pmc2_1$	$Pmc2_1$	$Pmc2_1$	
27	C_{2v}^3	$(c:(a:b)):\tilde{c}\cdot 2$	*Pcc*	*Pcc*2	*Pcc*2	*Pcc*2	
28	C_{2v}^4	$(c:(a:b)):\tilde{a}\cdot 2$	*Pma*	*Pma*2	*Pma*2	*Pma*2	
29	C_{2v}^5	$(c:(a:b)):\tilde{a}\cdot 2_1$	*Pca*	$Pca2_1$	$Pca2_1$	$Pca2_1$	
30	C_{2v}^6	$(c:(a:b)):\tilde{c}\odot 2$	*Pnc*	*Pnc*2	*Pnc*2	*Pnc*2	$(c:(a:b)):\widetilde{ac}\cdot 2$ (Sh–K)
31	C_{2v}^7	$(c:(a:b)):\widetilde{ac}\cdot 2_1$	*Pmn*	$Pmn2_1$	$Pmn2_1$	$Pmn2_1$	
32	C_{2v}^8	$(c:(a:b)):\tilde{a}\odot 2$	*Pba*	*Pba*2	*Pba*2	*Pba*2	
33	C_{2v}^9	$(c:(a:b)):\tilde{a}\odot 2_1$	*Pna*	$Pna2_1$	$Pna2_1$	$Pna2_1$	
34	C_{2v}^{10}	$(c:(a:b)):\widetilde{ac}\odot 2$	*Pnn*	*Pnn*2	*Pnn*2	*Pnn*2	
35	C_{2v}^{11}	$\left(\frac{a+b}{2}:c:(a:b)\right):m\cdot 2$	*Cmm*	*Cmm*2	*Cmm*2	*Cmm*2	
36	C_{2v}^{12}	$\left(\frac{a+b}{2}:c:(a:b)\right):\tilde{c}\cdot 2_1$	*Cmc*	$Cmc2_1$	$Cmc2_1$	$Cmc2_1$	
37	C_{2v}^{13}	$\left(\frac{a+b}{2}:c:(a:b)\right):\tilde{c}\cdot 2$	*Ccc*	*Ccc*2	*Ccc*2	*Ccc*2	
38	C_{2v}^{14}	$\left(\frac{b+c}{2}/c:(a:b)\right):m\cdot 2$	*Amm*	*Amm*2	*Amm*2	*Amm*2	
39	C_{2v}^{15}	$\left(\frac{b+c}{2}/c:(a:b)\right):m\cdot 2_1$	*Abm*	*Abm*2	*Aem*2	*Aem*2	$\left(\frac{b+c}{2}/c:(a:b)\right):\tilde{c}\cdot 2$ (Sh−K) Use former symbol *Abm*2 for generation
40	C_{2v}^{16}	$\left(\frac{b+c}{2}/c:(a:b)\right):\tilde{a}\cdot 2$	*Ama*	*Ama*2	*Ama*2	*Ama*2	
41	C_{2v}^{17}	$\left(\frac{b+c}{2}/c:(a:b)\right):\tilde{a}\cdot 2_1$	*Aba*	*Aba*2	*Aea*2	*Aea*2	$\left(\frac{b+c}{2}/c:(a:b)\right):\widetilde{ac}\cdot 2$ (Sh−K) Use former symbol *Aba*2 for generation
42	C_{2v}^{18}	$\left(\frac{a+c}{2}/\frac{b+c}{2}/\frac{a+b}{2}:c:(a:b)\right):m\cdot 2$	*Fmm*	*Fmm*2	*Fmm*2	*Fmm*2	
43	C_{2v}^{19}	$\left(\frac{a+c}{2}/\frac{b+c}{2}/\frac{a+b}{2}:\tilde{c}:(a:b)\right)$ $:\frac{1}{2}\widetilde{ac}\odot 2$	*Fdd*	*Fdd*2	*Fdd*2	*Fdd*2	
44	C_{2v}^{20}	$\left(\frac{a+b+c}{2}/c:(a:b)\right):m\cdot 2$	*Imm*	*Imm*2	*Imm*2	*Imm*2	
45	C_{2v}^{21}	$\left(\frac{a+b+c}{2}/c:(a:b)\right):\tilde{c}\cdot 2$	*Iba*	*Iba*2	*Iba*2	*Iba*2	$\left(\frac{a+b+c}{2}/c:(a:b)\right):\tilde{a}\cdot 2_1$ (Sh−K)
46	C_{2v}^{22}	$\left(\frac{a+b+c}{2}/c:(a:b)\right):\tilde{a}\cdot 2$	*Ima*	*Ima*2	*Ima*2	*Ima*2	

between symmetry operations. It is possible, however, to derive the glide/screw parts of the elements in the full symbol directly from the glide/screw parts of the short symbol.

The product of operations corresponding to non-parallel glide or mirror planes generates a rotation or screw axis parallel to the intersection line. The screw part of the rotation is equal to the sum of the projections of the glide components of the planes on the axis. The angle between the planes determines the rotation part of the axis. For 90°, we obtain a twofold, for 60° a threefold, for 45° a fourfold and for 30° a sixfold axis.

Example: $Pbcn = D_{2h}^{14}$ (60)

The product of *b* and *c* generates a screw axis 2_1 in the *z* direction because the sum of the glide components in the *z* direction is $\frac{1}{2}$. The product of *c* and *n* generates a screw axis 2_1 in the *x* direction and the product between *b* and *n* produces a rotation axis 2 in the *y* direction because the *y* components for *b* and *n* add up to $1 \equiv 0$ modulo integers.

Thus, the full symbol is

$$P\frac{2_1}{b}\frac{2}{c}\frac{2_1}{n}.$$

In most cases, the full symbol is identical with the short symbol; differences between full and short symbols can only occur for space groups corresponding to lattice point groups (holohedries) and to the point group $m\bar{3}$. In all these cases, the short symbol is extended to the full symbol by adding the symbol for the maximal purely rotational subgroup. A special procedure is in use for monoclinic space groups. To indicate the choice of coordinate axes, the full symbol is treated like an orthorhombic symbol, in which the directions without symmetry are indicated by ‘1’, *even though they do not correspond to lattice symmetry directions in the monoclinic case.*

Table 12.3.4.1. *Standard space-group symbols* (*cont*.)

			Symbols of *International Tables*				
			1935 Edition		Present Edition		
No.	Schoenflies symbol	Shubnikov symbol	Short	Full	Short	Full	Comments*†
47	D_{2h}^{1}	$(c:(a:b))\cdot m:2\cdot m$	*Pmmm*	$P2/m\ 2/m\ 2/m$	*Pmmm*	$P2/m\ 2/m\ 2/m$	
48	D_{2h}^{2}	$(c:(a:b))\cdot\widetilde{ab}:2\odot\widetilde{ac}$	*Pnnn*	$P2/n\ 2/n\ 2/n$	*Pnnn*	$P2/n\ 2/n\ 2/n$	
49	D_{2h}^{3}	$(c:(a:b))\cdot m:2\cdot\tilde{c}$	*Pccm*	$P2/c\ 2/c\ 2/m$	*Pccm*	$P2/c\ 2/c\ 2/m$	
50	D_{2h}^{4}	$(c:(a:b))\cdot\widetilde{ab}:2\odot\tilde{a}$	*Pban*	$P2/b\ 2/a\ 2/n$	*Pban*	$P2/b\ 2/a\ 2/n$	
51	D_{2h}^{5}	$(c:(a:b))\cdot\tilde{a}:2\cdot m$	*Pmma*	$P2_1/m\ 2/m\ 2/a$	*Pmma*	$P2_1/m\ 2/m\ 2/a$	
52	D_{2h}^{6}	$(c:(a:b))\cdot\tilde{a}:2\odot\widetilde{ac}$	*Pnna*	$P2/n\ 2_1/n\ 2/a$	*Pnna*	$P2/n\ 2_1/n\ 2/a$	
53	D_{2h}^{7}	$(c:(a:b))\cdot\tilde{a}:2_1\cdot\widetilde{ac}$	*Pmna*	$P2/m\ 2/n\ 2_1/a$	*Pmna*	$P2/m\ 2/n\ 2_1/a$	
54	D_{2h}^{8}	$(c:(a:b))\cdot\tilde{a}:2\cdot\tilde{c}$	*Pcca*	$P2_1/c\ 2/c\ 2/a$	*Pcca*	$P2_1/c\ 2/c\ 2/a$	
55	D_{2h}^{9}	$(c:(a:b))\cdot m:2\odot\tilde{a}$	*Pbam*	$P2_1/b\ 2_1/a\ 2/m$	*Pbam*	$P2_1/b\ 2_1/a\ 2/m$	
56	D_{2h}^{10}	$(c:(a:b))\cdot\widetilde{ab}:2\cdot\tilde{c}$	*Pccn*	$P2_1/c\ 2_1/c\ 2/n$	*Pccn*	$P2_1/c\ 2_1/c\ 2/n$	
57	D_{2h}^{11}	$(c:(a:b))\cdot m:2_1\odot\tilde{c}$	*Pbcm*	$P2/b\ 2_1/c\ 2_1/m$	*Pbcm*	$P2/b\ 2_1/c\ 2_1/m$	
58	D_{2h}^{12}	$(c:(a:b))\cdot m:2\odot\widetilde{ac}$	*Pnnm*	$P2_1/n\ 2_1/n\ 2/m$	*Pnnm*	$P2_1/n\ 2_1/n\ 2/m$	
59	D_{2h}^{13}	$(c:(a:b))\cdot\widetilde{ab}:2\cdot m$	*Pmmn*	$P2_1/m\ 2_1/m\ 2/n$	*Pmmn*	$P2_1/m\ 2_1/m\ 2/n$	
60	D_{2h}^{14}	$(c:(a:b))\cdot\widetilde{ab}:2_1\odot\tilde{c}$	*Pbcn*	$P2_1/b\ 2/c\ 2_1/n$	*Pbcn*	$P2_1/b\ 2/c\ 2_1/n$	
61	D_{2h}^{15}	$(c:(a:b))\cdot\tilde{a}:2_1\odot\tilde{c}$	*Pbca*	$P2_1/b\ 2_1/c\ 2_1/a$	*Pbca*	$P2_1/b\ 2_1/c\ 2_1/a$	
62	D_{2h}^{16}	$(c:(a:b))\cdot\tilde{a}:2_1\odot m$	*Pnma*	$P2_1/n\ 2_1/m\ 2_1/a$	*Pnma*	$P2_1/n\ 2_1/m\ 2_1/a$	
63	D_{2h}^{17}	$\left(\frac{a+b}{2}:c:(a:b)\right)\cdot m:2_1\cdot\tilde{c}$	*Cmcm*	$C2/m\ 2/c\ 2_1/m$	*Cmcm*	$C2/m\ 2/c\ 2_1/m$	
64	D_{2h}^{18}	$\left(\frac{a+b}{2}:c:(a:b)\right)\cdot\tilde{a}:2_1\cdot\tilde{c}$	*Cmca*	$C2/m\ 2/c\ 2_1/a$	*Cmce*	$C2/m\ 2/c\ 2_1/e$	Use former symbol *Cmca* for generation
65	D_{2h}^{19}	$\left(\frac{a+b}{2}:c:(a:b)\right)\cdot m:2\cdot m$	*Cmmm*	$C2/m\ 2/m\ 2/m$	*Cmmm*	$C2/m\ 2/m\ 2/m$	
66	D_{2h}^{20}	$\left(\frac{a+b}{2}:c:(a:b)\right)\cdot m:2\cdot\tilde{c}$	*Cccm*	$C2/c\ 2/c\ 2/m$	*Cccm*	$C2/c\ 2/c\ 2/m$	
67	D_{2h}^{21}	$\left(\frac{a+b}{2}:c:(a:b)\right)\cdot\tilde{a}:2\cdot m$	*Cmma*	$C2/m\ 2/m\ 2/a$	*Cmme*	$C2/m\ 2/m\ 2/e$	Use former symbol *Cmma* for generation
68	D_{2h}^{22}	$\left(\frac{a+b}{2}:c:(a:b)\right)\cdot\tilde{a}:2\cdot\tilde{c}$	*Ccca*	$C2/c\ 2/c\ 2/a$	*Ccce*	$C2/c\ 2/c\ 2/e$	Use former symbol *Ccca* for generation
69	D_{2h}^{23}	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:c:(a:b)\right)\cdot m:2\cdot m$	*Fmmm*	$F2/m\ 2/m\ 2/m$	*Fmmm*	$F2/m\ 2/m\ 2/m$	
70	D_{2h}^{24}	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:c:(a:b)\right)\cdot\frac{1}{2}\widetilde{ab}:2\odot\frac{1}{2}\widetilde{ac}$	*Fddd*	$F2/d\ 2/d\ 2/d$	*Fddd*	$F2/d\ 2/d\ 2/d$	
71	D_{2h}^{25}	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right)\cdot m:2\cdot m$	*Immm*	$I2/m\ 2/m\ 2/m$	*Immm*	$I2/m\ 2/m\ 2/m$	
72	D_{2h}^{26}	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right)\cdot m:2\cdot\tilde{c}$	*Ibam*	$I2/b\ 2/a\ 2/m$	*Ibam*	$I2/b\ 2/a\ 2/m$	
73	D_{2h}^{27}	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right)\cdot\tilde{a}:2\cdot\tilde{c}$	*Ibca*	$I2_1/b\ 2_1/c\ 2_1/a$	*Ibca*	$I2_1/b\ 2_1/c\ 2_1/a$	$I2/b\ 2/c\ 2/a$ (*IT*, 1952)
74	D_{2h}^{28}	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right)\cdot\tilde{a}:2\cdot m$	*Imma*	$I2_1/m\ 2_1/m\ 2_1/a$	*Imma*	$I2_1/m\ 2_1/m\ 2_1/a$	$I2/m\ 2/m\ 2/a$ (*IT*, 1952)
75	C_{4}^{1}	$(c:(a:a)):4$	$P4$	$P4$	$P4$	$P4$	
76	C_{4}^{2}	$(c:(a:a)):4_1$	$P4_1$	$P4_1$	$P4_1$	$P4_1$	
77	C_{4}^{3}	$(c:(a:a)):4_2$	$P4_2$	$P4_2$	$P4_2$	$P4_2$	
78	C_{4}^{4}	$(c:(a:a)):4_3$	$P4_3$	$P4_3$	$P4_3$	$P4_3$	
79	C_{4}^{5}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):4$	$I4$	$I4$	$I4$	$I4$	
80	C_{4}^{6}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):4_1$	$I4_1$	$I4_1$	$I4_1$	$I4_1$	

Table 12.3.4.1. *Standard space-group symbols* (*cont.*)

			Symbols of *International Tables*				
			1935 Edition		Present Edition		
No.	Schoenflies symbol	Shubnikov symbol	Short	Full	Short	Full	Comments*†
81	S_4^1	$(c:(a:a)):\tilde{4}$	$P\bar{4}$	$P\bar{4}$	$P\bar{4}$	$P\bar{4}$	
82	S_4^2	$\left(\frac{a+b+c}{2}\middle/ c:(a:a)\right):\tilde{4}$	$I\bar{4}$	$I\bar{4}$	$I\bar{4}$	$I\bar{4}$	
83	C_{4h}^1	$(c:(a:a))\cdot m:4$	$P4/m$	$P4/m$	$P4/m$	$P4/m$	
84	C_{4h}^2	$(c:(a:a))\cdot m:4_2$	$P4_2/m$	$P4_2/m$	$P4_2/m$	$P4_2/m$	
85	C_{4h}^3	$(c:(a:a))\cdot\widetilde{ab}:4$	$P4/n$	$P4/n$	$P4/n$	$P4/n$	
86	C_{4h}^4	$(c:(a:a))\cdot\widetilde{ab}:4_2$	$P4_2/n$	$P4_2/n$	$P4_2/n$	$P4_2/n$	
87	C_{4h}^5	$\left(\frac{a+b+c}{2}\middle/ c:(a:a)\right)\cdot m:4$	$I4/m$	$I4/m$	$I4/m$	$I4/m$	
88	C_{4h}^6	$\left(\frac{a+b+c}{2}\middle/ c:(a:a)\right)\cdot\tilde{a}:4_1$	$I4_1/a$	$I4_1/a$	$I4_1/a$	$I4_1/a$	
89	D_4^1	$(c:(a:a)):4:2$	$P42$	$P422$	$P422$	$P422$	
90	D_4^2	$(c:(a:a)):4\odot 2_1$	$P42_1$	$P42_12$	$P42_12$	$P42_12$	
91	D_4^3	$(c:(a:a)):4_1:2$	$P4_12$	$P4_122$	$P4_122$	$P4_122$	
92	D_4^4	$(c:(a:a)):4_1\odot 2_1$	$P4_12_1$	$P4_12_12$	$P4_12_12$	$P4_12_12$	
93	D_4^5	$(c:(a:a)):4_2:2$	$P4_22$	$P4_222$	$P4_222$	$P4_222$	
94	D_4^6	$(c:(a:a)):4_2\odot 2_1$	$P4_22_1$	$P4_22_12$	$P4_22_12$	$P4_22_12$	
95	D_4^7	$(c:(a:a)):4_3:2$	$P4_32$	$P4_322$	$P4_322$	$P4_322$	
96	D_4^8	$(c:(a:a)):4_3\odot 2_1$	$P4_32_1$	$P4_32_12$	$P4_32_12$	$P4_32_12$	
97	D_4^9	$\left(\frac{a+b+c}{2}\middle/ c:(a:a)\right):4:2$	$I42$	$I422$	$I422$	$I422$	
98	D_4^{10}	$\left(\frac{a+b+c}{2}\middle/ c:(a:a)\right):4_1:2$	$I4_12$	$I4_122$	$I4_122$	$I4_122$	
99	C_{4v}^1	$(c:(a:a)):4\cdot m$	$P4mm$	$P4mm$	$P4mm$	$P4mm$	
100	C_{4v}^2	$(c:(a:a)):4\odot\tilde{a}$	$P4bm$	$P4bm$	$P4bm$	$P4bm$	
101	C_{4v}^3	$(c:(a:a)):4_2\cdot\tilde{c}$	$P4cm$	$P4_2cm$	$P4_2cm$	$P4_2cm$	
102	C_{4v}^4	$(c:(a:a)):4_2\odot\widetilde{ac}$	$P4nm$	$P4_2nm$	$P4_2nm$	$P4_2nm$	
103	C_{4v}^5	$(c:(a:a)):4\cdot\tilde{c}$	$P4cc$	$P4cc$	$P4cc$	$P4cc$	
104	C_{4v}^6	$(c:(a:a)):4\odot\widetilde{ac}$	$P4nc$	$P4nc$	$P4nc$	$P4nc$	
105	C_{4v}^7	$(c:(a:a)):4_2\cdot m$	$P4mc$	$P4_2mc$	$P4_2mc$	$P4_2mc$	
106	C_{4v}^8	$(c:(a:a)):4_2\odot\tilde{a}$	$P4bc$	$P4_2bc$	$P4_2bc$	$P4_2bc$	
107	C_{4v}^9	$\left(\frac{a+b+c}{2}\middle/ c:(a:a)\right):4\cdot m$	$I4mm$	$I4mm$	$I4mm$	$I4mm$	
108	C_{4v}^{10}	$\left(\frac{a+b+c}{2}\middle/ c:(a:a)\right):4\cdot\tilde{c}$	$I4cm$	$I4cm$	$I4cm$	$I4cm$	
109	C_{4v}^{11}	$\left(\frac{a+b+c}{2}\middle/ c:(a:a)\right):4_1\odot m$	$I4md$	$I4_1md$	$I4_1md$	$I4_1md$	
110	C_{4v}^{12}	$\left(\frac{a+b+c}{2}\middle/ c:(a:a)\right):4_1\odot\tilde{c}$	$I4cd$	$I4_1cd$	$I4_1cd$	$I4_1cd$	$\left(\frac{a+b+c}{2}\middle/ c:a:a\right):4_1\cdot\tilde{a}$ (Sh–K)
111	D_{2d}^1	$(c:(a:a)):\tilde{4}:2$	$P\bar{4}2m$	$P\bar{4}2m$	$P\bar{4}2m$	$P\bar{4}2m$	
112	D_{2d}^2	$(c:(a:a)):\tilde{4}\odot 2$	$P\bar{4}2c$	$P\bar{4}2c$	$P\bar{4}2c$	$P\bar{4}2c$	
113	D_{2d}^3	$(c:(a:a)):\tilde{4}\cdot\widetilde{ab}$	$P\bar{4}2_1m$	$P\bar{4}2_1m$	$P\bar{4}2_1m$	$P\bar{4}2_1m$	
114	D_{2d}^4	$(c:(a:a)):\tilde{4}\cdot\widetilde{abc}$	$P\bar{4}2_1c$	$P\bar{4}2_1c$	$P\bar{4}2_1c$	$P\bar{4}2_1c$	
115	D_{2d}^5	$(c:(a:a)):\tilde{4}\cdot m$	$C\bar{4}2m$	$C\bar{4}2m$	$P\bar{4}m2$	$P\bar{4}m2$	
116	D_{2d}^6	$(c:(a:a)):\tilde{4}\cdot\tilde{c}$	$C\bar{4}2c$	$C\bar{4}2c$	$P\bar{4}c2$	$P\bar{4}c2$	
117	D_{2d}^7	$(c:(a:a)):\tilde{4}\odot\tilde{a}$	$C\bar{4}2b$	$C\bar{4}2b$	$P\bar{4}b2$	$P\bar{4}b2$	
118	D_{2d}^8	$(c:(a:a)):\tilde{4}\cdot\widetilde{ac}$	$C\bar{4}2n$	$C\bar{4}2n$	$P\bar{4}n2$	$P\bar{4}n2$	
119	D_{2d}^9	$\left(\frac{a+b+c}{2}\middle/ c:(a:a)\right):\tilde{4}\cdot m$	$F\bar{4}2m$	$F\bar{4}2m$	$I\bar{4}m2$	$I\bar{4}m2$	
120	D_{2d}^{10}	$\left(\frac{a+b+c}{2}\middle/ c:(a:a)\right):\tilde{4}\cdot\tilde{c}$	$F\bar{4}2c$	$F\bar{4}2c$	$I\bar{4}c2$	$I\bar{4}c2$	

Table 12.3.4.1. *Standard space-group symbols* (*cont.*)

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*: 1935 Edition, Short	1935 Edition, Full	Present Edition, Short	Present Edition, Full	Comments*†
121	D_{2d}^{11}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):\tilde{4}:2$	$I\bar{4}2m$	$I\bar{4}2m$	$I\bar{4}2m$	$I\bar{4}2m$	
122	D_{2d}^{12}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):\tilde{4}\odot\frac{1}{2}\widetilde{abc}$	$I\bar{4}2d$	$I\bar{4}2d$	$I\bar{4}2d$	$I\bar{4}2d$	
123	D_{4h}^{1}	$(c:(a:a))\cdot m:4\cdot m$	$P4/mmm$	$P4/m\ 2/m\ 2/m$	$P4/mmm$	$P4/m\ 2/m\ 2/m$	
124	D_{4h}^{2}	$(c:(a:a))\cdot m:4\cdot\tilde{c}$	$P4/mcc$	$P4/m\ 2/c\ 2/c$	$P4/mcc$	$P4/m\ 2/c\ 2/c$	
125	D_{4h}^{3}	$(c:(a:a))\cdot\widetilde{ab}:4\odot\tilde{a}$	$P4/nbm$	$P4/n\ 2/b\ 2/m$	$P4/nbm$	$P4/n\ 2/b\ 2/m$	$(c:a:a)\cdot\widetilde{ab}:4\odot\tilde{b}$ (Sh–K)
126	D_{4h}^{4}	$(c:(a:a))\cdot\widetilde{ab}:4\odot\widetilde{ac}$	$P4/nnc$	$P4/n\ 2/n\ 2/c$	$P4/nnc$	$P4/n\ 2/n\ 2/c$	
127	D_{4h}^{5}	$(c:(a:a))\cdot m:4\odot\tilde{a}$	$P4/mbm$	$P4/m\ 2_1/b\ 2/m$	$P4/mbm$	$P4/m\ 2_1/b\ 2/m$	$(c:a:a)\cdot m:4\odot\tilde{b}$ (Sh–K)
128	D_{4h}^{6}	$(c:(a:a))\cdot m:4\odot\widetilde{ac}$	$P4/mnc$	$P4/m\ 2_1/n\ 2/c$	$P4/mnc$	$P4/m\ 2_1/n\ 2/c$	
129	D_{4h}^{7}	$(c:(a:a))\cdot\widetilde{ab}:4\cdot m$	$P4/nmm$	$P4/n\ 2_1/m\ 2/m$	$P4/nmm$	$P4/n\ 2_1/m\ 2/m$	
130	D_{4h}^{8}	$(c:(a:a)\cdot\widetilde{ab}:4\cdot\tilde{c}$	$P4/ncc$	$P4/n\ 2/c\ 2/c$	$P4/ncc$	$P4/n\ 2/c\ 2/c$	
131	D_{4h}^{9}	$(c:(a:a))\cdot m:4_2\cdot m$	$P4/mmc$	$P4_2/m\ 2/m\ 2/c$	$P4_2/mmc$	$P4_2/m\ 2/m\ 2/c$	
132	D_{4h}^{10}	$(c:(a:a))\cdot m:4_2\cdot\tilde{c}$	$P4/mcm$	$P4_2/m\ 2/c\ 2/m$	$P4_2/mcm$	$P4_2/m\ 2/c\ 2/m$	
133	D_{4h}^{11}	$(c:(a:a))\cdot\widetilde{ab}:4_2\odot\tilde{a}$	$P4/nbc$	$P4_2/n\ 2/b\ 2/c$	$P4_2/nbc$	$P4_2/n\ 2/b\ 2/c$	$(c:a:a)\cdot\widetilde{ab}:4_2\odot\tilde{b}$ (Sh–K)
134	D_{4h}^{12}	$(c:(a:a))\cdot\widetilde{ab}:4_2\odot\widetilde{ac}$	$P4/nnm$	$P4_2/n\ 2/n\ 2/m$	$P4_2/nnm$	$P4_2/n\ 2/n\ 2/m$	
135	D_{4h}^{13}	$(c:(a:a))\cdot n:4_2\odot\tilde{a}$	$P4/mbc$	$P4_2/m\ 2_1/b\ 2/c$	$P4_2/mbc$	$P4_2/m\ 2_1/b\ 2/c$	$(c:a:a)\cdot m:4_2\odot\tilde{b}$ (Sh–K)
136	D_{4h}^{14}	$(c:(a:a))\cdot m:4_2\odot\widetilde{ac}$	$P4/mnm$	$P4_2/m\ 2_1/n\ 2/m$	$P4_2/mnm$	$P4_2/m\ 2_1/n\ 2/m$	
137	D_{4h}^{15}	$(c:(a:a))\cdot\widetilde{ab}:4_2\cdot m$	$P4/nmc$	$P4_2/n\ 2_1/m\ 2/c$	$P4_2/nmc$	$P4_2/n\ 2_1/m\ 2/c$	
138	D_{4h}^{16}	$(c:(a:a))\cdot ab:4_2\cdot\tilde{c}$	$P4/ncm$	$P4_2/n\ 2_1/c\ 2/m$	$P4_2/ncm$	$P4_2/n\ 2_1/c\ 2/m$	
139	D_{4h}^{17}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right)\cdot m:4\cdot m$	$I4/mmm$	$I4/m\ 2/m\ 2/m$	$I4/mmm$	$I4/m\ 2/m\ 2/m$	
140	D_{4h}^{18}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right)\cdot m:4\cdot\tilde{c}$	$I4/mcm$	$I4/m\ 2/c\ 2/m$	$I4/mcm$	$I4/m\ 2/c\ 2/m$	
141	D_{4h}^{19}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right)\cdot\tilde{a}:4_1\odot m$	$I4/amd$	$I4_1/a\ 2/m\ 2/d$	$I4_1/amd$	$I4_1/a\ 2/m\ 2/d$	
142	D_{4h}^{20}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right)\cdot\tilde{a}:4_1\odot\tilde{c}$	$I4/acd$	$I4_1/a\ 2/c\ 2/d$	$I4_1/acd$	$I4_1/a\ 2/c\ 2/d$	
143	C_{3}^{1}	$(c:(a/a)):3$	$C3$	$C3$	$P3$	$P3$	
144	C_{3}^{2}	$(c:(a/a)):3_1$	$C3_1$	$C3_1$	$P3_1$	$P3_1$	
145	C_{3}^{3}	$(c:(a/a)):3_2$	$C3_2$	$C3_2$	$P3_2$	$P3_2$	
146	C_{3}^{4}	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c:(a/a)\right):3$	$R3$	$R3$	$R3$	$R3$	Hexagonal setting (Sh–K)
		$(a/a/a)/3$					Rhombohedral setting (Sh–K)
147	C_{3i}^{1}	$(c:(a/a)):\tilde{6}$	$C\bar{3}$	$C\bar{3}$	$P\bar{3}$	$P\bar{3}$	
148	C_{3i}^{2}	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c:(a/a)\right):\tilde{6}$	$R\bar{3}$	$R\bar{3}$	$R\bar{3}$	$R\bar{3}$	Hexagonal setting (Sh–K)
		$(a/a/a)/\tilde{6}$					Rhombohedral setting (Sh–K)
149	D_{3}^{1}	$(c:(a/a)):2:3$	$H32$	$H321$	$P312$	$P312$	
150	D_{3}^{2}	$(c:(a/a))\cdot 2:3$	$C32$	$C321$	$P321$	$P321$	
151	D_{3}^{3}	$(c:(a/a)):2:3_1$	$H3_12$	$H3_121$	$P3_112$	$P3_112$	
152	D_{3}^{4}	$(c:(a/a))\cdot 2:3_1$	$C3_12$	$C3_121$	$P3_121$	$P3_121$	
153	D_{3}^{5}	$(c:(a/a)):2:3_2$	$H3_22$	$H3_221$	$P3_212$	$P3_212$	
154	D_{3}^{6}	$(c:(a/a))\cdot 2:3_2$	$C3_22$	$C3_221$	$P3_221$	$P3_221$	
155	D_{3}^{7}	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c:(a/a)\right)\cdot 2:3$	$R32$	$R32$	$R32$	$R32$	Hexagonal setting (Sh–K)
		$(a/a/a)/3:2$					Rhombohedral setting (Sh–K)

Table 12.3.4.1. *Standard space-group symbols* (*cont.*)

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*				Comments*†
			1935 Edition		Present Edition		
			Short	Full	Short	Full	
156	C_{3v}^1	$(c:(a/a)):m\cdot 3$	$C3m$	$C3m1$	$P3m1$	$P3m1$	
157	C_{3v}^2	$(a:c:a)\cdot m\cdot 3$	$H3m$	$H3m1$	$P31m$	$P31m$	$(c:(a/a))\cdot m\cdot 3$ (Sh–K) with special comment
158	C_{3v}^3	$(c:(a/a)):\tilde{c}\cdot 3$	$C3c$	$C3c1$	$P3c1$	$P3c1$	
159	C_{3v}^4	$(a:c:a)\cdot\tilde{c}\cdot 3$	$H3c$	$H3c1$	$P31c$	$P31c$	$(c:(a/a))\cdot\tilde{c}\cdot 3$ (Sh–K) with special comment
160	C_{3v}^5	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c:(a/a)\right)\cdot m\cdot 3$	$R3m$	$R3m$	$R3m$	$R3m$	Hexagonal setting (Sh–K)
		$(a/a/a)/3\cdot m$					Rhombohedral setting (Sh–K)
161	C_{3v}^6	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c:(a/a)\right)\cdot\tilde{c}\cdot 3$	$R3c$	$R3c$	$R3c$	$R3c$	Hexagonal setting (Sh–K)
		$(a/a/a)/3\cdot\widetilde{abc}$					Rhombohedral setting (Sh–K)
162	D_{3d}^1	$(a:c:a)\cdot m\cdot\tilde{6}$	$H\bar{3}m$	$H\bar{3}\ 2/m\ 1$	$P\bar{3}1m$	$P\bar{3}1\ 2/m$	$(c:(a/a))\cdot m\cdot\tilde{6}$ (Sh–K) with special comment
163	D_{3d}^2	$(a:c:a)\cdot\tilde{c}\cdot\tilde{6}$	$H\bar{3}c$	$H\bar{3}\ 2/c\ 1$	$P\bar{3}1c$	$P\bar{3}1\ 2/c$	$(c:(a/a))\cdot\tilde{c}\cdot\tilde{6}$ (Sh–K) with special comment
164	D_{3d}^3	$(c:(a/a)):m\cdot\tilde{6}$	$C\bar{3}m$	$C\bar{3}\ 2/m\ 1$	$P\bar{3}m1$	$P\bar{3}\ 2/m\ 1$	
165	D_{3d}^4	$(c:(a/a)):\tilde{c}\cdot\tilde{6}$	$C\bar{3}c$	$C\bar{3}\ 2/c\ 1$	$P\bar{3}c1$	$P\bar{3}\ 2/c\ 1$	
166	D_{3d}^5	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c:(a/a)\right):m\cdot\tilde{6}$	$R\bar{3}m$	$R\bar{3}\ 2/m$	$R\bar{3}m$	$R\bar{3}\ 2/m$	Hexagonal setting (Sh–K)
		$(a/a/a)/\tilde{6}\cdot m$					Rhombohedral setting (Sh–K)
167	D_{3d}^6	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c:(a/a)\right):\tilde{c}\cdot\tilde{6}$	$R\bar{3}c$	$R\bar{3}\ 2/c$	$R\bar{3}c$	$R\bar{3}\ 2/c$	Hexagonal setting (Sh–K)
		$(a/a/a)/\tilde{6}\cdot\widetilde{abc}$					Rhombohedral setting (Sh–K)
168	C_6^1	$(c:(a/a)):6$	$C6$	$C6$	$P6$	$P6$	
169	C_6^2	$(c:(a/a)):6_1$	$C6_1$	$C6_1$	$P6_1$	$P6_1$	
170	C_6^3	$(c:(a/a)):6_5$	$C6_5$	$C6_5$	$P6_5$	$P6_5$	
171	C_6^4	$(c:(a/a)):6_2$	$C6_2$	$C6_2$	$P6_2$	$P6_2$	
172	C_6^5	$(c:(a/a)):6_4$	$C6_4$	$C6_4$	$P6_4$	$P6_4$	
173	C_6^6	$(c:(a/a)):6_3$	$C6_3$	$C6_3$	$P6_3$	$P6_3$	
174	C_{3h}^1	$(c:(a/a)):3:m$	$C\bar{6}$	$C\bar{6}$	$P\bar{6}$	$P\bar{6}$	
175	C_{6h}^1	$(c:(a/a))\cdot m:6$	$C6/m$	$C6/m$	$P6/m$	$P6/m$	
176	C_{6h}^2	$(c:(a/a))\cdot m:6_3$	$C6_3/m$	$C6_3/m$	$P6_3/m$	$P6_3/m$	
177	D_6^1	$(c:(a/a))\cdot 2:6$	$C62$	$C622$	$P622$	$P622$	
178	D_6^2	$(c:(a/a))\cdot 2:6_1$	$C6_12$	$C6_122$	$P6_122$	$P6_122$	
179	D_6^3	$(c:(a/a))\cdot 2:6_5$	$C6_52$	$C6_522$	$P6_522$	$P6_522$	
180	D_6^4	$(c:(a/a))\cdot 2:6_2$	$C6_22$	$C6_222$	$P6_222$	$P6_222$	
181	D_6^5	$(c:(a/a))\cdot 2:6_4$	$C6_42$	$C6_422$	$P6_422$	$P6_422$	
182	D_6^6	$(c:(a/a))\cdot 2:6_3$	$C6_32$	$C6_322$	$P6_322$	$P6_322$	
183	C_{6v}^1	$(c:(a/a)):m\cdot 6$	$C6mm$	$C6mm$	$P6mm$	$P6mm$	
184	C_{6v}^2	$(c:(a/a)):\tilde{c}\cdot 6$	$C6cc$	$C6cc$	$P6cc$	$P6cc$	
185	C_{6v}^3	$(c:(a/a)):\tilde{c}\cdot 6_3$	$C6cm$	$C6_3cm$	$P6_3cm$	$P6_3cm$	
186	C_{6v}^4	$(c:(a/a)):m\cdot 6_3$	$C6mc$	$C6_3mc$	$P6_3mc$	$P6_3mc$	
187	D_{3h}^1	$(c:(a/a)):m\cdot 3:m$	$C\bar{6}m2$	$C\bar{6}m2$	$P\bar{6}m2$	$P\bar{6}m2$	
188	D_{3h}^2	$(c:(a/a)):\tilde{c}\cdot 3:m$	$C\bar{6}c2$	$C\bar{6}c2$	$P\bar{6}c2$	$P\bar{6}c2$	
189	D_{3h}^3	$(c:(a/a))\cdot m:3\cdot m$	$H\bar{6}m2$	$H\bar{6}m2$	$P\bar{6}2m$	$P\bar{6}2m$	
190	D_{3h}^4	$(c:(a/a))\cdot m:3\cdot\tilde{c}$	$H\bar{6}c2$	$H\bar{6}c2$	$P\bar{6}2c$	$P\bar{6}2c$	

Table 12.3.4.1. *Standard space-group symbols* (*cont.*)

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*: 1935 Edition Short	1935 Edition Full	Present Edition Short	Present Edition Full	Comments*†
191	D_{6h}^1	$(c{:}(a/a))\cdot m{:}6\cdot m$	$C6/mmm$	$C6/m\ 2/m\ 2/m$	$P6/mmm$	$P6/m\ 2/m\ 2/m$	
192	D_{6h}^2	$(c{:}(a/a))\cdot m{:}6\cdot\tilde{c}$	$C6/mcc$	$C6/m\ 2/c\ 2/c$	$P6/mcc$	$P6/m\ 2/c\ 2/c$	
193	D_{6h}^3	$(c{:}(a/a))\cdot m{:}6_3\cdot\tilde{c}$	$C6/mcm$	$C6_3/m\ 2/c\ 2/m$	$P6_3/mcm$	$P6_3/m\ 2/c\ 2/m$	
194	D_{6h}^4	$(c{:}(a/a))\cdot m{:}6_3\cdot m$	$C6/mmc$	$C6_3/m\ 2/m\ 2/c$	$P6_3/mmc$	$P6_3/m\ 2/m\ 2/c$	
195	T^1	$(a{:}(a/a)){:}2/3$	$P23$	$P23$	$P23$	$P23$	
196	T^2	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}{:}a{:}(a{:}a)\right){:}2/3$	$F23$	$F23$	$F23$	$F23$	
197	T^3	$\left(\frac{a+b+c}{2}\Big/a{:}(a{:}a)\right){:}2/3$	$I23$	$I23$	$I23$	$I23$	
198	T^4	$(a{:}(a{:}a)){:}2_1//3$	$P2_13$	$P2_13$	$P2_13$	$P2_13$	
199	T^5	$\left(\frac{a+b+c}{2}\Big/a{:}(a{:}a)\right){:}2_1//3$	$I2_13$	$I2_13$	$I2_13$	$I2_13$	
200	T_h^1	$(a{:}(a{:}a))\cdot m/\tilde{6}$	$Pm3$	$P2/m\ \bar{3}$	$Pm\bar{3}$	$P2/m\ \bar{3}$	$Pm3$ (*IT*, 1952)
201	T_h^2	$(a{:}(a{:}a))\cdot\widetilde{ab}/\tilde{6}$	$Pn3$	$P2/n\ \bar{3}$	$Pn\bar{3}$	$P2/n\ \bar{3}$	$Pn3$ (*IT*, 1952)
202	T_h^3	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}{:}a{:}(a{:}a)\right)\cdot m/\tilde{6}$	$Fm3$	$F2/m\ \bar{3}$	$Fm\bar{3}$	$F2/m\ \bar{3}$	$Fm3$ (*IT*, 1952)
203	T_h^4	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}{:}a{:}(a{:}a)\right)\cdot\frac{1}{2}ab/\tilde{6}$	$Fd3$	$F2/d\ \bar{3}$	$Fd\bar{3}$	$F2/d\ \bar{3}$	$Fd3$ (*IT*, 1952)
204	T_h^5	$\left(\frac{a+b+c}{2}\Big/a{:}(a{:}a)\right)\cdot m/\tilde{6}$	$Im3$	$I2/m\ \bar{3}$	$Im\bar{3}$	$I2/m\ \bar{3}$	$Im3$ (*IT*, 1952)
205	T_h^6	$(a{:}(a{:}a))\cdot\tilde{a}/\tilde{6}$	$Pa3$	$P2_1/a\ \bar{3}$	$Pa\bar{3}$	$P2_1/a\ \bar{3}$	$Pa3$ (*IT*, 1952)
206	T_h^7	$\left(\frac{a+b+c}{2}\Big/a{:}(a{:}a)\right)\cdot\tilde{a}/\tilde{6}$	$Ia3$	$I2_1/a\ \bar{3}$	$Ia\bar{3}$	$I2_1/a\ \bar{3}$	$Ia3$ (*IT*, 1952)
207	O^1	$(a{:}(a{:}a)){:}4/3$	$P43$	$P432$	$P432$	$P432$	
208	O^2	$(a{:}(a{:}a)){:}4_2//3$	$P4_23$	$P4_232$	$P4_232$	$P4_232$	
209	O^3	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}{:}a{:}(a{:}a)\right){:}4/3$	$F43$	$F432$	$F432$	$F432$	
210	O^4	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}{:}a{:}(a{:}a)\right){:}4_1//3$	$F4_13$	$F4_132$	$F4_132$	$F4_132$	
211	O^5	$\left(\frac{a+b+c}{2}\Big/a{:}(a{:}a)\right){:}4/3$	$I43$	$I432$	$I432$	$I432$	
212	O^6	$(a{:}(a{:}a)){:}4_3//3$	$P4_33$	$P4_332$	$P4_332$	$P4_332$	
213	O^7	$(a{:}(a{:}a)){:}4_1//3$	$P4_13$	$P4_132$	$P4_132$	$P4_132$	
214	O^8	$\left(\frac{a+b+c}{2}\Big/a{:}(a{:}a)\right){:}4_1//3$	$I4_13$	$I4_132$	$I4_132$	$I4_132$	
215	T_d^1	$(a{:}(a{:}a)){:}\tilde{4}/3$	$P\bar{4}3m$	$P\bar{4}3m$	$P\bar{4}3m$	$P\bar{4}3m$	
216	T_d^2	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}{:}a{:}(a{:}a)\right){:}\tilde{4}/3$	$F\bar{4}3m$	$F\bar{4}3m$	$F\bar{4}3m$	$F\bar{4}3m$	
217	T_d^3	$\left(\frac{a+b+c}{2}\Big/a{:}(a{:}a)\right){:}\tilde{4}/3$	$I\bar{4}3m$	$I\bar{4}3m$	$I\bar{4}3m$	$I\bar{4}3m$	
218	T_d^4	$(a{:}(a{:}a)){:}\tilde{4}//3$	$P\bar{4}3n$	$P\bar{4}3n$	$P\bar{4}3n$	$P\bar{4}3n$	
219	T_d^5	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}{:}a{:}(a{:}a)\right){:}\tilde{4}//3$	$F\bar{4}3c$	$F\bar{4}3c$	$F\bar{4}3c$	$F\bar{4}3c$	
220	T_d^6	$\left(\frac{a+b+c}{2}\Big/a{:}(a{:}a)\right){:}\tilde{4}//3$	$I\bar{4}3d$	$I\bar{4}3d$	$I\bar{4}3d$	$I\bar{4}3d$	

Table 12.3.4.1. *Standard space-group symbols* (*cont.*)

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*				Comments*†
			1935 Edition		Present Edition		
			Short	Full	Short	Full	
221	O_h^1	$(a:(a:a)):4/\tilde{6}\cdot m$	$Pm3m$	$P4/m\,\bar{3}\,2/m$	$Pm\bar{3}m$	$P4/m\,\bar{3}\,2/m$	$Pm3m$ (*IT*, 1952)
222	O_h^2	$(a:(a:a)):4/\tilde{6}\cdot \widetilde{abc}$	$Pn3n$	$P4/n\,\bar{3}\,2/n$	$Pn\bar{3}n$	$P4/n\,\bar{3}\,2/n$	$Pn3n$ (*IT*, 1952)
223	O_h^3	$(a:(a:a)):4_2//\tilde{6}\cdot \widetilde{abc}$	$Pm3n$	$P4_2/m\,\bar{3}\,2/n$	$Pm\bar{3}n$	$P4_2/m\,\bar{3}\,2/n$	$Pm3n$ (*IT*, 1952)
224	O_h^4	$(a:(a:a)):4_2//\tilde{6}\cdot m$	$Pn3m$	$P4_2/n\,\bar{3}\,2/m$	$Pn\bar{3}m$	$P4_2/n\,\bar{3}\,2/m$	$Pn3m$ (*IT*, 1952)
225	O_h^5	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right):4/\tilde{6}\cdot m$	$Fm3m$	$F4/m\,\bar{3}\,2/m$	$Fm\bar{3}m$	$F4/m\,\bar{3}\,2/m$	$Fm3m$ (*IT*, 1952)
226	O_h^6	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right):4/\tilde{6}\cdot \tilde{c}$	$Fm3c$	$F4/m\,\bar{3}\,2/c$	$Fm\bar{3}c$	$F4/m\,\bar{3}\,2/c$	$Fm3c$ (*IT*, 1952)
227	O_h^7	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a(a:a)\right)$ $:4_1//\tilde{6}\cdot m$	$Fd3m$	$F4_1/d\,\bar{3}\,2/m$	$Fd\bar{3}m$	$F4_1/d\,\bar{3}\,2/m$	$Fd3m$ (*IT*, 1952)
228	O_h^8	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right)$ $:4_1//\tilde{6}\cdot \tilde{c}$	$Fd3c$	$F4_1/d\,\bar{3}\,2/c$	$Fd\bar{3}c$	$F4_1/d\,\bar{3}\,2/c$	$Fd3c$ (*IT*, 1952)
229	O_h^9	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right):4/\tilde{6}\cdot m$	$Im3m$	$I4/m\,\bar{3}\,2/m$	$Im\bar{3}m$	$I4/m\,\bar{3}\,2/m$	$Im3m$ (*IT*, 1952)
230	O_h^{10}	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right):4_1//\tilde{6}\cdot \frac{1}{2}\widetilde{abc}$	$Ia3d$	$I4_1/a\,\bar{3}\,2/d$	$Ia\bar{3}d$	$I4_1/a\,\bar{3}\,2/d$	$Ia3d$ (*IT*, 1952)

* Abbreviations used in the column *Comments*: *IT*, 1952: *International Tables for X-ray Crystallography,* Vol. 1 (1952); Sh–K; Shubnikov & Koptsik (1972).
† Note that this table contains only one notation for the *b*-unique setting and one notation for the *c*-unique setting in the monoclinic case, always referring to cell choice 1 of the space-group tables.

12.3.3. Non-symbolized symmetry elements

Certain symmetry elements are not given explicitly in the full symbol because they can easily be derived. They are:

(i) Rotoinversion axes that are not used to indicate the lattice symmetry directions.

(ii) Rotation axes 2 included in the axes 4, $\bar{4}$ and 6 and rotation axes 3 included in the axes $\bar{3}$, 6 and $\bar{6}$.

(iii) Additional symmetry elements occurring in space groups with centred unit cells. These types of operation can be deduced from the product of the centring translation $(\boldsymbol{I}, \boldsymbol{g})$ with a symmetry operation $(\boldsymbol{W}, \boldsymbol{w})$. The new symmetry operation $(\boldsymbol{W}, \boldsymbol{g}+\boldsymbol{w})$ again has $\boldsymbol{W}$ as rotation part but a different glide/screw part if the component of $\boldsymbol{g}$ parallel to the symmetry element corresponding to $\boldsymbol{W}$ is not a lattice vector; *cf.* Chapter 4.1.

Example

Space group $C2/c$ (15) has a twofold axis along **b** with screw part $\boldsymbol{w}_g = (0,0,0)$. The translational part of the centring operation is $\boldsymbol{g} = (\frac{1}{2}, \frac{1}{2}, 0)$.

An additional axis parallel to **b** thus has a translation part $\boldsymbol{g} + \boldsymbol{w}_g = (\frac{1}{2}, \frac{1}{2}, 0)$. The component $(0, \frac{1}{2}, 0)$ indicates a screw axis 2_1 in the y direction, whereas the component $(\frac{1}{2}, 0, 0)$ indicates the location of this axis in $(\frac{1}{4}, y, 0)$. Similarly, it can be shown that glide plane *c* combined with the centring gives a glide plane *n*.

In the same way, in rhombohedral and cubic space groups, a rotation axis 3 is accompanied by screw axes 3_1 and 3_2.

In space groups with centred unit cells, the location parts of different symmetry elements may coincide. In $I\bar{4}2m$, for example, the mirror plane *m* contains simultaneously a non-symbolized glide plane *n*. The same applies to all mirror planes in *Fmmm.*

(iv) Symmetry elements with diagonal orientation always occur with different types of glide/screw parts simultaneously. In space group $P\bar{4}2m$ the translation vector along *a* can be decomposed as

$$\boldsymbol{w} = (1,0,0) = (\tfrac{1}{2}, \tfrac{1}{2}, 0) + (\tfrac{1}{2}, -\tfrac{1}{2}, 0) = \boldsymbol{w}_g + \boldsymbol{w}_l.$$

The diagonal mirror plane with normal along $[1\bar{1}0]$ passing through the origin is accompanied by a parallel glide plane with glide part $(\frac{1}{2}, \frac{1}{2}, 0)$ shifted by $(\frac{1}{4}, -\frac{1}{4}, 0)$. The same arguments lead to the occurrence of screw axes 2_1, 3_1 and 3_2 connected with diagonal rotation axes 2 or 3.

(v) For some investigations connected with *klassengleiche* subgroups, it is convenient to introduce an *extended full space-group symbol* that comprises all symmetry elements indicated in (iii) and (iv). The basic concept may be found in papers by Hermann (1929) and in *IT* (1952). These concepts have been applied by Bertaut (1976) and Zimmermann (1976); *cf.* Part 4.

Example

The full symbol of space group *Imma* (74) is

$$I\frac{2_1}{m}\frac{2_1}{m}\frac{2_1}{a}.$$

The *I*-centring operation introduces additional rotation axes and glide planes for all three sets of lattice symmetry directions. The extended full symbol is

$$I\frac{2,2_1}{m,n}\frac{2,2_1}{m,n}\frac{2,2_1}{a,b} \quad \text{or} \quad I\begin{matrix}\frac{2_1}{m} & \frac{2_1}{m} & \frac{2_1}{a}\\ \frac{2}{n} & \frac{2}{n} & \frac{2}{b}\end{matrix}.$$

This symbol shows immediately the eight subgroups with a *P* lattice corresponding to point group *mmm*:

$Pmma \sim Pmmb$, $Pnma \sim Pmnb$, $Pmna \sim Pnmb$ and $Pnna \sim Pnnb$.

12.3.4. Standardization rules for short symbols

The symbols of Bravais lattices and glide planes depend on the choice of basis vectors. As shown in the preceding section, additional translation vectors in centred unit cells produce new symmetry operations with the same rotation but different glide/screw parts. Moreover, it was shown that for diagonal orientations symmetry operations may be represented by different symbols. Thus, different short symbols for the same space group can be derived even if the rules for the selection of the generators and indicators are obeyed.

For the unique designation of a space-group type, a standardization of the short symbol is necessary. Rules for standardization were given first by Hermann (1931) and later in a slightly modified form in *IT* (1952).

These rules, which are generally followed in the present tables, are given below. Because of the historical development of the symbols (*cf.* Chapter 12.4), some of the present symbols do not obey the rules, whereas others depending on the crystal class need additional rules for them to be uniquely determined. These exceptions and additions are not explicitly mentioned, but may be discovered from Table 12.3.4.1 in which the short symbols are listed for all space groups. A table for all settings may be found in Chapter 4.3.

Triclinic symbols are unique if the unit cell is primitive. For the standard setting of *monoclinic* space groups, the lattice symmetry direction is labelled b. From the three possible centrings A, I and C, the latter one is favoured. If glide components occur in the plane perpendicular to [010], the glide direction c is preferred. In the space groups corresponding to the *orthorhombic* group $mm2$, the unique direction of the twofold axis is chosen along **c**. Accordingly, the face centring C is employed for centrings perpendicular to the privileged direction. For space groups with possible A or B centring, the first one is preferred. For groups 222 and *mmm*, no privileged symmetry direction exists, so the different possibilities of one-face centring can be reduced to C centring by change of the setting. The choices of unit cell and centring type are fixed by the conventional basis in systems with higher symmetry.

When more than one kind of symmetry elements exist in one representative direction, in most cases the choice for the space-group symbol is made in order of decreasing priority: for reflections and glide reflections m, a, b, c, n, d, for proper rotations and screw rotations 6, 6_1, 6_2, 6_3, 6_4, 6_5; 4, 4_1, 4_2, 4_3; 3, 3_1, 3_2; 2, 2_1 [*cf.* *IT* (1952), p. 55, and Chapter 4.1].

12.3.5. Systematic absences

Hermann (1928) emphasized that the short symbols permit the derivation of systematic absences of X-ray reflections caused by the glide/screw parts of the symmetry operations. If $\boldsymbol{H} = (h, k, l)$ describes the X-ray reflection and $(\boldsymbol{W}, \boldsymbol{w})$ is the matrix representation of a symmetry operation, the matrix can be expanded as follows:

$$(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{W}, \boldsymbol{w}_g + \mathbf{w}_l) = (\boldsymbol{W}, \begin{pmatrix} w_g^1 \\ w_g^2 \\ w_g^3 \end{pmatrix} + \boldsymbol{w}_l).$$

The absence of a reflection is governed by the relation (i) $\boldsymbol{H} \cdot \boldsymbol{W} = \boldsymbol{H}$ and the scalar product (ii) $\boldsymbol{H} \cdot \boldsymbol{w}_g = hw_g^1 + kw_g^2 + lw_g^3$. A reflection $\boldsymbol{H}$ is absent if condition (i) holds and the scalar product (ii) is not an integer. The calculation must be made for all generators and indicators of the short symbol. Systematic absences, introduced by the further symmetry operations generated, are obtained by the combination of the extinction rules derived for the generators and indicators.

Example: Space group $D_4^{10} = I4_122$ (98)

The generators of the space group are the integral translations and the centring translation $(xyz, \frac{1}{2}\frac{1}{2}\frac{1}{2})$, the rotation 2 in direction [100]: $(x\bar{y}\bar{z}, 000)$ and the rotation 2 in direction $[1\bar{1}0]$: $(\bar{y}\bar{x}\bar{z}, 00-\frac{1}{4})$. The operation corresponding to the indicator is the product of the two generators:

$$(x\bar{y}\bar{z}, 000)\ (\bar{y}\bar{x}\bar{z}, 00-\tfrac{1}{4}) = (\bar{y}xz, 00\tfrac{1}{4}).$$

The integral translations imply no restriction because the scalar product is always an integer. For the centring, condition (i) with $\boldsymbol{W} = \boldsymbol{I}$ holds for all reflections (integral condition), but the scalar product (ii) is an integer only for $h + k + l = 2n$. Thus, reflections hkl with $h + k + l \neq 2n$ are absent. The screw rotation 4 has the screw part $\boldsymbol{w}_g = (0, 0, \frac{1}{4})$. Only $00l$ reflections obey condition (i) (serial extinction). An integral value for the scalar product (ii) requires $l = 4n$. The twofold axes in the directions [100] and $[1\bar{1}0]$ do not imply further absences because $\boldsymbol{w}_g = \boldsymbol{0}$.

12.3.6. Generalized symmetry

The international symbols can be suitably modified to describe generalized symmetry, *e.g.* colour groups, which occur when the symmetry operations are combined with changes of physical properties. For the description of antisymmetry (or 'black–white' symmetry), the symbols of the Bravais lattices are supplemented by additional letters for centrings accompanied by a change in colour. For symmetry operations that are not translations, a prime is added to the usual symbol if a change of colour takes place. A complete description of the symbols and a detailed list of references are given by Koptsik (1966). The Shubnikov symbols have not been extended to colour symmetry.

International Tables for Crystallography (2006). Vol. A, Chapter 12.4, pp. 833–834.

12.4. Changes introduced in space-group symbols since 1935

BY H. BURZLAFF AND H. ZIMMERMANN

Before the appearance of the first edition of *International Tables* in 1935, different notations for space groups were in use. A summary and comparative tables may be found in the introduction to that edition. The international notation was proposed by Hermann (1928*a*,*b*) and Mauguin (1931), who used the concept of lattice symmetry directions (see Chapter 12.1) and gave preference to reflections or glide reflections as generators. Considerable changes to the original Hermann–Mauguin short symbols were made in *IT* (1952).

The most important change refers to the symmetry directions. In the original Hermann–Mauguin symbols [(*IT*, 1935)], the distribution of symmetry elements is prescribed by the point-group symbol in the traditional setting, for example $\bar{4}2m$ (not $\bar{4}m2$) but $\bar{6}m2$ (not $\bar{6}2m$). This procedure sometimes implies the use of a larger unit cell than would be necessary. In *IT* (1952) and in the present *Tables*, however, the lattice symmetry directions always refer to the conventional cell (*cf.* Part 9) of the Bravais lattice. The results of this change are (*a*) different symbols for centring types and (*b*) different sequences of the symbols referring to the point group. These differences occur only in some space groups that have a tetragonal or hexagonal lattice.

Thus, the two different space groups D^1_{2d} and D^5_{2d} were symbolized by $P\bar{4}2m$ and $C\bar{4}2m$ in *IT* (1935) because in both cases the twofold axis had to be connected with the secondary set of symmetry directions. The new international symbols are $P\bar{4}2m$ and $P\bar{4}m2$; since in the point group $4/m\ 2/m\ 2/m$ of the Bravais lattice the secondary and tertiary set cannot be distinguished, the twofold axis in the subgroups $\bar{4}2m$ and $\bar{4}m2$ may occur in either the secondary or the tertiary set. Accordingly, the *C*-centred cell of $D^5_{2d} - C\bar{4}2m$, used in *IT* (1935), was transformed to a primitive one with the twofold axis along the tertiary set, resulting in the symbol $P\bar{4}m2$.

The same considerations hold for $\bar{6}m2$ and $\bar{6}2m$ and for space groups with a hexagonal lattice belonging to the point groups 32, $3m$ and $\bar{3}m$, which can be oriented in two ways with respect to the lattice.

For example, the point group $3m$ has two sets of symmetry directions. If the basis vector **a** is normal to the mirror plane *m*, two hexagonal cells with different centrings are possible:

(i) the hexagonal primitive cell, always described by *C* in *IT* (1935), leads to $C3m = C^1_{3v}$;

(ii) the hexagonal *H*-centred cell, with centring points in $\frac{2}{3}\frac{1}{3}0$ and $\frac{1}{3}\frac{2}{3}0$, leads to $H3m = C^2_{3v}$ (*cf.* Part 9).

The latter can be transformed to a primitive cell in which the mirror plane is normal to the representative of the tertiary set of the hexagonal lattice. In *IT* (1952) and the present editions, the primitive hexagonal cell is described by *P*. Thus, the above space groups receive the symbols $P3m1 = C^1_{3v}$ and $P31m = C^2_{3v}$.

Further changes are:

(i) In *IT* (1952), symbols for space groups related to the point groups 422, 622 and 432 contain the twofold axis of the tertiary set. The advantage is that these groups can be generated by operations of the secondary and tertiary set. The symbol of the indicator is provided with the appropriate index to identify the screw part, thus fixing the intersection parameter.

(ii) Some standard settings are changed in the monoclinic system. In *IT* (1935), only one setting (*b* unique, one cell choice) was tabulated for the monoclinic space groups. In *IT* (1952), two choices were offered, *b* and *c* unique, each with one cell choice. In the present edition, the two choices (*b* and *c* unique) are retained but for each one three different cells are available. The standard short symbol, however, is that of *IT* (1935) (*b*-unique setting).

(iii) In the short symbols of centrosymmetric space groups in the cubic system, $\bar{3}$ is written instead of 3, *e.g.* $Pm\bar{3}$ instead of $Pm3$ [as in *IT* (1935) and *IT* (1952)].

(iv) Beginning with the Fourth Edition of this volume (1995), the following five orthorhombic space-group symbols have been modified by introducing the new glide-plane symbol *e*, according to a Nomenclature Report of the IUCr (de Wolff *et al.*, 1992).

Space group No.	39	41	64	67	68
Former symbol:	*Abm*2	*Aba*2	*Cmca*	*Cmma*	*Ccca*
New symbol:	*Aem*2	*Aea*2	*Cmce*	*Cmme*	*Ccce*

The new symbol is indicated in the headline of these space groups. Further details are given in Chapter 1.3.

Difficulties arising from these changes are avoided by selecting the lexicographically first one of the two possible glide parts for the generating operation.

Example: $Aea2 \sim Aba2 = C^{17}_{2v}$ (41)

The generators are

A centring:	$(xyz, 0\frac{1}{2}\frac{1}{2})$	$(1) + (0\frac{1}{2}\frac{1}{2})$
glide reflection $b_{[100]}$:	$(\bar{x}yz, 0\frac{1}{2}0)$	(4)
or glide reflection $c_{[100]}$:	$(\bar{x}yz, 00\frac{1}{2})$	$(4) + (0\frac{1}{2}\frac{1}{2})$
The first possibility is selected.		
glide reflection $a_{[010]}$:	$(x\bar{y}z, \frac{1}{2}00)$	(3).

A shift of origin by $(-\frac{1}{4}, -\frac{1}{4}, 0)$ is necessary

The 1935 symbols and all the changes adopted in the present edition of *International Tables* can be seen in Table 12.3.4.1. Differences in the symbols between *IT* (1952) and the present edition may be found in the last column of this table; *cf.* also Section 2.2.4.

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13.1. Isomorphic subgroups

BY Y. BILLIET AND E. F. BERTAUT

13.1.1. Definitions

A subgroup $\mathcal{H}$ of a space group $\mathcal{G}$ is an *isomorphic subgroup* if $\mathcal{H}$ is of the same or the enantiomorphic space-group type as $\mathcal{G}$. Thus, isomorphic space groups are a special subset of *klassengleiche subgroups*. The *maximal isomorphic subgroups of lowest index* are listed under **IIc** in the space-group tables of this volume (Part 7) (*cf.* Section 2.2.15). Isomorphic subgroups can easily be recognized because the standard space-group symbols of $\mathcal{G}$ and $\mathcal{H}$ are the same [isosymbolic subgroups (Billiet, 1973)] or the symbol of $\mathcal{H}$ is enantiomorphic to that of $\mathcal{G}$. Every space group has an infinite number of maximal isomorphic subgroups, whereas the number of maximal non-isomorphic subgroups is finite (*cf.* Section 8.3.3). For this reason, isomorphic subgroups are discussed in more detail in the present section.

If **a**, **b**, **c** are the basis vectors defining the conventional unit cell of $\mathcal{G}$ and **a**′, **b**′, **c**′ the basis vectors corresponding to $\mathcal{H}$ the relation

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{S} \qquad (13.1.1.1)$$

holds, where $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ and $(\mathbf{a}', \mathbf{b}', \mathbf{c}')$ are row matrices and $\boldsymbol{S}$ is a (3×3) matrix. The coefficients S_{ij} of $\boldsymbol{S}$ are integers.*

The index of $\mathcal{H}$ in $\mathcal{G}$ is equal to $|\det(\boldsymbol{S})|$*, which is the ratio of the volumes $[\mathbf{a}'\mathbf{b}'\mathbf{c}']$ and $[\mathbf{abc}]$ of the two cells. $\det(\boldsymbol{S})$ is positive if the bases of the two cells have the same handedness and negative if they have opposite handedness.

If O and O' are the origins of the coordinate systems $(O, \mathbf{a}, \mathbf{b}, \mathbf{c})$ and $(O', \mathbf{a}', \mathbf{b}', \mathbf{c}')$, used for the description of $\mathcal{G}$ and $\mathcal{H}$, the column matrix of the coordinates of O' referred to the system $(O, \mathbf{a}, \mathbf{b}, \mathbf{c})$ will be denoted by $\boldsymbol{s}$. Thus, the coordinate system $(O', \mathbf{a}', \mathbf{b}', \mathbf{c}')$ will be specified completely by the square matrix $\boldsymbol{S}$ and the column matrix $\boldsymbol{s}$, symbolized by $\mathbb{S} : (\boldsymbol{S}, \boldsymbol{s})$.

An example of the application of equation (13.1.1.1) is given at the end of this chapter.

13.1.1.1. *The mathematical expression of equivalence*

Let $\mathbb{W} = (\boldsymbol{W}, \boldsymbol{w})$ be the operator of a given symmetry operation of $\mathcal{H}$ referred to $(O, \mathbf{a}, \mathbf{b}, \mathbf{c})$ and $\mathbb{W}' = (\boldsymbol{W}', \boldsymbol{w}')$ the operator of the same operation referred to $(O', \mathbf{a}', \mathbf{b}', \mathbf{c})$. Then the following relation applies

$$\mathbb{S}\mathbb{W}' = \mathbb{W}\mathbb{S} \quad \text{or} \quad \mathbb{W}' = \mathbb{S}^{-1}\mathbb{W}\mathbb{S} \qquad (13.1.1.2)$$

(*cf.* Bertaut & Billiet, 1979). The latter expression is more conventional, the former is easier to manipulate. Identifying the rotational (matrix) and translational (column) parts of $\mathbb{W}$, one obtains the following two conditions:

$$\begin{aligned} \boldsymbol{S}\boldsymbol{W}' &= \boldsymbol{W}\boldsymbol{S}, \\ \boldsymbol{s} + \boldsymbol{S}\boldsymbol{w}' &= \boldsymbol{w} + \boldsymbol{W}\boldsymbol{s} = \hat{\boldsymbol{w}} + \boldsymbol{t}_{\mathcal{G}} + \boldsymbol{W}\boldsymbol{s} \end{aligned} \qquad (13.1.1.2a)$$

or

$$\boldsymbol{S}\boldsymbol{w}' - \hat{\boldsymbol{w}} + (\boldsymbol{I} - \boldsymbol{W})\boldsymbol{s} = \boldsymbol{t}_{\mathcal{G}}. \qquad (13.1.1.2b)$$

Here we have split $\boldsymbol{w}$ into a fractional part $\hat{\boldsymbol{w}}$ (smaller than any lattice translation) and $\boldsymbol{t}_{\mathcal{G}}$ which describes a lattice translation in $\mathcal{G}$.

The general expression of the matrix $\boldsymbol{S}$ is

$$\boldsymbol{S} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix}. \qquad (13.1.1.3)$$

* In general, this does not hold for non-isomorphic subgroups.

This general form, without any restrictions on the coefficients, applies only to the triclinic space groups $P1$ and $P\bar{1}$; $P1$ has only isomorphic subgroups (*cf.* Billiet, 1979; Billiet & Rolley Le Coz, 1980). For other space groups, restrictions have to be imposed on the coefficients S_{ij}.

13.1.2. Isomorphic subgroups

For convenience, we consider first those crystal systems that possess a unique direction (the privileged axis being taken parallel to **c**). We also include here the monoclinic system (unique axis either c or b).

13.1.2.1. *Monoclinic, tetragonal, trigonal, hexagonal systems*

If $\boldsymbol{W}$ is the matrix corresponding to a rotation about the c axis, $\boldsymbol{W}' = \boldsymbol{W}$ holds if the positive direction is the same for c and c'.† In consequence, $\boldsymbol{W}$ *must commute with* $\boldsymbol{S}$ [*cf.* equation (13.1.1.2*a*)]. This condition imposes relations on the coefficients S_{ij} of the matrix so that $\boldsymbol{S}$ and $\det(\boldsymbol{S})$ take the following forms:

Monoclinic system

$$\boldsymbol{M}_c = \begin{pmatrix} S_{11} & S_{12} & 0 \\ S_{21} & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(\boldsymbol{M}_c) = S_{33}(S_{11}S_{22} - S_{12}S_{21});$$

or if b instead of c is used

$$\boldsymbol{M}_b = \begin{pmatrix} S_{11} & 0 & S_{13} \\ 0 & S_{22} & 0 \\ S_{31} & 0 & S_{33} \end{pmatrix}, \quad \det(\boldsymbol{M}_b) = S_{22}(S_{11}S_{33} - S_{13}S_{31}).$$

Tetragonal system

$$\boldsymbol{T}_1 = \begin{pmatrix} S_{11} & -S_{21} & 0 \\ S_{21} & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(\boldsymbol{T}_1) = S_{33}(S_{11}^2 + S_{21}^2).$$

Hexagonal and trigonal systems

$$\boldsymbol{H}_1 = \begin{pmatrix} S_{11} & -S_{21} & 0 \\ S_{21} & S_{11} - S_{21} & 0 \\ 0 & 0 & S_{33} \end{pmatrix},$$
$$\det(\boldsymbol{H}_1) = S_{33}(S_{11}^2 + S_{21}^2 - S_{11}S_{21}).$$

For *rhombohedral* space groups, the matrix $\boldsymbol{H}_1$ applies only when hexagonal axes are used. If rhombohedral axes are used, the matrix $\boldsymbol{S}$ has the form

$$\boldsymbol{R}_1 = \begin{pmatrix} S_0 & S_2 & S_1 \\ S_1 & S_0 & S_2 \\ S_2 & S_1 & S_0 \end{pmatrix},$$
$$\begin{aligned} \det(\boldsymbol{R}_1) &= S_0^3 + S_1^3 + S_2^3 - 3S_0S_1S_2 \\ &= (S_0 + S_1 + S_2) \\ &\quad \times (S_0^2 + S_1^2 + S_2^2 - S_0S_1 - S_1S_2 - S_2S_0). \end{aligned}$$

† If the positive directions of c and c' are opposite, $\boldsymbol{W}' = \boldsymbol{W}^{-1}$, but this does not bring in any new features.

Table 13.1.2.1. *Isomorphic subgroups of the plane groups*

OBLIQUE SYSTEM

$$\boldsymbol{S} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{22} > 0, S_{11}S_{22} > 1, S_{21} = 0, -S_{11}/2 < S_{12} \leq S_{11}/2$

RECTANGULAR SYSTEM

$$\boldsymbol{O} = \begin{pmatrix} S_{11} & 0 \\ 0 & S_{22} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{22} > 0, S_{11}S_{22} > 1$

	$\boldsymbol{O}^a$	$\boldsymbol{O}^b$	$\boldsymbol{O}^c$	$\boldsymbol{O}^d$	$\boldsymbol{O}^e$
S_{11}	n_1	n_1	$2n_1+1$	$2n_1$	$2n_1+1$
S_{22}	n_2	$2n_2+1$	$2n_2+1$	$2n_2$	n_2

SQUARE SYSTEM

$$\boldsymbol{T}_1 = \begin{pmatrix} S_{11} & -S_{21} \\ S_{21} & S_{11} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{21} \geq 0, S_{11}^2 + S_{21}^2 > 1$

$$\boldsymbol{T}_2 = \begin{pmatrix} S_{11} & 0 \\ 0 & S_{11} \end{pmatrix}$$

Conditions: $\boldsymbol{T}_2^a : S_{11} > 1;\ \boldsymbol{T}_2^b : S_{11} = 2n_1 + 1 > 1$

$$\boldsymbol{T}_3 = \begin{pmatrix} S_{11} & -S_{11} \\ S_{11} & S_{11} \end{pmatrix}$$

Condition: $S_{11} > 0$

HEXAGONAL SYSTEM

$$\boldsymbol{H}_1 = \begin{pmatrix} S_{11} & -S_{21} \\ S_{21} & S_{11} - S_{21} \end{pmatrix}$$

Conditions: $S_{11} > 0, 0 \leq S_{21} < S_{11}, (S_{11}^2 + S_{21}^2 - S_{11}S_{21}) > 1$

$$\boldsymbol{H}_2 = \begin{pmatrix} S_{11} & 0 \\ 0 & S_{11} \end{pmatrix}$$

Condition: $S_{11} > 1$

$$\boldsymbol{H}_3 = \begin{pmatrix} 2S_{11} & -S_{11} \\ S_{11} & S_{11} \end{pmatrix}$$

Condition: $S_{11} > 0$

Table of plane subgroups

No. 1 $p1 : \boldsymbol{S}$; No. 2 $p2 : \boldsymbol{S}$; No. 3 $pm : \boldsymbol{O}^a$; No. 4 $pg : \boldsymbol{O}^b$;
No. 5 $cm : \boldsymbol{O}^c, \boldsymbol{O}^d$; No. 6 $p2mm : \boldsymbol{O}^a$; No. 7 $p2mg : \boldsymbol{O}^e$; No. 8 $p2gg : \boldsymbol{O}^c$;
No. 9 $c2mm : \boldsymbol{O}^c, \boldsymbol{O}^d$; No. 10 $p4 : \boldsymbol{T}_1$; No. 11 $p4mm : \boldsymbol{T}_2^a, \boldsymbol{T}_3$;
No. 12 $p4gm : \boldsymbol{T}_2^b$; No. 13 $p3 : \boldsymbol{H}_1$; No. 14 $p3m1 : \boldsymbol{H}_2$; No. 15 $p31m : \boldsymbol{H}_2$;
No. 16 $p6 : \boldsymbol{H}_1$; No. 17 $p6mm : \boldsymbol{H}_2, \boldsymbol{H}_3$.

13.1.2.1.1. *Additional restrictions*

If mirror or glide planes parallel to and/or twofold rotation or screw axes perpendicular to the principal rotation axis exist, further conditions are imposed upon the coefficients S_{ij} and these are indicated below (*cf.* Bertaut & Billiet, 1979).

Monoclinic system

The matrices $\boldsymbol{M}_c$ and $\boldsymbol{M}_b$ apply without any further restrictions on the coefficients.

Tetragonal system

The matrix $\boldsymbol{T}_1$ is valid for all space groups belonging to the crystal classes 4, $\bar{4}$ and $4/m$.

For all other space groups, restrictions apply to the coefficients S_{21} according to the following two rules which are consequences of equation (13.1.1.2*a*):

(i) If the last two letters of the Hermann–Mauguin symbol are different, $S_{21} = 0$; the corresponding matrix is called $\boldsymbol{T}_2$.

Example: $P4_2/mmc$

$$\boldsymbol{T}_2 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(\boldsymbol{T}_2) = S_{33}S_{11}^2.$$

(ii) If the last two letters are the same (except for the three cases mentioned below), two matrices have to be applied, the matrix $\boldsymbol{T}_2$ introduced above and the matrix $\boldsymbol{T}_1$ with $S_{21} = S_{11}$; the corresponding matrix is called $\boldsymbol{T}_3$.

$$\boldsymbol{T}_3 = \begin{pmatrix} S_{11} & -S_{11} & 0 \\ S_{11} & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(\boldsymbol{T}_3) = 2S_{33}S_{11}^2.$$

The following space groups have matrices $\boldsymbol{T}_2$ and $\boldsymbol{T}_3$: $P422$, $P4mm$, $P4/mmm$, $P4_122$, $P4_322$, $P4_222$, $P4cc$, $P4/mcc$, $I422$, $I4mm$ and $I4/mmm$. The three exceptions to the rule mentioned above are the space groups $P4/nmm$, $P4/ncc$ and $I4_122$, which allow only $\boldsymbol{T}_2$.

Hexagonal and trigonal systems

The matrix $\boldsymbol{H}_1$ is valid for all space groups belonging to the crystal classes 6, $\bar{6}$, $6/m$, 3 and $\bar{3}$.

For all other space groups for which the last two letters of the Hermann–Mauguin symbol are different, $S_{22} = S_{11}$, and the matrix is called $\boldsymbol{H}_2$. Examples are $P6_3/mcm$, $P312$ and $P\bar{6}2m$.

$$\boldsymbol{H}_2 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(\boldsymbol{H}_2) = S_{33}S_{11}^2.$$

If the last two letters of the Hermann–Mauguin symbol are the same, two matrices have to be applied, the matrix $\boldsymbol{H}_2$ introduced above and the matrix $\boldsymbol{H}_1$ with $S_{11} = 2S'_{11}$ and $S_{21} = S'_{11}$; this matrix is called $\boldsymbol{H}_3$,

$$\boldsymbol{H}_3 = \begin{pmatrix} 2S'_{11} & -S'_{11} & 0 \\ S'_{11} & S'_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(\boldsymbol{H}_3) = 3S_{33}S'^2_{11}.$$

Examples are $P622$, $P6/mmm$ and $P6cc$.

Rhombohedral space groups

For $R3$ and $R\bar{3}$, one has the matrix $\boldsymbol{H}_1$ for hexagonal axes and $\boldsymbol{R}_1$ for rhombohedral axes. For all other rhombohedral space groups, one has $\boldsymbol{H}_2$ (hexagonal axes) and the matrix $\boldsymbol{R}_1$ with $S_1 = S_2$ (rhombohedral axes). This last matrix is called $\boldsymbol{R}_2$. Example: $R32$.

Table 13.1.2.2. *Isomorphic subgroups of the space groups*

TRICLINIC SYSTEM

$$\boldsymbol{S} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{22} > 0, S_{33} > 0, S_{11}S_{22}S_{33} > 1,$
$S_{21} = S_{31} = S_{32} = 0,\ -S_{11}/2 < S_{12} \leq S_{11}/2,$
$-S_{11}/2 < S_{13} \leq S_{11}/2,\ -S_{22}/2 < S_{23} \leq S_{22}/2$

MONOCLINIC SYSTEM

Unique axis c

$$\boldsymbol{M}_c = \begin{pmatrix} S_{11} & S_{12} & 0 \\ S_{21} & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{33} > 0, (S_{11}S_{22} - S_{12}S_{21})S_{33} > 1$

	S_{11}	S_{12}	S_{21}	S_{22}	S_{33}	Extra condition
$\boldsymbol{M}_c^a$	$n_1 > 0$	0	n_3	$n_4 > 0$	n_5	$-n_4/2 < n_3 \leq n_4/2$
$\boldsymbol{M}_c^b$	$n_1 > 0$	0	n_3	$n_4 > 0$	$2n_5 + 1$	$-n_4/2 < n_3 \leq n_4/2$
$\boldsymbol{M}_c^c$	$n_1 > 0$	$2n_2$	0	$2n_4 + 1 > 0$	$2n_5 + 1$	$-n_1/2 < n_2 \leq n_1/2$
$\boldsymbol{M}_c^d$	$n_1 > 0$	$2n_2$	0	$2n_4 > 0$	$2n_5$	$-n_1/2 < n_2 \leq n_1/2$
$\boldsymbol{M}_c^e$	n_1	$2n_2 > 0$	$n_3 < 0$	0	$2n_5$	$-n_2 < n_1 \leq n_2$
$\boldsymbol{M}_c^f$	$2n_1 + 1 > 0$	0	$2n_3$	$n_4 > 0$	n_5	$-n_4/2 < n_3 \leq n_4/2$
$\boldsymbol{M}_c^g$	$2n_1 + 1 > 0$	$2n_2$	0	$2n_4 + 1 > 0$	$2n_5 + 1$	$-(2n_1 + 1)/2 < n_2 \leq (2n_1 + 1)/2$
$\boldsymbol{M}_c^h$	$2n_1 + 1 > 0$	$2n_2$	0	$2n_4 > 0$	$2n_5$	$-(2n_1 + 1)/2 < n_2 \leq (2n_1 + 1)/2$
$\boldsymbol{M}_c^i$	$2n_1 + 1$	$2n_2 > 0$	$n_3 < 0$	0	$2n_5$	$-(n_2 + 1)/2 < n_1 \leq (n_2 - 1)/2$
$\boldsymbol{M}_c^j$	$2n_1 + 1 > 0$	0	$2n_3$	$n_4 > 0$	$2n_5 + 1$	$-n_4/2 < n_3 \leq n_4/2$

Unique axis b

$$\boldsymbol{M}_b = \begin{pmatrix} S_{11} & 0 & S_{13} \\ 0 & S_{22} & 0 \\ S_{31} & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{22} > 0, (S_{11}S_{33} - S_{13}S_{31})S_{22} > 1$

	S_{11}	S_{13}	S_{22}	S_{31}	S_{33}	Extra condition
$\boldsymbol{M}_b^a$	$n_1 > 0$	n_2	n_3	0	$n_5 > 0$	$-n_1/2 < n_2 \leq n_1/2$
$\boldsymbol{M}_b^b$	$n_1 > 0$	n_2	$2n_3 + 1$	0	$n_5 > 0$	$-n_1/2 < n_2 \leq n_1/2$
$\boldsymbol{M}_b^c$	$2n_1 + 1 > 0$	0	$2n_3 + 1$	$2n_4$	$n_5 > 0$	$-n_5/2 < n_4 \leq n_5/2$
$\boldsymbol{M}_b^d$	$2n_1 > 0$	0	$2n_3$	$2n_4$	$n_5 > 0$	$-n_5/2 < n_4 \leq n_5/2$
$\boldsymbol{M}_b^e$	0	$n_2 < 0$	$2n_3$	$2n_4 > 0$	n_5	$-n_4 < n_5 \leq n_4$
$\boldsymbol{M}_b^f$	n_1	$2n_2$	n_3	0	$2n_5 + 1 > 0$	$-n_1/2 < n_2 \leq n_1/2$
$\boldsymbol{M}_b^g$	$2n_1 + 1 > 0$	0	$2n_3 + 1$	$2n_4$	$2n_5 + 1 > 0$	$-(2n_5 + 1)/2 < n_4 \leq (2n_5 + 1)/2$
$\boldsymbol{M}_b^h$	$2n_1 > 0$	0	$2n_3$	$2n_4$	$2n_5 + 1 > 0$	$-(2n_5 + 1)/2 < n_4 \leq (2n_5 + 1)/2$
$\boldsymbol{M}_b^i$	0	$n_2 < 0$	$2n_3$	$2n_4 > 0$	$2n_5 + 1$	$-(n_4 + 1)/2 < n_5 \leq (n_4 - 1)/2$
$\boldsymbol{M}_b^j$	$n_1 > 0$	$2n_2$	$2n_3 + 1$	0	$2n_5 + 1 > 0$	$-n_1/2 < n_2 \leq n_1/2$

$$\boldsymbol{R}_2 = \begin{pmatrix} S_0 & S_1 & S_1 \\ S_1 & S_0 & S_1 \\ S_1 & S_1 & S_0 \end{pmatrix}, \quad \det(\boldsymbol{R}_2) = (S_0 + 2S_1)(S_0 - S_1)^2.$$

13.1.2.2. *Cubic and orthorhombic systems*

Cubic system

For cubic space groups, equation (13.1.1.2*a*) leads to the matrix $\boldsymbol{C}$:

$$\boldsymbol{C} = \begin{pmatrix} S & 0 & 0 \\ 0 & S & 0 \\ 0 & 0 & S \end{pmatrix}, \quad \det(\boldsymbol{C}) = S^3.$$

Orthorhombic system

There are six choices of matrices $\boldsymbol{O}_i$ $(i = 1, 2, 3, 4, 5, 6)$ corresponding to the identical orientation ($\boldsymbol{O}_1$), to cyclic permutations of the three axes ($\boldsymbol{O}_2$ and $\boldsymbol{O}_3$) and to the interchange of two axes ($\boldsymbol{O}_4, \boldsymbol{O}_5$ and $\boldsymbol{O}_6$), *i.e.* to the six orthorhombic 'settings'.

$$\boldsymbol{O}_1 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}; \quad \boldsymbol{O}_2 = \begin{pmatrix} 0 & S_{12} & 0 \\ 0 & 0 & S_{23} \\ S_{31} & 0 & 0 \end{pmatrix};$$

$$\boldsymbol{O}_3 = \begin{pmatrix} 0 & 0 & S_{13} \\ S_{21} & 0 & 0 \\ 0 & S_{32} & 0 \end{pmatrix}; \quad \boldsymbol{O}_4 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & 0 & S_{23} \\ 0 & S_{32} & 0 \end{pmatrix};$$

$$\boldsymbol{O}_5 = \begin{pmatrix} 0 & 0 & S_{13} \\ 0 & S_{22} & 0 \\ S_{31} & 0 & 0 \end{pmatrix}; \quad \boldsymbol{O}_6 = \begin{pmatrix} 0 & S_{12} & 0 \\ S_{21} & 0 & 0 \\ 0 & 0 & S_{33} \end{pmatrix}.$$

The determinant is always equal to the product of the three non-zero coefficients, $\det(\boldsymbol{O}_i) = \pm S_{1j}S_{2k}S_{3l}$.

Table 13.1.2.2. *Isomorphic subgroups of the space groups* (*cont.*)

ORTHORHOMBIC SYSTEM

$$\boldsymbol{O}_1 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{22} > 0, S_{33} > 0, S_{11}S_{22}S_{33} > 1$

	S_{11}	S_{22}	S_{33}
$\boldsymbol{O}_1^a$	n_1	n_2	n_3
$\boldsymbol{O}_1^b$	n_1	n_2	$2n_3+1$
$\boldsymbol{O}_1^c$	$2n_1+1$	$2n_2+1$	n_3
$\boldsymbol{O}_1^d$	$2n_1+1$	$2n_2+1$	$2n_3+1$
$\boldsymbol{O}_1^e$	$2n_1$	$2n_2$	$2n_3+1$
$\boldsymbol{O}_1^f$	$2n_1$	$2n_2$	n_3
$\boldsymbol{O}_1^g$	$2n_1$	$2n_2$	$2n_3$
$\boldsymbol{O}_1^h$	$2n_1+1$	n_2	n_3
$\boldsymbol{O}_1^i$	$2n_1+1$	n_2	$2n_3+1$
$\boldsymbol{O}_1^j$	n_1	$2n_2+1$	$2n_3+1$
$\boldsymbol{O}_1^k$	n_1	$2n_2$	$2n_3$
$\boldsymbol{O}_1^l$	$2n_1+1$	$2n_2$	$2n_3$

$$\boldsymbol{O}_4 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & 0 & S_{23} \\ 0 & S_{32} & 0 \end{pmatrix}$$

Conditions: $S_{11} = 2n_1 > 0, S_{23} = -n_2 < 0, S_{32} = 2n_3 > 0$

$$\boldsymbol{O}_5 = \begin{pmatrix} 0 & 0 & S_{13} \\ 0 & S_{22} & 0 \\ S_{31} & 0 & 0 \end{pmatrix}$$

Conditions: $S_{13} = -n_1 < 0, S_{22} = 2n_2 > 0, S_{31} = 2n_3 > 0$

$$\boldsymbol{O}_6 = \begin{pmatrix} 0 & S_{12} & 0 \\ S_{21} & 0 & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{12} = 2n_1 > 0, S_{21} = -n_2 < 0, S_{33} = 2n_3 > 0$

The following general rule exists: only those matrices $\boldsymbol{O}_i$ are permissible for which, if the non-zero coefficients are replaced by 1, the corresponding transformation of the axes conserves the Hermann–Mauguin symbol.

Examples

(1) When the three letters of the Hermann–Mauguin symbol are the same, as in *P*222, *Pmmm*, *Pnnn etc.*, the Hermann–Mauguin symbol does not change and all six matrices are valid.

(2) When the *z* axis plays a privileged role and when the *x* and *y* axes are equivalent, only $\boldsymbol{O}_1$ and $\boldsymbol{O}_6$ apply. Examples are $P222_1$, *Pbam* and *Ccca*. In *Pmma*, the *x* and *y* axes are not equivalent because the interchange leads to *Pmmb* (the non-equivalence of the *x* and *y* axes can also be recognized by inspection of the full symbol $P2_1/m\ 2/m\ 2/a$).

(3) Matrix $\boldsymbol{O}_1$ always applies.

13.1.2.3. *Triclinic system*

As stated above, *P*1 has only isomorphic subgroups and the general nature of the matrix $\boldsymbol{S}$ [equation (13.1.1.3)] requires the use of special techniques (*cf.* Chapter 13.2, *Derivative lattices*); they apply also to $P\bar{1}$.

Table 13.1.2.2. *Isomorphic subgroups of the space groups* (*cont.*)

TETRAGONAL SYSTEM

$$\boldsymbol{T}_1 = \begin{pmatrix} S_{11} & -S_{21} & 0 \\ S_{21} & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{21} \geq 0, S_{33} > 0, (S_{11}^2 + S_{21}^2)S_{33} > 1$

	S_{11}	S_{21}	S_{33}
$\boldsymbol{T}_1^a$	n_1	n_2	n_3
$\boldsymbol{T}_1^b$	n_1	n_2	$4n_3+1$
$\boldsymbol{T}_1^c$	n_1	n_2	$4n_3+3$
$\boldsymbol{T}_1^d$	n_1	n_2	$2n_3+1$
$\boldsymbol{T}_1^e$	$2n_1+1$	$2n_2$	$2n_3+1$
$\boldsymbol{T}_1^f$	$2n_1$	$2n_2+1$	$2n_3+1$
$\boldsymbol{T}_1^g$	$2n_1+1$	$2n_2+1$	$2n_3$
$\boldsymbol{T}_1^h$	$2n_1$	$2n_2$	$2n_3$
$\boldsymbol{T}_1^i$	$2n_1+1$	$2n_2$	n_3
$\boldsymbol{T}_1^j$	$2n_1$	$2n_2+1$	n_3

$$\boldsymbol{T}_2 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{33} > 0, S_{11}S_{33} > 1$

	S_{11}		S_{33}
$\boldsymbol{T}_2^a$	n_1		n_2
$\boldsymbol{T}_2^b$	$2n_1+1$		n_2
$\boldsymbol{T}_2^c$	n_1		$4n_2+1$
$\boldsymbol{T}_2^d$	n_1		$4n_2+3$
$\boldsymbol{T}_2^e$	$2n_1+1$		$4n_2+1$
$\boldsymbol{T}_2^f$	$2n_1+1$		$4n_2+3$
$\boldsymbol{T}_2^g$	n_1		$2n_2+1$
$\boldsymbol{T}_2^h$	$2n_1+1$		$2n_2+1$
$\boldsymbol{T}_2^i$	$2n_1$		$2n_2$

$$\boldsymbol{T}_3 = \begin{pmatrix} S_{11} & -S_{11} & 0 \\ S_{11} & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions : $S_{11} > 0, S_{33} > 0$

$\boldsymbol{T}_3^a : S_{33} = n_1$; $\boldsymbol{T}_3^b : S_{33} = 4n_1 + 1$; $\boldsymbol{T}_3^c : S_{33} = 4n_1 + 1$;

$\boldsymbol{T}_3^d : S_{33} = 2n_1 + 1$; $\boldsymbol{T}_3^e : S_{33} = 2n_1$

13.1.2.4. *Parity conditions*

In equation (13.1.1.2*b*), there occurs the choice of the origin by means of *s*, the nature of the lattice by means of $\boldsymbol{t}_\mathcal{G}$ and the nature of the symmetry operations by means of the column matrices $\boldsymbol{w}$ and $\boldsymbol{w}'$. The three factors, origin, lattice type, screw and glide components, impose parity conditions on the coefficients of the matrix $\boldsymbol{S}$. Only a few examples are given here.

When $(\boldsymbol{W}, \boldsymbol{w})$ and $(\boldsymbol{W}', \boldsymbol{w}')$ are operators of lattice translations of $\mathcal{H}$, say $(\boldsymbol{I}, \boldsymbol{t}_\mathcal{G})$ and $(\boldsymbol{I}, \boldsymbol{t}_\mathcal{H})$, equation (13.1.1.2*b*) reduces to

$$\boldsymbol{S} \cdot \boldsymbol{t}_\mathcal{H} = \boldsymbol{t}_\mathcal{G}. \qquad (13.1.1.4)$$

Example

In a tetragonal *I* lattice, $\boldsymbol{t}_\mathcal{G}$ is either an integral or a fractional translation. If $\boldsymbol{t}_\mathcal{H}$ is $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and the matrix $\boldsymbol{S}$ is replaced by $\boldsymbol{T}_1$, one obtains

Table 13.1.2.2. *Isomorphic subgroups of the space groups* (*cont.*)

TRIGONAL AND HEXAGONAL SYSTEMS

Hexagonal axes

$$\boldsymbol{H}_1 = \begin{pmatrix} S_{11} & -S_{21} & 0 \\ S_{21} & S_{11}-S_{21} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{11} > 0, 0 \leq S_{21} < S_{11}, S_{33} > 0, (S_{11}^2 + S_{21}^2 - S_{11}S_{21})S_{33} > 1$

$\boldsymbol{H}_1^a : S_{33} = n_1$; $\boldsymbol{H}_1^b : S_{33} = 3n_1 + 1$; $\boldsymbol{H}_1^c : S_{33} = 3n_1 + 2$;

$\boldsymbol{H}_1^d : S_{33} = 6n_1 + 1$; $\boldsymbol{H}_1^e : S_{33} = 6n_1 + 5$; $\boldsymbol{H}_1^f : S_{33} = 2n_3 + 1$

Conditions: $S_{11} > 0, S_{21} \geq 0, S_{33} > 0, (S_{11}^2 + S_{21}^2 - S_{11}S_{21})S_{33} > 1$

	S_{11}	S_{21}	S_{33}
$\boldsymbol{H}_1^g$	$3n_1+1$	$3n_2$	$3n_3+1$
$\boldsymbol{H}_1^h$	$3n_1+2$	$3n_2+2$	$3n_3+1$
$\boldsymbol{H}_1^i$	$3n_1$	$3n_2+1$	$3n_3+1$
$\boldsymbol{H}_1^j$	$3n_1+1$	$3n_2+1$	$3n_3+2$
$\boldsymbol{H}_1^k$	$3n_1+2$	$3n_2$	$3n_3+2$
$\boldsymbol{H}_1^l$	$3n_1$	$3n_2+2$	$3n_3+2$
$\boldsymbol{H}_1^m$	$3n_1+1$	$3n_2+2$	$3n_3$
$\boldsymbol{H}_1^n$	$3n_1+2$	$3n_2+1$	$3n_3$
$\boldsymbol{H}_1^o$	$3n_1$	$3n_2$	$3n_3$

$$\boldsymbol{H}_2 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{33} > 0, S_{11}S_{33} > 1$

	S_{11}		S_{33}
$\boldsymbol{H}_2^a$	n_1		n_2
$\boldsymbol{H}_2^b$	n_1		$3n_2+1$
$\boldsymbol{H}_2^c$	n_1		$3n_2+2$
$\boldsymbol{H}_2^d$	$3n_1+1$		$3n_2+1$
$\boldsymbol{H}_2^e$	$3n_1+2$		$3n_2+2$
$\boldsymbol{H}_2^f$	$3n_1$		$3n_2$
$\boldsymbol{H}_2^g$	n_1		$2n_2+1$
$\boldsymbol{H}_2^h$	$3n_1+1$		$6n_2+1$
$\boldsymbol{H}_2^i$	$3n_1+2$		$6n_2+5$
$\boldsymbol{H}_2^j$	$3n_1$		$6n_2+3$
$\boldsymbol{H}_2^k$	n_1		$6n_2+1$
$\boldsymbol{H}_2^l$	n_1		$6n_2+5$

$$\boldsymbol{H}_3 = \begin{pmatrix} 2S_{11} & -S_{11} & 0 \\ S_{11} & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{33} > 0$

$\boldsymbol{H}_3^a : S_{33} = n_1$; $\boldsymbol{H}_3^b : S_{33} = 6n_1 + 1$; $\boldsymbol{H}_3^c : S_{33} = 6n_1 + 5$;

$\boldsymbol{H}_3^d : S_{33} = 3n_1 + 1$; $\boldsymbol{H}_3^e : S_{33} = 3n_1 + 2$; $\boldsymbol{H}_3^f : S_{33} = 2n_1 + 1$

Rhombohedral axes

$$\boldsymbol{R}_1 = \begin{pmatrix} S_0 & S_2 & S_1 \\ S_1 & S_0 & S_2 \\ S_2 & S_1 & S_0 \end{pmatrix}$$

Conditions: $S_0 > 0, S_1 \leq S_0, -(S_0 + S_1) < S_2 < S_0$,

$(S_0 + S_1 + S_2)(S_0^2 + S_1^2 + S_2^2 - S_0S_1 - S_1S_2 - S_2S_0) > 1$

$$\boldsymbol{R}_2 = \begin{pmatrix} S_0 & S_1 & S_1 \\ S_1 & S_0 & S_1 \\ S_1 & S_1 & S_0 \end{pmatrix}$$

Conditions: $\boldsymbol{R}_2^a : S_0 > 0, -S_0/2 < S_1 < S_0$;

$\boldsymbol{R}_b^2 : S_0 > 0, -S_0/2 < S_1 < S_0, S_0 + 2S_1 = 2n + 1$

Table 13.1.2.2. *Isomorphic subgroups of the space groups* (*cont.*)

CUBIC SYSTEM

$$\boldsymbol{C} = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{11} \end{pmatrix}$$

Condition: $S_{11} > 1$

$\boldsymbol{C}^a : S_{11} = n_1$; $\boldsymbol{C}^b : S_{11} = 2n_1 + 1$;

$\boldsymbol{C}^c : S_{11} = 4n_1 + 1$; $\boldsymbol{C}^d : S_{11} = 4n_1 + 3$

Table of space subgroups

No. 1 $P1 : \boldsymbol{S}$; No. 2 $P\bar{1} : \boldsymbol{S}$; No. 3 $P112 : \boldsymbol{M}_c^a$; $P121 : \boldsymbol{M}_a^b$;
No. 4 $P112_1 : \boldsymbol{M}_c^b$; $P12_11 : \boldsymbol{M}_b^b$; No. 5 $A112 : \boldsymbol{M}_c^c, \boldsymbol{M}_c^d, \boldsymbol{M}_c^e$;
$C121 : \boldsymbol{M}_b^c, \boldsymbol{M}_b^d, \boldsymbol{M}_b^e$; No. 6 $P11m : \boldsymbol{M}_c^a$; $P1m1 : \boldsymbol{M}_b^a$; No. 7 $P11a : \boldsymbol{M}_c^f$;
$P1c1 : \boldsymbol{M}_b^f$; No. 8 $A11m : \boldsymbol{M}_c^c, \boldsymbol{M}_c^d, \boldsymbol{M}_c^e$; $C1m1 : \boldsymbol{M}_b^c, \boldsymbol{M}_b^d, \boldsymbol{M}_b^e$;
No. 9 $A11a : \boldsymbol{M}_c^g, \boldsymbol{M}_c^h, \boldsymbol{M}_c^i$; $C1c1 : \boldsymbol{M}_b^g, \boldsymbol{M}_b^h, \boldsymbol{M}_b^i$; No. 10 $P112/m : \boldsymbol{M}_c^a$;
$P12/m1 : \boldsymbol{M}_b^a$; No. 11 $P112_1/m : \boldsymbol{M}_c^b$; $P12_1/m1 : \boldsymbol{M}_b^b$;
No. 12 $A112/m : \boldsymbol{M}_c^c, \boldsymbol{M}_c^d, \boldsymbol{M}_c^e$; $C12/m1 : \boldsymbol{M}_b^c, \boldsymbol{M}_b^d, \boldsymbol{M}_b^e$;
No. 13 $P112/a : \boldsymbol{M}_c^f$; $P12/c1 : \boldsymbol{M}_b^f$;
No. 14 $P112_1/a : \boldsymbol{M}_c^j$; $P12_1/c1 : \boldsymbol{M}_b^j$;
No. 15 $A112/a : \boldsymbol{M}_c^g, \boldsymbol{M}_c^h, \boldsymbol{M}_c^i$; $C12/c1$; $\boldsymbol{M}_b^g, \boldsymbol{M}_b^h, \boldsymbol{M}_b^i$; No. 16 $P222 : \boldsymbol{O}_1^a$;
No. 17 $P222_1 : \boldsymbol{O}_1^b$; No. 18 $P2_12_12 : \boldsymbol{O}_1^c$; No. 19 $P2_12_12_1 : \boldsymbol{O}_1^d$;
No. 20 $C222_1 : \boldsymbol{O}_1^d, \boldsymbol{O}_1^e$; No. 21 $C222 : \boldsymbol{O}_1^c, \boldsymbol{O}_1^f, \boldsymbol{O}_4, \boldsymbol{O}_5$;
No. 22 $F222 : \boldsymbol{O}_1^d, \boldsymbol{O}_1^g$; No. 23 $I222 : \boldsymbol{O}_1^d, \boldsymbol{O}_1^g$; No. 24 $I2_12_12_1 : \boldsymbol{O}_1^d$;
No. 25 $Pmm2 : \boldsymbol{O}_1^a$; No. 26 $Pmc2_1$; $\boldsymbol{O}_1^b$; No. 27 $Pcc2 : \boldsymbol{O}_1^b$;
No. 28 $Pma2 : \boldsymbol{O}_1^h$; No. 29 $Pca2_1 : \boldsymbol{O}_1^i$; No. 30 $Pnc2 : \boldsymbol{O}_1^j$;
No. 31 $Pmn2_1 : \boldsymbol{O}_1^i$; No. 32 $Pba2 : \boldsymbol{O}_1^c$; No. 33 $Pna2 : \boldsymbol{O}_1^d$;
No. 34 $Pnn2 : \boldsymbol{O}_1^d$; No. 35 $Cmm2 : \boldsymbol{O}_1^c, \boldsymbol{O}_1^f$; No. 36 $Cmc2_1 : \boldsymbol{O}_1^d$;
No. 37 $Ccc2 : \boldsymbol{O}_1^d, \boldsymbol{O}_1^e$; No. 38 $Amm2 : \boldsymbol{O}_1^j, \boldsymbol{O}_1^k, \boldsymbol{O}_6$; No. 39 $Abm2 : \boldsymbol{O}_1^j$;
No. 40 $Ama2 : \boldsymbol{O}_1^d, \boldsymbol{O}_1^l$; No. 41 $Aba2 : \boldsymbol{O}_1^d$; No. 42 $Fmm2 : \boldsymbol{O}_1^d, \boldsymbol{O}_1^g$;
No. 43 $Fdd2 : \boldsymbol{O}_1^d$; No. 44 $Imm2 : \boldsymbol{O}_1^d, \boldsymbol{O}_1^g$; No. 45 $Iba2 : \boldsymbol{O}_1^d$;
No. 46 $Ima2 : \boldsymbol{O}_1^d$; No. 47 $Pmmm : \boldsymbol{O}_1^a$; No. 48 $Pnnn : \boldsymbol{O}_1^d$;
No. 49 $Pccm : \boldsymbol{O}_1^b$; No. 50 $Pban : \boldsymbol{O}_1^c$; No. 51 $Pmma : \boldsymbol{O}_1^h$
No. 52 $Pnna : \boldsymbol{O}_1^d$; No. 53 $Pmna : \boldsymbol{O}_1^i$; No. 54 $Pcca : \boldsymbol{O}_1^i$;
No. 55 $Pbam : \boldsymbol{O}_1^c$; No. 56 $Pccn : \boldsymbol{O}_1^d$; No. 57 $Pbcm : \boldsymbol{O}_1^j$;
No. 58 $Pnnm : \boldsymbol{O}_1^d$; No. 59 $Pmmn : \boldsymbol{O}_1^c$; No. 60 $Pbcn : \boldsymbol{O}_1^d$;
No. 61 $Pbca : \boldsymbol{O}_1^d$; No. 62 $Pnma : \boldsymbol{O}_1^d$; No. 63 $Cmcm : \boldsymbol{O}_1^d, \boldsymbol{O}_1^e$;
No. 64 $Cmca : \boldsymbol{O}_1^d$; No. 65 $Cmmm : \boldsymbol{O}_1^c, \boldsymbol{O}_1^f, \boldsymbol{O}_4, \boldsymbol{O}_5$;
No. 66 $Cccm : \boldsymbol{O}_1^d, \boldsymbol{O}_1^e$; No. 67 $Cmma : \boldsymbol{O}_1^c$; No. 68 $Ccca : \boldsymbol{O}_1^d$;
No. 69 $Fmmm : \boldsymbol{O}_1^d, \boldsymbol{O}_1^g$; No. 70 $Fddd : \boldsymbol{O}_1^d$; No. 71 $Immm : \boldsymbol{O}_1^d, \boldsymbol{O}_1^g$;
No. 72 $Ibam : \boldsymbol{O}_1^d$; No. 73 $Ibca : \boldsymbol{O}_1^d$; No. 74 $Imma : \boldsymbol{O}_1^d$;
No. 75 $P4 : \boldsymbol{T}_1^a$; No. 76 $P4_1 : \boldsymbol{T}_1^b$(subgroups $P4_1$), $\boldsymbol{T}_1^c$(subgroups $P4_3$);
No. 77 $P4_2 : \boldsymbol{T}_1^d$; No. 78 $P4_3 : \boldsymbol{T}_1^b$(subgroups $P4_3$), $\boldsymbol{T}_1^c$(subgroups $P4_1$);
No. 79 $I4 : \boldsymbol{T}_1^e, \boldsymbol{T}_1^f, \boldsymbol{T}_1^g, \boldsymbol{T}_1^h$; No. 80 $I4_1 : \boldsymbol{T}_1^e, \boldsymbol{T}_1^f$; No. 81 $P\bar{4} : \boldsymbol{T}_1^a$;
No. 82 $I\bar{4} : \boldsymbol{T}_1^e, \boldsymbol{T}_1^f, \boldsymbol{T}_1^g, \boldsymbol{T}_1^h$; No. 83 $P4/m : \boldsymbol{T}_1^a$; No. 84 $P4_2/m : \boldsymbol{T}_1^d$;
No. 85 $P4/n : \boldsymbol{T}_1^i, \boldsymbol{T}_1^j$; No. 86 $P4_2/n : \boldsymbol{T}_1^e, \boldsymbol{T}_1^f$;
No. 87 $I4/m : \boldsymbol{T}_1^e, \boldsymbol{T}_1^f, \boldsymbol{T}_1^g, \boldsymbol{T}_1^h$; No. 88 $I4_1/a : \boldsymbol{T}_1^e, \boldsymbol{T}_1^f$;
No. 89 $P422 : \boldsymbol{T}_2^a, \boldsymbol{T}_3^a$; No. 90 $P42_12 : \boldsymbol{T}_2^b$;
No. 91 $P4_122 : \boldsymbol{T}_2^c$(subgroups $P4_122$), $\boldsymbol{T}_2^d$(subgroups $P4_322$),
$\boldsymbol{T}_3^b$(subgroups $P4_122$), $\boldsymbol{T}_3^c$(subgroups $P4_322$);
No. 92 $P4_12_12 : \boldsymbol{T}_2^e$(subgroups $P4_12_12$), $\boldsymbol{T}_2^f$(subgroups $P4_32_12$);
No. 93 $P4_222 : \boldsymbol{T}_2^g, \boldsymbol{T}_3^d$; No. 94 $P4_22_12 : \boldsymbol{T}_2^h$;
No. 95 $P4_322 : \boldsymbol{T}_2^c$(subgroups $P4_322$), $\boldsymbol{T}_2^d$(subgroups $P4_122$),
$\boldsymbol{T}_3^b$(subgroups $P4_322$), $\boldsymbol{T}_3^c$(subgroups $P4_122$);
No. 96 $P4_32_12 : \boldsymbol{T}_2^e$(subgroups $P4_32_12$), $\boldsymbol{T}_2^f$(subgroups $P4_12_12$);
No. 97 $I422 : \boldsymbol{T}_2^h, \boldsymbol{T}_2^i, \boldsymbol{T}_3^e$; No. 98 $I4_122 : \boldsymbol{T}_2^h$; No. 99 $P4mm : \boldsymbol{T}_2^a, \boldsymbol{T}_3^a$;
No. 100 $P4bm : \boldsymbol{T}_2^b$; No. 101 $P4_2cm : \boldsymbol{T}_2^g$; No. 102 $P4_2nm : \boldsymbol{T}_2^h$;

Table 13.1.2.2. *Isomorphic subgroups of the space groups* (*cont.*)

Table of space subgroups (*cont.*)

No. 103 $P4cc$: $\boldsymbol{T}_2^g, \boldsymbol{T}_3^d$; No. 104 $P4nc$: $\boldsymbol{T}_2^h$; No. 105 $P4_2mc$: $\boldsymbol{T}_2^g$;
No. 106 $P4_2bc$: $\boldsymbol{T}_2^h$; No. 107 $I4mm$: $\boldsymbol{T}_2^h, \boldsymbol{T}_2^i, \boldsymbol{T}_3^e$; No. 108 $I4cm$: $\boldsymbol{T}_2^h$;
No. 109 $I4_1md$: $\boldsymbol{T}_2^h$; No. 110 $I4_1cd$: $\boldsymbol{T}_2^h$; No. 111 $P\bar{4}2m$: $\boldsymbol{T}_2^a$;
No. 112 $P\bar{4}2c$: $\boldsymbol{T}_2^g$; No. 113 $P\bar{4}2_1m$: $\boldsymbol{T}_2^b$; No. 114 $P\bar{4}2_1c$: $\boldsymbol{T}_2^h$;
No. 115 $P\bar{4}m2$: $\boldsymbol{T}_2^a$; No. 116 $P\bar{4}c2$: $\boldsymbol{T}_2^g$; No. 117 $P\bar{4}b2$: $\boldsymbol{T}_2^b$;
No. 118 $P\bar{4}n2$: $\boldsymbol{T}_2^h$; No. 119 $I\bar{4}m2$: $\boldsymbol{T}_2^h, \boldsymbol{T}_2^i$; No. 120 $I\bar{4}c2$: $\boldsymbol{T}_2^h$;
No. 121 $I\bar{4}2m$: $\boldsymbol{T}_2^h, \boldsymbol{T}_2^i$; No. 122 $I\bar{4}2d$: $\boldsymbol{T}_2^h$; No. 123 $P4/mmm$: $\boldsymbol{T}_2^a, \boldsymbol{T}_3^a$;
No. 124 $P4/mcc$: $\boldsymbol{T}_2^g, \boldsymbol{T}_3^d$; No. 125 $P4/nbm$: $\boldsymbol{T}_2^b$; No. 126 $P4/nnc$: $\boldsymbol{T}_2^h$;
No. 127 $P4/mbm$: $\boldsymbol{T}_2^b$; No. 128 $P4/mnc$: $\boldsymbol{T}_2^h$; No. 129 $P4/nmm$: $\boldsymbol{T}_2^b$;
No. 130 $P4/ncc$: $\boldsymbol{T}_2^h$; No. 131 $P4_2/mmc$: $\boldsymbol{T}_2^g$; No. 132 $P4_2/mcm$: $\boldsymbol{T}_2^g$;
No. 133 $P4_2/nbc$: $\boldsymbol{T}_2^h$; No. 134 $P4_2/nnm$: $\boldsymbol{T}_2^h$; No. 135 $P4_2/mbc$: $\boldsymbol{T}_2^h$;
No. 136 $P4_2/mnm$: $\boldsymbol{T}_2^h$; No. 137 $P4_2/nmc$: $\boldsymbol{T}_2^h$; No. 138 $P4_2/ncm$: $\boldsymbol{T}_2^h$;
No. 139 $I4/mmm$: $\boldsymbol{T}_2^h$, $\boldsymbol{T}_2^i$, $\boldsymbol{T}_3^e$; No. 140 $I4/mcm$: $\boldsymbol{T}_2^h$;
No. 141 $I4_1/amd$: $\boldsymbol{T}_2^h$; No. 142 $I4_1/acd$: $\boldsymbol{T}_2^h$; No. 143 $P3$: $\boldsymbol{H}_1^a$;
No. 144 $P3_1$: $\boldsymbol{H}_1^b$(subgroups $P3_1$), $\boldsymbol{H}_1^c$(subgroups $P3_2$);
No. 145 $P3_2$: $\boldsymbol{H}_1^b$(subgroups $P3_2$), $\boldsymbol{H}_1^c$(subgroups $P3_1$);
No. 146 $R3$ (hexagonal axes): $\boldsymbol{H}_1^g$, $\boldsymbol{H}_1^h$, $\boldsymbol{H}_1^i$, $\boldsymbol{H}_1^j$, $\boldsymbol{H}_1^k$, $\boldsymbol{H}_1^l$, $\boldsymbol{H}_1^m$, $\boldsymbol{H}_1^n$, $\boldsymbol{H}_1^o$;
$R3$ (rhombohedral axes): $\boldsymbol{R}_1$; No. 147 $P\bar{3}$: $\boldsymbol{H}_1^a$;
No. 148 $R\bar{3}$ (hexagonal axes): $\boldsymbol{H}_1^g$, $\boldsymbol{H}_1^h$, $\boldsymbol{H}_1^i$, $\boldsymbol{H}_1^j$, $\boldsymbol{H}_1^k$, $\boldsymbol{H}_1^l$, $\boldsymbol{H}_1^m$, $\boldsymbol{H}_1^n$, $\boldsymbol{H}_1^o$;
$R\bar{3}$ (rhombohedral axes): $\boldsymbol{R}_1$; No. 149 $P312$: $\boldsymbol{H}_2^a$; No. 150 $P321$: $\boldsymbol{H}_2^a$;
No. 151 $P3_112$: $\boldsymbol{H}_2^b$(subgroups $P3_112$), $\boldsymbol{H}_2^c$(subgroups $P3_212$);
No. 152 $P3_121$: $\boldsymbol{H}_2^b$(subgroups $P3_121$), $\boldsymbol{H}_2^c$(subgroups $P3_221$);
No. 153 $P3_212$: $\boldsymbol{H}_2^b$(subgroups $P3_212$), $\boldsymbol{H}_2^c$(subgroups $P3_112$);
No. 154 $P3_221$: $\boldsymbol{H}_2^b$(subgroups $P3_221$), $\boldsymbol{H}_2^c$(subgroups $P3_121$);
No. 155 $R32$ (hexagonal axes): $\boldsymbol{H}_2^d$, $\boldsymbol{H}_2^e$, $\boldsymbol{H}_2^f$; $R32$ (rhombohedral axes): $\boldsymbol{R}_2^a$; No. 156 $P3m1$: $\boldsymbol{H}_2^a$; No. 157 $P31m$: $\boldsymbol{H}_2^a$; No. 158 $P3c1$: $\boldsymbol{H}_2^g$;
No. 159 $P31c$: $\boldsymbol{H}_2^g$; No. 160 $R3m$ (hexagonal axes): $\boldsymbol{H}_2^d, \boldsymbol{H}_2^e, \boldsymbol{H}_2^f$;
$R3m$ (rhombohedral axes): $\boldsymbol{R}_2^a$; No. 161 $R3c$ (hexagonal axes): $\boldsymbol{H}_2^h, \boldsymbol{H}_2^i, \boldsymbol{H}_2^j$; $R3c$ (rhombohedral axes): $\boldsymbol{R}_2^b$; No. 162 $P\bar{3}1m$: $\boldsymbol{H}_2^a$;
No. 163 $P\bar{3}1c$: $\boldsymbol{H}_2^g$; No. 164 $P\bar{3}m1$: $\boldsymbol{H}_2^a$; No. 165 $P\bar{3}c1$: $\boldsymbol{H}_2^g$;
No. 166 $R\bar{3}m$ (hexagonal axes): $\boldsymbol{H}_2^d, \boldsymbol{H}_2^e, \boldsymbol{H}_2^f$; $R\bar{3}m$ (rhombohedral axes): $\boldsymbol{R}_2^a$; No. 167 $R\bar{3}c$ (hexagonal axes): $\boldsymbol{H}_2^h, \boldsymbol{H}_2^i, \boldsymbol{H}_2^j$;
$R\bar{3}c$ (rhombohedral axes): $\boldsymbol{R}_2^b$; No. 168 $P6$: $\boldsymbol{H}_1^a$;
No. 169 $P6_1$: $\boldsymbol{H}_1^d$(subgroups $P6_1$), $\boldsymbol{H}_1^e$(subgroups $P6_5$);
No. 170 $P6_5$: $\boldsymbol{H}_1^d$(subgroups $P6_5$), $\boldsymbol{H}_1^e$(subgroups $P6_1$);
No. 171 $P6_2$: $\boldsymbol{H}_1^b$(subgroups $P6_2$), $\boldsymbol{H}_1^c$(subgroups $P6_4$);
No. 172 $P6_4$: $\boldsymbol{H}_1^b$(subgroups $P6_4$), $\boldsymbol{H}_1^c$(subgroups $P6_2$);
No. 173 $P6_3$: $\boldsymbol{H}_1^f$; No. 174 $P\bar{6}$: $\boldsymbol{H}_1^a$; No. 175 $P6/m$: $\boldsymbol{H}_1^a$;
No. 176 $P6_3/m$: $\boldsymbol{H}_1^f$; No. 177 $P622$: $\boldsymbol{H}_2^a$; $\boldsymbol{H}_3^a$;
No. 178 $P6_122$: $\boldsymbol{H}_2^k$(subgroups $P6_122$), $\boldsymbol{H}_2^l$(subgroups $P6_522$), $\boldsymbol{H}_3^b$(subgroups $P6_122$), $\boldsymbol{H}_3^c$(subgroups $P6_522$);
No. 179 $P6_522$: $\boldsymbol{H}_2^k$(subgroups $P6_522$), $\boldsymbol{H}_2^l$(subgroups $P6_122$), $\boldsymbol{H}_3^b$(subgroups $P6_522$), $\boldsymbol{H}_3^c$(subgroups $P6_122$);
No. 180 $P6_222$: $\boldsymbol{H}_2^b$(subgroups $P6_222$), $\boldsymbol{H}_2^c$(subgroups $P6_422$), $\boldsymbol{H}_3^d$(subgroups $P6_222$), $\boldsymbol{H}_3^e$(subgroups $P6_422$);
No. 181 $P6_422$: $\boldsymbol{H}_2^b$(subgroups $P6_422$), $\boldsymbol{H}_2^c$(subgroups $P6_222$), $\boldsymbol{H}_3^d$(subgroups $P6_422$), $\boldsymbol{H}_3^e$(subgroups $P6_222$); No. 182 $P6_322$: $\boldsymbol{H}_2^g, \boldsymbol{H}_3^f$;
No. 183 $P6mm$: $\boldsymbol{H}_2^a, \boldsymbol{H}_3^a$; No. 184 $P6cc$: $\boldsymbol{H}_2^g, \boldsymbol{H}_3^f$; No. 185 $P6_3cm$: $\boldsymbol{H}_2^g$;
No. 186 $P6_3mc$: $\boldsymbol{H}_2^g$; No. 187 $P\bar{6}m2$: $\boldsymbol{H}_2^a$; No. 188 $P\bar{6}c2$: $\boldsymbol{H}_2^g$;
No. 189 $P\bar{6}2m$: $\boldsymbol{H}_2^a$; No. 190 $P\bar{6}2c$: $\boldsymbol{H}_2^g$; No. 191 $P6/mmm$: $\boldsymbol{H}_2^a, \boldsymbol{H}_3^a$;
No. 192 $P6/mcc$: $\boldsymbol{H}_2^g, \boldsymbol{H}_3^f$; No. 193 $P6_3/mcm$: $\boldsymbol{H}_2^g$;
No. 194 $P6_3/mmc$: $\boldsymbol{H}_2^g$; No. 195 $P23$: $\boldsymbol{C}^a$; No. 196 $F23$: $\boldsymbol{C}^a$;
No. 197 $I23$: $\boldsymbol{C}^a$; No. 198 $P2_13$: $\boldsymbol{C}^b$; No. 199 $I2_13$: $\boldsymbol{C}^b$;
No. 200 $Pm\bar{3}$: $\boldsymbol{C}^a$; No. 201 $Pn\bar{3}$: $\boldsymbol{C}^b$; No. 202 $Fm\bar{3}$: $\boldsymbol{C}^a$;
No. 203 $Fd\bar{3}$: $\boldsymbol{C}^b$; No. 204 $Im\bar{3}$: $\boldsymbol{C}^a$; No. 205 $Pa\bar{3}$: $\boldsymbol{C}^b$;
No. 206 $Ia\bar{3}$: $\boldsymbol{C}^b$; No. 207 $P432$: $\boldsymbol{C}^a$; No. 208 $P4_232$: $\boldsymbol{C}^b$;

Table 13.1.2.2. *Isomorphic subgroups of the space groups* (*cont.*)

Table of space subgroups (*cont.*)

No. 209 $F432$: $\boldsymbol{C}^a$; No. 210 $F4_132$: $\boldsymbol{C}^b$; No. 211 $I432$: $\boldsymbol{C}^a$;
No. 212 $P4_332$: $\boldsymbol{C}^c$(subgroups $P4_332$), $\boldsymbol{C}^d$(subgroups $P4_132$);
No. 213 $P4_132$: $\boldsymbol{C}^c$(subgroups $P4_132$), $\boldsymbol{C}^d$(subgroups $P4_332$);
No. 214 $I4_132$: $\boldsymbol{C}^b$; No. 215 $P\bar{4}3m$: $\boldsymbol{C}^a$; No. 216 $F\bar{4}3m$: $\boldsymbol{C}^a$;
No. 217 $I\bar{4}3m$: $\boldsymbol{C}^a$: No. 218 $P\bar{4}3n$: $\boldsymbol{C}^b$; No. 219 $F\bar{4}3c$: $\boldsymbol{C}^b$;
No. 220 $I\bar{4}3d$: $\boldsymbol{C}^b$; No. 221 $Pm\bar{3}m$: $\boldsymbol{C}^a$; No. 222 $Pn\bar{3}n$: $\boldsymbol{C}^b$;
No. 223 $Pm\bar{3}n$: $\boldsymbol{C}^b$; No. 224 $Pn\bar{3}m$: $\boldsymbol{C}^b$; No. 225 $Fm\bar{3}m$: $\boldsymbol{C}^a$;
No. 226 $Fm\bar{3}c$: $\boldsymbol{C}^b$; No. 227 $Fd\bar{3}m$: $\boldsymbol{C}^b$; No. 228 $Fd\bar{3}c$: $\boldsymbol{C}^b$;
No. 229 $Im\bar{3}m$: $\boldsymbol{C}^a$; No. 230 $Ia\bar{3}d$: $\boldsymbol{C}^b$.

$$\boldsymbol{S}\begin{pmatrix}\frac{1}{2}\\ \frac{1}{2}\\ \frac{1}{2}\end{pmatrix} = \begin{pmatrix}\frac{1}{2}(S_{11}-S_{21})\\ \frac{1}{2}(S_{11}+S_{21})\\ \frac{1}{2}S_{33}\end{pmatrix} = \begin{pmatrix}n_1\\ n_2\\ n_3\end{pmatrix} \text{ or } \begin{pmatrix}n_1+\frac{1}{2}\\ n_2+\frac{1}{2}\\ n_3+\frac{1}{2}\end{pmatrix} \quad (13.1.1.4a)$$

with n_1, n_2, n_3 integers.

From this it follows that either S_{11} and S_{21} have the same parity and S_{33} is even, or else S_{11} and S_{21} have opposite parities and S_{33} is odd.

If $(\boldsymbol{W}, \boldsymbol{w})$ and $(\boldsymbol{W}', \boldsymbol{w}')$ represent the same operation 4_1 in the two P lattices of $\mathcal{G}$ and $\mathcal{H}$, with $\hat{\boldsymbol{w}} = \boldsymbol{w}' = (00\frac{1}{4})$, for $\boldsymbol{s} = \boldsymbol{0}$, equation (13.1.1.2$b$) reduces to

$$\tfrac{1}{4}(S_{33}-1) = n \quad \text{or} \quad S_{33} = 4n+1, \quad n \text{ integer}.$$

There are similar conditions for glide and other screw operations.

The location part $\boldsymbol{s}$, *i.e.* the relative positions of the origins O and O' of group and subgroup, is another important problem. This problem can be approached in two ways. First, only standard settings and origins (as defined in the space-group tables of this volume) of the group $\mathcal{G}$ and its subgroup $\mathcal{H}$ are considered. In this case, the origin relation between $\mathcal{G}$ and $\mathcal{H}$ must be indicated by the appropriate column $\boldsymbol{s}$. For instance, in $P2_12_12_1$ the matrices $\boldsymbol{O}_4$, $\boldsymbol{O}_5$, $\boldsymbol{O}_6$ are only possible for $s \neq o$, say $s = (-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4})$. Second, one can describe $\mathcal{H}$ based on the same origin as $\mathcal{G}$, *i.e.* O and O' coincide. In this case, nonstandard descriptions of $\mathcal{H}$ frequently result and one has to indicate the location of the symmetry elements of $\mathcal{H}$ with respect to the origin of $\mathcal{G}$.

Unfortunately, it was not possible to incorporate in the present tables the implications that the choice of the origin has on the coefficients S_{ij} (*cf.* Bertaut, 1956; Billiet, 1978; Bertaut & Billiet, 1979).

The explicit forms of the matrices $\boldsymbol{S}$ for each space group and each plane group are given in Tables 13.1.2.1 and 13.1.2.2 without origin indications.

Example

Consider space groups $P4/mmm$ and $P4/mcc$ and envisage the matrix $\boldsymbol{T}_3$ which has the determinant $2S_{33}S_{11}^2$. Its lowest value is 2 with $S_{11} = S_{33} = 1$. The matrix $\boldsymbol{T}_3$ then implies the axis transformation

$$\mathbf{a}' = \mathbf{a} + \mathbf{b}, \quad \mathbf{b}' = -\mathbf{a} + \mathbf{b}, \quad \mathbf{c}' = \mathbf{c}.$$

Envisage also the matrix $\boldsymbol{T}_2$ which has the determinant $S_{11}^2S_{33}$. Its lowest value for a proper subgroup is 2 with $S_{11} = 1$ and $S_{33} = 2$. The axis transformation is here

$$\mathbf{a}' = \mathbf{a}, \quad \mathbf{b}' = \mathbf{b}, \quad \mathbf{c}' = 2\mathbf{c}.$$

This transformation is permitted for $P4/mmm$ but not for $P4/mcc$ where the parity rules require $S_{33} = 2n + 1$. Thus, the lowest value of $S_{11}^2 S_{33}$ for a subgroup of space group $P4/mcc$ is 3 and the axis transformation is

$$\mathbf{a}' = \mathbf{a}, \quad \mathbf{b}' = \mathbf{b}, \quad \mathbf{c}' = 3\mathbf{c}.$$

13.1.2.5. *Plane groups*

There is no difficulty in reducing the preceding considerations to plane groups, where $\boldsymbol{S}$ is a (2×2) matrix and $\boldsymbol{s}$ a (2×1) matrix.

13.1.2.6. *Tables of matrices for isomorphic subgroups*

The matrices and the restrictions on the coefficients are listed for the plane groups in Table 13.1.2.1 and for the space groups in Table 13.1.2.2.

For the triclinic and monoclinic systems, there is an infinite choice of matrices for each index, owing to the infinite number of equivalent unit cells. For the other space groups, several different (but finitely many) choices of matrix occur. In all cases, we have restricted this choice to *one* matrix for each group–subgroup relation so that *each subgroup is listed exactly once* (apart from origin choice).

Example

No. 178, $P6_122$, has the matrix $\boldsymbol{H}_2^k$ for *all isomorphic and isosymbolic* subgroups $P6_122$, having the lattices $n_{11}\mathbf{a}$, $n_{11}\mathbf{b}$, $(6n_{33}+1)\mathbf{c}$ $(n_{11} \geq 1, n_{33} \geq 0)$, whilst $\boldsymbol{H}_3^b$ is used for *all isomorphic and isosymbolic* subgroups with the lattices $n_{11}(2\mathbf{a}+\mathbf{b})$, $n_{11}(-\mathbf{a}+\mathbf{b})$, $(6n_{33}+1)\mathbf{c}$ $(n_{11} \geq 1, n_{33} \geq 0)$. These two kinds of subgroups are obviously different, having different translation lattices. The same group, $P6_122$, has the matrix $\boldsymbol{H}_2^l$ for the *isomorphic and enantiomorphic subgroups* $P6_522$ of lattices $n_{11}\mathbf{a}$, $n_{11}\mathbf{b}$, $(6n_{33}+5)\mathbf{c}$ whilst $\boldsymbol{H}_3^c$ is used for the *isomorphic and enantiomorphic subgroups* $P6_522$ of lattices $n_{11}(2\mathbf{a}+\mathbf{b})$, $n_{11}(-\mathbf{a}+\mathbf{b})$, $(6n_{33}+5)\mathbf{c}$.

In the tables, each system is preceded by the appropriate general form of the matrix, which is also given in this chapter, followed by the more specialized matrices such as $\boldsymbol{T}_2, \boldsymbol{T}_3$. Under *Conditions*, we have listed the nonredundant inequalities and parity conditions* that ensure the uniqueness of the matrix for each subgroup. Also, we have used rules in order to avoid repetition of equivalent unit cells. For instance, for trigonal and hexagonal groups (rhombohedral groups excepted), we have restricted $\mathbf{a}'$ to lie between $\mathbf{a}$ and $\mathbf{a}+\mathbf{b}$ excluding this last vector from the sector of 60° because there is a repetition after a 60° rotation of the unit cell.

* More exactly 'congruence modulo $\mathbb{Z}$ conditions'.

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13.2. Derivative lattices

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13.2.1. Introduction

The three-dimensional subgroups of space group $P1$ and the two-dimensional subgroups of plane group $p1$ are all isomorphic subgroups; *i.e.* these subgroups are pure translation groups and correspond to lattices. In the past, these lattices have often been called 'superlattices' (the term 'sublattice' perhaps would be more precise). To avoid confusion, the lattices that correspond to the isomorphic subgroups of $P1$ and $p1$ are designated here as *derivative lattices.*

The number of derivative lattices (both maximal and nonmaximal) of a lattice is infinite and always several derivative lattices of index $[i] \geq 2$ exist. Only for prime indices are maximal derivative lattices obtained; for any prime p, there are (p^2+p+1) three-dimensional derivative lattices of $P1$, whereas there are $(p+1)$ two-dimensional derivative lattices of $p1$. The number of nonmaximal derivative lattices is given by more complicated formulae (*cf.* Billiet & Rolley Le Coz, 1980).

Table 13.2.2.1. *Three-dimensional derivative lattices of indices 2 to 7*

The entry for each derivative lattice starts with a running number which is followed, between parentheses, by the appropriate basis-vector relations. It should be noted that the seven derivative lattices of index 2 are also recorded in the space-group table of $P1$ (No. 1) under *Maximal isomorphic subgroups of lowest index* but in the slightly different sequence 1, 2, 3, 6, 5, 4, 7.

Index 2	$1(2\mathbf{a},\mathbf{b},\mathbf{c})$; $2(\mathbf{a},2\mathbf{b},\mathbf{c})$; $3(\mathbf{a},\mathbf{b},2\mathbf{c})$; $4(2\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c})$; $5(2\mathbf{a},\mathbf{b},\mathbf{c}+\mathbf{a})$; $6(\mathbf{a},2\mathbf{b},\mathbf{c}+\mathbf{b})$; $7(2\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{a})$
Index 3	$1(3\mathbf{a},\mathbf{b},\mathbf{c})$; $2(\mathbf{a},3\mathbf{b},\mathbf{c})$; $3(\mathbf{a},\mathbf{b},3\mathbf{c})$; $4(3\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c})$; $5(3\mathbf{a},\mathbf{b},\mathbf{c}+\mathbf{a})$; $6(\mathbf{a},3\mathbf{b},\mathbf{c}+\mathbf{b})$; $7(3\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c})$; $8(3\mathbf{a},\mathbf{b},\mathbf{c}-\mathbf{a})$; $9(\mathbf{a},3\mathbf{b},\mathbf{c}-\mathbf{b})$; $10(3\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{a})$; $11(3\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}-\mathbf{a})$; $12(3\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}+\mathbf{a})$; $13(3\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}-\mathbf{a})$
Index 4	$1(4\mathbf{a},\mathbf{b},\mathbf{c})$; $2(\mathbf{a},4\mathbf{b},\mathbf{c})$; $3(\mathbf{a},\mathbf{b},4\mathbf{c})$; $4(4\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c})$; $5(4\mathbf{a},\mathbf{b},\mathbf{c}+\mathbf{a})$; $6(\mathbf{a},4\mathbf{b},\mathbf{c}+\mathbf{b})$; $7(4\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c})$; $8(4\mathbf{a},\mathbf{b},\mathbf{c}-\mathbf{a})$; $9(\mathbf{a},4\mathbf{b},\mathbf{c}-\mathbf{b})$; $10(4\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c})$; $11(4\mathbf{a},\mathbf{b},\mathbf{c}+2\mathbf{a})$; $12(2\mathbf{a},2\mathbf{b}+\mathbf{a},\mathbf{c})$; $13(\mathbf{a},4\mathbf{b},\mathbf{c}+2\mathbf{b})$; $14(2\mathbf{a},\mathbf{b},2\mathbf{c}+\mathbf{a})$; $15(\mathbf{a},2\mathbf{b},2\mathbf{c}+\mathbf{b})$; $16(4\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{a})$; $17(4\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}-\mathbf{a})$; $18(4\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}+\mathbf{a})$; $19(4\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}-\mathbf{a})$; $20(4\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}+2\mathbf{a})$; $21(4\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}+\mathbf{a})$; $22(2\mathbf{a},2\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{b})$; $23(4\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}+2\mathbf{a})$; $24(4\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}-\mathbf{a})$; $25(2\mathbf{a},2\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{a}+\mathbf{b})$; $26(4\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}+2\mathbf{a})$; $27(2\mathbf{a},2\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{a})$; $28(2\mathbf{a},\mathbf{b}+\mathbf{a},2\mathbf{c}+\mathbf{a})$; $29(2\mathbf{a},2\mathbf{b},\mathbf{c})$; $30(2\mathbf{a},\mathbf{b},2\mathbf{c})$; $31(\mathbf{a},2\mathbf{b},2\mathbf{c})$; $32(2\mathbf{a},2\mathbf{b},\mathbf{c}+\mathbf{a})$; $33(2\mathbf{a},2\mathbf{b},\mathbf{c}+\mathbf{b})$; $34(2\mathbf{a},\mathbf{b}+\mathbf{a},2\mathbf{c})$; $35(2\mathbf{a},2\mathbf{b},\mathbf{c}+\mathbf{a}+\mathbf{b})$
Index 5	$1(5\mathbf{a},\mathbf{b},\mathbf{c})$; $2(\mathbf{a},5\mathbf{b},\mathbf{c})$; $3(\mathbf{a},\mathbf{b},5\mathbf{c})$; $4(5\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c})$; $5(5\mathbf{a},\mathbf{b},\mathbf{c}+\mathbf{a})$; $6(\mathbf{a},5\mathbf{b},\mathbf{c}+\mathbf{b})$; $7(5\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c})$; $8(5\mathbf{a},\mathbf{b},\mathbf{c}-\mathbf{a})$; $9(\mathbf{a},5\mathbf{b},\mathbf{c}-\mathbf{b})$; $10(5\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c})$; $11(5\mathbf{a},\mathbf{b},\mathbf{c}-2\mathbf{a})$; $12(\mathbf{a},5\mathbf{b},\mathbf{c}+2\mathbf{b})$; $13(5\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c})$; $14(5\mathbf{a},\mathbf{b},\mathbf{c}+2\mathbf{a})$; $15(\mathbf{a},5\mathbf{b},\mathbf{c}-2\mathbf{b})$; $16(5\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{a})$; $17(5\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}-\mathbf{a})$; $18(5\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}+\mathbf{a})$; $19(5\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}-\mathbf{a})$; $20(5\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}+2\mathbf{a})$; $21(5\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}-2\mathbf{a})$; $22(5\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}+\mathbf{a})$; $23(5\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c}+\mathbf{a})$; $24(5\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}-2\mathbf{a})$; $25(5\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c}+2\mathbf{a})$; $26(5\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}+2\mathbf{a})$; $27(5\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c}-\mathbf{a})$; $28(5\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}-2\mathbf{a})$; $29(5\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c}-2\mathbf{a})$; $30(5\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}-\mathbf{a})$; $31(5\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}+2\mathbf{a})$

13.2.2. Construction of three-dimensional derivative lattices

It is possible to construct in a *simple way* all three-dimensional derivative lattices of a lattice (Table 13.2.2.1). Starting from a primitive unit cell defined by $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, *each* derivative lattice possesses exactly *one* primitive unit cell defined by $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ by means of the following relation

$$\mathbf{a}' = p_1\mathbf{a}, \quad \mathbf{b}' = p_2\mathbf{b} + q_1\mathbf{a}, \quad \mathbf{c}' = p_3\mathbf{c} + r_1\mathbf{a} + q_2\mathbf{b}$$

$$(p_1, p_2, p_3 \text{ positive integers, not necessarily prime;}$$
$$\text{index} = p_1p_2p_3 > 1; q_1, q_2, r_1 \text{ integers;}$$
$$-p_1/2 < q_1 \leq p_1/2; -p_2/2 < q_2 \leq p_2/2;$$
$$-p_1/2 < r_1 \leq p_1/2).$$

Note that *the vector* $\mathbf{a}'$ *has the same direction as the vector* $\mathbf{a}$ *and the plane* $(\mathbf{a}', \mathbf{b}')$ *is parallel to the plane* $(\mathbf{a}, \mathbf{b})$, *i.e.* the matrix of the transformation is *triangular.* Equivalent formulae can be derived by permutations of the vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ which keep the directions of $\mathbf{b}'$ or $\mathbf{c}'$ and which preserve the parallelism of the planes $(\mathbf{b}', \mathbf{c}')$ with $(\mathbf{b}, \mathbf{c})$ or $(\mathbf{a}', \mathbf{c}')$ with $(\mathbf{a}, \mathbf{c})$.

Table 13.2.2.1. *Three-dimensional derivative lattices of indices 2 to 7* (*cont.*)

Index 6	$1(6\mathbf{a},\mathbf{b},\mathbf{c})$; $2(\mathbf{a},6\mathbf{b},\mathbf{c})$; $3(\mathbf{a},\mathbf{b},6\mathbf{c})$; $4(6\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c})$; $5(6\mathbf{a},\mathbf{b},\mathbf{c}+\mathbf{a})$; $6(\mathbf{a},6\mathbf{b},\mathbf{c}+\mathbf{b})$; $7(6\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c})$; $8(6\mathbf{a},\mathbf{b},\mathbf{c}-\mathbf{a})$; $9(\mathbf{a},6\mathbf{b},\mathbf{c}-\mathbf{b})$; $10(6\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c})$; $11(6\mathbf{a},\mathbf{b},\mathbf{c}+2\mathbf{a})$; $12(\mathbf{a},6\mathbf{b},\mathbf{c}+2\mathbf{b})$; $13(3\mathbf{a},2\mathbf{b}+\mathbf{a},\mathbf{c})$; $14(\mathbf{a},3\mathbf{b},2\mathbf{c}+\mathbf{b})$; $15(3\mathbf{a},\mathbf{b},2\mathbf{c}+\mathbf{a})$; $16(6\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c})$; $17(6\mathbf{a},\mathbf{b},\mathbf{c}-2\mathbf{a})$; $18(\mathbf{a},6\mathbf{b},\mathbf{c}-2\mathbf{b})$; $19(3\mathbf{a},2\mathbf{b}-\mathbf{a},\mathbf{c})$; $20(\mathbf{a},3\mathbf{b},2\mathbf{c}-\mathbf{b})$; $21(3\mathbf{a},\mathbf{b},2\mathbf{c}-\mathbf{a})$; $22(6\mathbf{a},\mathbf{b}+3\mathbf{a},\mathbf{c})$; $23(6\mathbf{a},\mathbf{b},\mathbf{c}+3\mathbf{a})$; $24(\mathbf{a},6\mathbf{b},\mathbf{c}+3\mathbf{b})$; $25(2\mathbf{a},3\mathbf{b}+\mathbf{a},\mathbf{c})$; $26(\mathbf{a},2\mathbf{b},3\mathbf{c}+\mathbf{b})$; $27(2\mathbf{a},\mathbf{b},3\mathbf{c}+\mathbf{a})$; $28(6\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{a})$; $29(6\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}-\mathbf{a})$; $30(6\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}+\mathbf{a})$; $31(6\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}-\mathbf{a})$; $32(6\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}+2\mathbf{a})$; $33(6\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}-2\mathbf{a})$; $34(3\mathbf{a},2\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{b})$; $35(3\mathbf{a},2\mathbf{b}-\mathbf{a},\mathbf{c}+\mathbf{b})$; $36(6\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}+\mathbf{a})$; $37(6\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c}+\mathbf{a})$; $38(6\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}+2\mathbf{a})$; $39(6\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}-\mathbf{a})$; $40(3\mathbf{a},2\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{a}+\mathbf{b})$; $41(6\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}-2\mathbf{a})$; $42(6\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c}-\mathbf{a})$; $43(3\mathbf{a},2\mathbf{b}-\mathbf{a},\mathbf{c}-\mathbf{a}+\mathbf{b})$; $44(6\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}+3\mathbf{a})$; $45(6\mathbf{a},\mathbf{b}+3\mathbf{a},\mathbf{c}+\mathbf{a})$; $46(2\mathbf{a},3\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{b})$; $47(6\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}+3\mathbf{a})$; $48(6\mathbf{a},\mathbf{b}+3\mathbf{a},\mathbf{c}-\mathbf{a})$; $49(2\mathbf{a},3\mathbf{b}+\mathbf{a},\mathbf{c}-\mathbf{b})$; $50(6\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}+2\mathbf{a})$; $51(3\mathbf{a},2\mathbf{b}+\mathbf{a},\mathbf{c}-\mathbf{a})$; $52(3\mathbf{a},\mathbf{b}-\mathbf{a},2\mathbf{c}+\mathbf{a})$; $53(6\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c}-2\mathbf{a})$; $54(3\mathbf{a},2\mathbf{b}-\mathbf{a},\mathbf{c}-\mathbf{a})$; $55(3\mathbf{a},\mathbf{b}-\mathbf{a},2\mathbf{c}-\mathbf{a})$; $56(6\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}-2\mathbf{a})$; $57(3\mathbf{a},2\mathbf{b}-\mathbf{a},\mathbf{c}+\mathbf{a})$; $58(3\mathbf{a},\mathbf{b}+\mathbf{a},2\mathbf{c}+\mathbf{a})$; $59(6\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c}+2\mathbf{a})$; $60(3\mathbf{a},2\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{a})$; $61(3\mathbf{a},\mathbf{b}+\mathbf{a},2\mathbf{c}-\mathbf{a})$; $62(6\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}+3\mathbf{a})$; $63(2\mathbf{a},3\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{a}-\mathbf{b})$; $64(3\mathbf{a},2\mathbf{b},\mathbf{c}-\mathbf{a}+\mathbf{b})$; $65(6\mathbf{a},\mathbf{b}+3\mathbf{a},\mathbf{c}+2\mathbf{a})$; $66(3\mathbf{a},2\mathbf{b}+\mathbf{a},\mathbf{c}-\mathbf{a}+\mathbf{b})$; $67(2\mathbf{a},3\mathbf{b},\mathbf{c}+\mathbf{a}-\mathbf{b})$; $68(6\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c}+3\mathbf{a})$; $69(2\mathbf{a},3\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{b}+\mathbf{a})$; $70(3\mathbf{a},2\mathbf{b},\mathbf{c}+\mathbf{a}+\mathbf{b})$; $71(6\mathbf{a},\mathbf{b}+3\mathbf{a},\mathbf{c}-2\mathbf{a})$; $72(3\mathbf{a},2\mathbf{b}-\mathbf{a},\mathbf{c}+\mathbf{a}+\mathbf{b})$; $73(2\mathbf{a},3\mathbf{b},\mathbf{c}+\mathbf{a}+\mathbf{b})$; $74(6\mathbf{a},\mathbf{b}+3\mathbf{a},\mathbf{c}+3\mathbf{a})$; $75(2\mathbf{a},3\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{a})$; $76(2\mathbf{a},\mathbf{b}+\mathbf{a},3\mathbf{c}+\mathbf{a})$; $77(3\mathbf{a},2\mathbf{b},\mathbf{c})$; $78(3\mathbf{a},\mathbf{b},2\mathbf{c})$; $79(2\mathbf{a},3\mathbf{b},\mathbf{c})$; $80(2\mathbf{a},\mathbf{b},3\mathbf{c})$; $81(\mathbf{a},3\mathbf{b},2\mathbf{c})$; $82(\mathbf{a},2\mathbf{b},3\mathbf{c})$; $83(3\mathbf{a},2\mathbf{b},\mathbf{c}+\mathbf{a})$; $84(3\mathbf{a},\mathbf{b}+\mathbf{a},2\mathbf{c})$; $85(2\mathbf{a},3\mathbf{b},\mathbf{c}+\mathbf{b})$; $86(3\mathbf{a},2\mathbf{b},\mathbf{c}-\mathbf{a})$; $87(3\mathbf{a},\mathbf{b}-\mathbf{a},2\mathbf{c})$; $88(2\mathbf{a},3\mathbf{b},\mathbf{c}-\mathbf{b})$; $89(3\mathbf{a},2\mathbf{b},\mathbf{c}+\mathbf{b})$; $90(2\mathbf{a},3\mathbf{b},\mathbf{c}+\mathbf{a})$; $91(2\mathbf{a},\mathbf{a}+\mathbf{b},3\mathbf{c})$

Table 13.2.2.1. *Three-dimensional derivative lattices of indices 2 to 7* (*cont.*)

Index 7	$1(7\mathbf{a},\mathbf{b},\mathbf{c})$; $2(\mathbf{a},7\mathbf{b},\mathbf{c})$; $3(\mathbf{a},\mathbf{b},7\mathbf{c})$; $4(7\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c})$; $5(7\mathbf{a},\mathbf{b},\mathbf{c}+\mathbf{b})$; $6(\mathbf{a},7\mathbf{b},\mathbf{c}+\mathbf{b})$; $7(7\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c})$; $8(7\mathbf{a},\mathbf{b},\mathbf{c}-\mathbf{a})$; $9(\mathbf{a},7\mathbf{b},\mathbf{c}-\mathbf{b})$; $10(7\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c})$; $11(7\mathbf{a},\mathbf{b},\mathbf{c}-3\mathbf{a})$; $12(\mathbf{a},7\mathbf{b},\mathbf{c}+2\mathbf{b})$; $13(7\mathbf{a},\mathbf{b}-3\mathbf{a},\mathbf{c})$; $14(7\mathbf{a},\mathbf{b},\mathbf{c}+2\mathbf{a})$; $15(\mathbf{a},7\mathbf{b},\mathbf{c}-3\mathbf{b})$; $16(7\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c})$; $17(7\mathbf{a},\mathbf{b},\mathbf{c}+3\mathbf{a})$; $18(\mathbf{a},7\mathbf{b},\mathbf{c}-2\mathbf{b})$; $19(7\mathbf{a},\mathbf{b}+3\mathbf{a},\mathbf{c})$; $20(7\mathbf{a},\mathbf{b},\mathbf{c}-2\mathbf{a})$; $21(\mathbf{a},7\mathbf{b},\mathbf{c}+3\mathbf{b})$; $22(7\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{a})$; $23(7\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}-\mathbf{a})$; $24(7\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}+\mathbf{a})$; $25(7\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}-\mathbf{a})$; $26(7\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}+2\mathbf{a})$; $27(7\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}-2\mathbf{a})$; $28(7\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}+\mathbf{a})$; $29(7\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c}+\mathbf{a})$; $30(7\mathbf{a},\mathbf{b}+3\mathbf{a},\mathbf{c}-3\mathbf{a})$; $31(7\mathbf{a},\mathbf{b}-3\mathbf{a},\mathbf{c}+3\mathbf{a})$; $32(7\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}+3\mathbf{a})$; $33(7\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}-3\mathbf{a})$; $34(7\mathbf{a},\mathbf{b}+3\mathbf{a},\mathbf{c}+\mathbf{a})$; $35(7\mathbf{a},\mathbf{b}-3\mathbf{a},\mathbf{c}+\mathbf{a})$; $36(7\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}-2\mathbf{a})$; $37(7\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c}+2\mathbf{a})$; $38(7\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}+2\mathbf{a})$; $39(7\mathbf{a},\mathbf{b}-3\mathbf{a},\mathbf{c}-\mathbf{a})$; $40(7\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}-3\mathbf{a})$; $41(7\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c}-2\mathbf{a})$; $42(7\mathbf{a},\mathbf{b}+3\mathbf{a},\mathbf{c}-\mathbf{a})$; $43(7\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}+3\mathbf{a})$; $44(7\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}+3\mathbf{a})$; $45(7\mathbf{a},\mathbf{b}+3\mathbf{a},\mathbf{c}+2\mathbf{a})$; $46(7\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c}-3\mathbf{a})$; $47(7\mathbf{a},\mathbf{b}-3\mathbf{a},\mathbf{c}+2\mathbf{a})$; $48(7\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}-3\mathbf{a})$; $49(7\mathbf{a},\mathbf{b}-3\mathbf{a},\mathbf{c}-2\mathbf{a})$; $50(7\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c}+3\mathbf{a})$; $51(7\mathbf{a},\mathbf{b}+3\mathbf{a},\mathbf{c}-2\mathbf{a})$; $52(7\mathbf{a},\mathbf{b}+3\mathbf{a},\mathbf{c}+3\mathbf{a})$; $53(7\mathbf{a},\mathbf{b}-2\mathbf{a},\mathbf{c}-\mathbf{a})$; $54(7\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}-2\mathbf{a})$; $55(7\mathbf{a},\mathbf{b}-3\mathbf{a},\mathbf{c}-3\mathbf{a})$; $56(7\mathbf{a},\mathbf{b}+2\mathbf{a},\mathbf{c}-\mathbf{a})$; $57(7\mathbf{a},\mathbf{b}-\mathbf{a},\mathbf{c}+2\mathbf{a})$

Example

One can derive easily the 7 derivative lattices of index 2.

$$1(2\mathbf{a},\mathbf{b},\mathbf{c});\ 2(\mathbf{a},2\mathbf{b},\mathbf{c});\ 3(\mathbf{a},\mathbf{b},2\mathbf{c});\ 4(2\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c});$$
$$5(2\mathbf{a},\mathbf{b},\mathbf{c}+\mathbf{a});\ 6(\mathbf{a},2\mathbf{b},\mathbf{c}+\mathbf{b});\ 7(2\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{a}).$$

Another primitive cell of a given derivative lattice is obtained if one of the following three elementary transformations is performed on the vectors of a primitive cell of this derivative lattice:

(i) the sign of a vector is changed;
(ii) two vectors are interchanged;
(iii) to a vector is added q times another vector (q integer).

(i) and (ii) are left-handed transformations, (iii) is right-handed.

Example

The primitive cell $\mathbf{a}'', \mathbf{b}'', \mathbf{c}''$ ($\mathbf{a}''=-2\mathbf{b}-\mathbf{a}$, $\mathbf{b}''=9\mathbf{a}-2\mathbf{c}-2\mathbf{b}$, $\mathbf{c}''=\mathbf{c}-\mathbf{a}+3\mathbf{b}$) belongs to the derivative lattice of index 10 given by the primitive cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ ($\mathbf{a}'=5\mathbf{a}$, $\mathbf{b}'=2\mathbf{b}+\mathbf{a}$, $\mathbf{c}'=\mathbf{c}-2\mathbf{a}+\mathbf{b}$) because these two cells are related by the following sequence of elementary transformations:

$$(-2\mathbf{b}-\mathbf{a},\ 9\mathbf{a}-2\mathbf{c}-2\mathbf{b},\ \mathbf{c}-\mathbf{a}+3\mathbf{b})\overset{\text{(iii)}}{\to}$$
$$(-2\mathbf{b}-\mathbf{a},\ 9\mathbf{a}-2\mathbf{c}-2\mathbf{b},\ \mathbf{c}-2\mathbf{a}+\mathbf{b})\overset{\text{(iii)}}{\to}$$
$$(-2\mathbf{b}-\mathbf{a},\ 5\mathbf{a},\ \mathbf{c}-2\mathbf{a}+\mathbf{b})\overset{\text{(i)}}{\to}(2\mathbf{b}+\mathbf{a},\ 5\mathbf{a},\ \mathbf{c}-2\mathbf{a}+\mathbf{b})$$
$$\overset{\text{(ii)}}{\to}(5\mathbf{a},\ 2\mathbf{b}+\mathbf{a},\ \mathbf{c}-2\mathbf{a}+\mathbf{b});$$

($\mathbf{a}''$, $\mathbf{b}''$, $\mathbf{c}''$) and ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$) have the same handedness.

Table 13.2.3.1. *Two-dimensional derivative lattices of indices 2 to 7*

The entry for each derivative lattice starts with a running number which is followed, between parentheses, by the appropriate basis-vector relations.

Index 2	$1(2\mathbf{a},\mathbf{b})$; $2(\mathbf{a},2\mathbf{b})$; $3(2\mathbf{a},\mathbf{b}+\mathbf{a})$
Index 3	$1(3\mathbf{a},\mathbf{b})$; $2(\mathbf{a},3\mathbf{b})$; $3(3\mathbf{a},\mathbf{b}+\mathbf{a})$; $4(3\mathbf{a},\mathbf{b}-\mathbf{a})$
Index 4	$1(4\mathbf{a},\mathbf{b})$; $2(\mathbf{a},4\mathbf{b})$; $3(4\mathbf{a},\mathbf{b}+\mathbf{a})$; $4(4\mathbf{a},\mathbf{b}-\mathbf{a})$; $5(4\mathbf{a},\mathbf{b}+2\mathbf{a})$; $6(2\mathbf{a},2\mathbf{b}+\mathbf{a})$; $7(2\mathbf{a},2\mathbf{b})$
Index 5	$1(5\mathbf{a},\mathbf{b})$; $2(\mathbf{a},5\mathbf{b})$; $3(5\mathbf{a},\mathbf{b}+\mathbf{a})$; $4(5\mathbf{a},\mathbf{b}-\mathbf{a})$; $5(5\mathbf{a},\mathbf{b}+2\mathbf{a})$; $6(5\mathbf{a},\mathbf{b}-2\mathbf{a})$
Index 6	$1(6\mathbf{a},\mathbf{b})$; $2(\mathbf{a},6\mathbf{b})$; $3(6\mathbf{a},\mathbf{b}+\mathbf{a})$; $4(6\mathbf{a},\mathbf{b}-\mathbf{a})$; $5(6\mathbf{a},\mathbf{b}+2\mathbf{a})$; $6(3\mathbf{a},2\mathbf{b}+\mathbf{a})$; $7(6\mathbf{a},\mathbf{b}-2\mathbf{a})$; $8(3\mathbf{a},2\mathbf{b}-\mathbf{a})$; $9(6\mathbf{a},\mathbf{b}+3\mathbf{a})$; $10(2\mathbf{a},3\mathbf{b}+\mathbf{a})$; $11(3\mathbf{a},2\mathbf{b})$; $12(2\mathbf{a},3\mathbf{b})$
Index 7	$1(7\mathbf{a},\mathbf{b})$; $2(\mathbf{a},7\mathbf{b})$; $3(7\mathbf{a},\mathbf{b}+\mathbf{a})$; $4(7\mathbf{a},\mathbf{b}-\mathbf{a})$; $5(7\mathbf{a},\mathbf{b}+2\mathbf{a})$; $6(7\mathbf{a},\mathbf{b}-3\mathbf{a})$; $7(7\mathbf{a},\mathbf{b}-2\mathbf{a})$; $8(7\mathbf{a},\mathbf{b}+3\mathbf{a})$

13.2.3. Two-dimensional derivative lattices

All previous considerations are valid also for two-dimensional lattices and their derivative lattices (Table 13.2.3.1). The relevant formula for any index is

$$\mathbf{a}'=p_1\mathbf{a},\quad \mathbf{b}'=p_2\mathbf{b}+q\mathbf{a}$$

[**a** direction is kept]

(p_1, p_2 positive integers, not necessarily prime;

index $=p_1p_2>1$; q any integer; $-p_1/2<q\le p_1/2$).

A similar formula is obtained by interchange of **a** and **b**.

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13.1

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14.1. Introduction and definition

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14.1.1. Introduction

In crystal structures belonging to different structure types and showing different space-group symmetries, the relative locations of symmetrically equivalent atoms nevertheless may be the same (*e.g.* Cl in CsCl and F in CaF_2). The concept of *lattice complexes* can be used to reveal relationships between crystal structures even if they belong to different space-group types.

14.1.2. Definition

The term *lattice complex* (*Gitterkomplex*) had originally been created by P. Niggli (1919), but it was not used by him with an unambiguous meaning. Later on, Hermann (1935) modified and specified the concept of lattice complexes, but the rigorous definition used here was proposed much later by Fischer & Koch (1974) [*cf.* also Koch & Fischer (1978)]. An alternative definition was given by Zimmermann & Burzlaff (1974) at the same time.

To introduce the concept of lattice complexes, relationships between point configurations are regarded.

> The set of all points that are symmetrically equivalent to a given one with respect to a certain space group is called a *point configuration* (*cf.* also crystallographic orbit; Section 8.3.2).

In each space group, there exist infinitely many point configurations. Given a coordinate system, they may be obtained by varying the coordinates x, y, z of a starting point and by calculating all symmetrically equivalent points.

Point configurations refer to the arrangements of atoms in crystal structures. They are analogous to the crystal forms in crystal morphology, where a crystal form is a set of symmetrically equivalent faces. Crystal forms are grouped into types designated by names like 'cube', 'tetragonal dipyramid' *etc*. In a similar, though not strictly analogous way, point configurations are also grouped into types, called lattice complexes. For example, all point configurations forming a cubic primitive point lattice belong to the same lattice complex. Each lattice complex is thus a set of infinitely many point configurations. The following stepwise procedure describes all point configurations belonging to the same lattice complex:

(i) Take all point configurations of a particular Wyckoff position in a particular space group. Mathematically these point configurations are distinguished by the following property: the site-symmetry groups of two arbitrary points from any two of the point configurations are conjugate in the space group (*cf.* Section 8.3.2).

(ii) Collect all point configurations of Wyckoff positions that belong to the same Wyckoff set of a given space group (*cf.* Section 8.3.2). Such Wyckoff positions play an analogous role with respect to this space group. Their point configurations have the following property: the site-symmetry groups of two arbitrary points from any two point configurations are conjugate in the affine normalizer (*cf.* Section 15.3.2) of the space group considered.

(iii) Assemble all point configurations of corresponding Wyckoff sets from all space groups of one of the 219 (affine) space-group types, *i.e.* take all point configurations belonging to a particular type of Wyckoff set (Section 8.3.2). Each affine mapping that maps two space groups of the same type onto each other simultaneously maps onto each other the site-symmetry groups of the points from the point configurations of the corresponding Wyckoff sets.

According to (i), (ii) and (iii), a lattice complex* is defined as follows:

> A *lattice complex* is the set of all point configurations that may be generated within one type of Wyckoff set.

Example

> Take, in a particular space group of type $P4/mmm$, the Wyckoff position $4l$ $x00$. The points of each corresponding point configuration form squares that replace the points of the tetragonal primitive lattice referring to Wyckoff position $1a$. For all conceivable point configurations of $4l$, the squares have the same orientation, but their edges have different lengths. Congruent arrangements of squares but shifted by $\frac{1}{2}\mathbf{c}$ or by $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ or by $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ give the point configurations of the Wyckoff positions $4m$, $4n$ and $4o$, respectively, in the same space group. The four Wyckoff positions $4l$ to $4o$, all with site symmetry $m2m.$, make up a Wyckoff set (*cf.* Table 14.2.3.2). They are mapped onto each other, for example, by the translations $\frac{1}{2}\mathbf{c}$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ and $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$, which belong to the Euclidean (and affine) normalizer of the group. If one space group of type $P4/mmm$ is mapped onto another space group of the same type, the Wyckoff set $4l$ to $4o$ as a whole is transformed to $4l$ to $4o$. The individual Wyckoff positions may be interchanged, however. The set of all point configurations from the Wyckoff positions $4l$ to $4o$ of all space groups of type $P4/mmm$ constitutes a lattice complex. Its point configurations may be derived as described above, but now starting from all space groups $P4/mmm$ with all conceivable lengths and orientations of the basis vectors instead of starting from just a particular group. Accordingly, the point configurations may differ in their orientation, in the size of their squares and in the distances between the centres of their squares.

Just as all crystal forms of a particular type may be found in different point-group types, the same lattice complex may occur in different space-group types.

Example

> The lattice complex 'cubic primitive lattice' may be generated, among others, in $Pm\bar{3}m$ $1a, b$, in $Fm\bar{3}m$ $8c$ and in $Ia\bar{3}$ $8a, b$ with site symmetry $m\bar{3}m$, $\bar{4}3m$ and $.\bar{3}.$, respectively. The type of Wyckoff set specified by $Pm\bar{3}m$ $1a, b$ leads to the same set of point configurations as $Fm\bar{3}m$ $8c$ or $Ia\bar{3}$ $8a, b$. Each point configuration of this lattice complex can be generated by a properly chosen space group in each of these space-group types.

All Wyckoff positions, Wyckoff sets and types of Wyckoff set that generate, as described above, the same set of point configurations are assigned to the same lattice complex. Accordingly, the following criterion holds: two Wyckoff positions are

* This definition agrees with that given by Fischer & Koch (1974) and Koch & Fischer (1978), but now the term Wyckoff position is used instead of *Punktlage* or point position, Wyckoff set instead of *Konfigurationslage* or configuration set, type of Wyckoff set instead of *Klasse von Konfigurationslagen* or class of configuration sets. New aspects have been taken into account by Koch & Fischer (1985).

assigned to the same lattice complex if there is a suitable transformation that maps the point configurations of the two Wyckoff positions onto each other and if their space groups belong to the same crystal family (*cf.* Sections 8.2.7 and 8.2.8). Suitable transformations are translations, proper or improper rotations, isotropic or anisotropic expansions or more general affine mappings (without violation of the metric conditions for the corresponding crystal family) and all their products.

By this criterion, the Wyckoff positions of all space groups (1731 entries in the space-group tables, 1128 types of Wyckoff set) are uniquely assigned to 402 lattice complexes.

The same concept has been used for the point configurations and Wyckoff positions in the plane groups. Here the Wyckoff positions (72 entries to the plane-group tables, 51 types of Wyckoff set) are assigned to 30 plane lattice complexes or net complexes (*cf.* Burzlaff *et al.*, 1968).

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14.2. Symbols and properties of lattice complexes

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14.2.1. Reference symbols and characteristic Wyckoff positions

If a lattice complex can be generated in different space-group types, one of them stands out because its corresponding Wyckoff positions show the highest site symmetry. This is called the *characteristic space-group type* of the lattice complex. The space groups of all the other types in which the lattice complex may be generated are subgroups of the space groups of the characteristic type.

Different lattice complexes may have the same characteristic space-group type but in that case they differ in the oriented site symmetry of their Wyckoff positions within the space groups of that type.

The characteristic space-group type and the corresponding oriented site symmetry express the common symmetry properties of all point configurations of a lattice complex. Therefore, they can be used to identify each lattice complex. Within the *reference symbols* of lattice complexes, however, instead of the site symmetry the Wyckoff letter of one of the Wyckoff positions with that site symmetry is given, as was first done by Hermann (1935). This Wyckoff position is called the *characteristic Wyckoff position* of the lattice complex.

Examples

(1) $Pm\bar{3}m$ is the characteristic space-group type for the lattice complex of all cubic primitive point lattices. The Wyckoff positions with the highest possible site symmetry $m\bar{3}m$ are $1a$ 000 and $1b$ $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, from which $1a$ has been chosen as the characteristic position. Thus, the lattice complex is designated $Pm\bar{3}m\ a$.

(2) $Pm\bar{3}m$ is also characteristic for another lattice complex that corresponds to Wyckoff position $8g$ xxx $.3m$. Thus, the reference symbol for this lattice complex is $Pm\bar{3}m\ g$. Each of its point configurations may be derived by replacing each point of a cubic primitive lattice by eight points arranged at the corners of a cube.

In Tables 14.2.3.1 and 14.2.3.2, the reference symbols denote the lattice complex of each Wyckoff position. The reference symbols of characteristic Wyckoff positions are marked by asterisks (*e.g.* $2e$ in $P2/c$). If in a particular space group several Wyckoff positions belong to the same Wyckoff set (*cf.* Koch & Fischer, 1975), the reference symbol is given only once (*e.g.* Wyckoff positions $4l$ to $4o$ in $P4/mmm$). To enable this, the usual sequence of Wyckoff positions had to be changed in a few cases (*e.g.* in $P4_2/mcm$). For Wyckoff positions assigned to the same lattice complex but belonging to different Wyckoff sets, the reference symbol is repeated. In $I4/m$, for example, Wyckoff positions $4c$ and $4d$ are both assigned to the lattice complex $P4/mmm\ a$. They do not belong, however, to the same Wyckoff set because the site-symmetry groups $2/m..$ of $4c$ and $\bar{4}..$ of $4d$ are different.

14.2.2. Additional properties of lattice complexes

14.2.2.1. *The degrees of freedom*

The number of coordinate parameters that can be varied independently within a Wyckoff position is called its number of degrees of freedom. For most lattice complexes, the number of *degrees of freedom* is the same as for any of its Wyckoff positions. The lattice complex with characteristic Wyckoff position $Pm\bar{3}$ $12j$ $m..$ $0yz$, for instance, has two degrees of freedom. If, however, the variation of a coordinate corresponds to a shift of the point configuration as a whole, one degree of freedom is lost. Therefore, $I4_1$ $8b$ xyz is the characteristic Wyckoff position of a lattice complex with only two degrees of freedom, although position $8b$ itself has three degrees of freedom. Another example is given by $P4/m$ $4j$ $m..$ $xy0$ and $P4$ $4d$ 1 xyz. Both Wyckoff positions belong to lattice complex $P4/m\ j$ with two degrees of freedom.

According to its number of degrees of freedom, a lattice complex is called *invariant, univariant, bivariant or trivariant.* In total, there exist 402 lattice complexes, 36 of which are invariant, 106 univariant, 105 bivariant and 155 trivariant. The 30 plane lattice complexes are made up of 7 invariant, 10 univariant and 13 bivariant ones.

Most of the invariant and univariant lattice complexes correspond to several types of Wyckoff set. In contrast to that, only one type of Wyckoff set belongs to each trivariant lattice complex. A bivariant lattice complex may either correspond to one type of Wyckoff set (*e.g.* $Pm\bar{3}\ j$) or to two types ($P4\ d$, for example, belongs to the lattice complex with the characteristic position $P4/m\ j$).

14.2.2.2. *Limiting complexes and comprehensive complexes*

For point groups, the occurrence of limiting crystal forms is well known. In $4/m$, for instance, any tetragonal prism $\{hk0\}$ is a special crystal form with face symmetry $m..$. In point group 4, on the other hand, the tetragonal prisms $\{hk0\}$ belong, as special cases, to the set of general crystal forms $\{hkl\}$, the tetragonal pyramids, and there is no difference between $\{hkl\}$ and $\{hk0\}$ in either the number or the symmetry of their faces. Therefore, the tetragonal prism is called a 'limiting form' of the tetragonal pyramid. In a case like this, all possible sets of equivalent faces belonging to a special type of crystal form (the tetragonal prism) may also be generated as a subset of another more comprehensive type of crystal form (the tetragonal pyramid). Of course, it is not possible, by considering a tetragonal prism by itself, to decide whether it has been generated by point group $4/m$ or by point group 4. This distinction can be made, however, if the tetragonal prism shows the right striations or occurs in combination with other appropriate crystal forms. Low quartz (oriented point group 321) gives a well known example: the hexagonal prism $\{10\bar{1}0\}$ has the same site symmetry 1 as any trigonal trapezohedron $\{hkil\}$. Therefore, $\{10\bar{1}0\}$ may be recognized as a limiting form only if the crystal shows in addition at least one trigonal trapezohedron.

A similar relation may exist between two lattice complexes. Let L be a lattice complex generated by a Wyckoff position of a space group $\mathcal{G}$ (*e.g.* by $P4/mmm$ $4l$ $m2m.$ $x00$). An appropriate Wyckoff position of a subgroup $\mathcal{H}$ of $\mathcal{G}$ (*e.g.* $P4/m$ $4j$ $m..$ $xy0$) may produce not only all point configurations of L but other point configurations in addition (with different orientations of the squares in the example). The complete set then forms a second lattice complex M. Such relationships led to the following definition (Fischer & Koch, 1974, 1978):

> If a lattice complex L forms a true subset of another lattice complex M, the lattice complex L is called a *limiting complex* of M and the lattice complex M a *comprehensive complex* of L.

The point configurations of the limiting complex L are generated within M by restrictions imposed on the coordinate or/and the metrical parameters.

In the above example, such a restriction holds for the y coordinate: the condition $y = 0$ for Wyckoff position $4j$ of $P4/m$ filters out exactly those point configurations that constitute the lattice complex $P4/mmm$ *l*. The latter complex is, therefore, a limiting complex of the lattice complex $P4/m$ *j*. In the present case of restricted coordinates, both complexes belong to the same crystal family and *L* has fewer degrees of freedom than *M*.

Another kind of limiting-complex relation is connected with restrictions for metrical parameters. All point configurations of the lattice complex $Pm\bar{3}m$ *a* are also generated by $P4/mmm$ *a* under the restriction $a = c$, *i.e.* in special space groups of type $P4/mmm$. Here *L* and *M* have the same number of degrees of freedom, but belong to different crystal families.

Finally, the two types of parameter restrictions for limiting complexes may also occur in combination. The trivariant lattice complex with characteristic Wyckoff position $P4_12_12$ 8*b* *xyz*, for example, contains the invariant cubic lattice complex $Fm\bar{3}m$ *a* as a limiting complex. The parameter restrictions necessary are $x = \frac{1}{2}, y = 0, z = \frac{1}{16}, c/a = 4\sqrt{2}$.

As for a limiting form in crystal morphology, it is often impossible to decide by which symmetry (space group and Wyckoff set) a particular point configuration, regarded by itself, has been generated. If a point configuration belongs to a lattice complex that is part of a comprehensive complex, this point configuration is a member of both complexes. As a consequence, the lattice complexes do not form equivalence classes of point configurations. Only if a point configuration is inspected in combination with a sufficient number of other point configurations – like sets of symmetrically equivalent atoms in a crystal structure – does it make sense to assign this point configuration to a particular lattice complex. An example is found in the crystal structures of the spinel type. Here, the oxygen atoms occupy Wyckoff position 32*e* *xxx* in $Fd\bar{3}m$ with $x \approx \frac{3}{8}$ (referred to origin choice 1). If *x* is restricted to $\frac{3}{8}$, the point configurations generated are those of the lattice complex $Fm\bar{3}m$ *a* (formed by all face-centred cubic point lattices). If for a spinel-type structure this restriction holds exactly, the point configurations of the cations would, nevertheless, reveal the true generating symmetry of the oxygen point configuration. It has, therefore, to be considered a member of the comprehensive complex $Fd\bar{3}m$ *e* rather than a member of the lattice complex $Fm\bar{3}m$ *a* (which includes among others the point configuration of the copper atoms in the crystal structure of copper). For practical applications, a point configuration contained in several lattice complexes may be investigated within the complex that is the least comprehensive but still allows the physical behaviour under discussion. This corresponds to the definition of the symmetry of a crystal generally used in crystallography: the highest symmetry that can be assigned to a crystal as a whole is that of its least symmetrical property known to date.

Even though limiting-complex relations are very useful for establishing crystallochemical relationships between different crystal structures, a complete study has not yet been carried out. Apart from isolated examples in the literature, systematic treatments have been given only for special aspects: plane lattice complexes (Burzlaff *et al.*, 1968); cubic lattice complexes (Koch, 1974); point complexes, rod complexes and layer complexes (Fischer & Koch, 1978); extraordinary orbits for plane groups (Lawrenson & Wondratschek, 1976); noncharacteristic orbits of space groups except those that are due to metrical specialization (Engel *et al.*, 1984). The closely related concepts of limiting complexes and noncharacteristic orbits have been compared by Koch & Fischer (1985).

14.2.2.3. *Weissenberg complexes*

Depending on their site-symmetry groups, two kinds of Wyckoff position may be distinguished:

(i) The site-symmetry group of any point is a proper subgroup of another site-symmetry group from the same space group. Then, the Wyckoff position contains, among others, point configurations with the property that the distance between two suitable chosen points is shorter than any small number $\varepsilon > 0$.

Example

Each point configuration of the lattice complex with the characteristic Wyckoff position $P4/mmm$ 4*j* *m*.2*m* *xx*0 may be imagined as squares of four points surrounding the points of a tetragonal primitive lattice. For $x \to 0$, the squares become infinitesimally small. Point configurations with $x = 0$ show site symmetry $4/mmm$, their multiplicity is decreased from 4 to 1, and they belong to lattice complex $P4/mmm$ *a*.

(ii) The site-symmetry group of any point belonging to the regarded Wyckoff position is not a subgroup of any other site-symmetry group from the same space group.

Example

In *Pmma*, there does not exist a site-symmetry group that is a proper supergroup of *mm*2, the site-symmetry group of Wyckoff position *Pmma* 2*e* $\frac{1}{4}0z$. As a consequence, the distance between any two symmetrically equivalent points belonging to *Pmma* *e* cannot become shorter than the minimum of $\frac{1}{2}a, b$ and *c*.

A lattice complex contains either Wyckoff positions exclusively of the first or exclusively of the second kind. Most lattice complexes are made up from Wyckoff positions of the first kind.

There exist, however, 67 lattice complexes that do not contain point configurations with infinitesimal short distances between symmetry-related points [*cf. Hauptgitter* (Weissenberg, 1925)]. These lattice complexes have been called *Weissenberg complexes* by Fischer *et al.* (1973). The 36 invariant lattice complexes are trivial examples of Weissenberg complexes. In addition, there exist 24 univariant (monoclinic 2, orthorhombic 5, tetragonal 7, hexagonal 5, cubic 5) and 6 bivariant Weissenberg complexes (monoclinic 1, orthorhombic 2, tetragonal 1, hexagonal 2). The only trivariant Weissenberg complex is $P2_12_12_1$ *a*. All Weissenberg complexes with degrees of freedom have the following common property: each Weissenberg complex contains at least two invariant limiting complexes belonging to the same crystal family.

Example

Pmma *e* is a comprehensive complex of *Pmmm* *a* and of *Cmmm* *a*. Within the characteristic Wyckoff position, $\frac{1}{4}00$ refers to *Pmmm* *a* and $\frac{1}{4}0\frac{1}{4}$ to *Cmmm* *a*.

Except for the seven invariant plane lattice complexes, there exists only one further Weissenberg complex within the plane groups, namely the univariant rectangular complex *p*2*mg* *c*.

14.2.3. Descriptive symbols

14.2.3.1. *Introduction*

For the study of relations between crystal structures, lattice-complex symbols are desirable that show as many relations between point configurations as possible. To this end, Hermann (1960) derived descriptive lattice-complex symbols that were further developed by Donnay *et al.* (1966) and completed by Fischer *et al.* (1973). These symbols describe the arrangements of the points in the point configurations and refer directly to the coordinate descriptions of the Wyckoff positions. Since a lattice complex, in general, contains Wyckoff positions with different coordinate descriptions, it may be represented by several different descriptive

(*continued on page* 870)

Table 14.2.3.1. *Plane groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes*

Wyckoff positions of the same Wyckoff set can be recognized by their consecutive listing without repetition of the reference symbol. Characteristic Wyckoff sets are marked by asterisks.

1	***p*1**			
1	a	1	p2 a	P[xy]
2	***p*2**			
1	a	2	* p2 a	P
1	b			$0\frac{1}{2}$ P
1	c			$\frac{1}{2}0$ P
1	d			$\frac{1}{2}\frac{1}{2}$ P
2	e	1	* p2 e	P2xy
3	***pm***			
1	a	.m.	p2mm a	P[y]
1	b			$\frac{1}{2}0$ P[y]
2	c	1	p2mm e	P2x[y]
4	***pg***			
2	a	1	p2mg c	2.. $P_bC1x[y]$
5	***cm***			
2	a	.m.	c2mm a	C[y]
4	b	1	c2mm d	C2x[y]
6	***p*2*mm***			
1	a	2mm	* p2mm a	P
1	b			$0\frac{1}{2}$ P
1	c			$\frac{1}{2}0$ P
1	d			$\frac{1}{2}\frac{1}{2}$ P
2	e	..m	* p2mm e	P2x
2	f			$0\frac{1}{2}$ P2x
2	g	.m.		P2y
2	h			$\frac{1}{2}0$ P2y
4	i	1	* p2mm i	P2x2y
7	***p*2*mg***			
2	a	2..	p2mm a	P_a
2	b			$0\frac{1}{2}$ P_a
2	c	.m.	* p2mg c	$\frac{1}{4}0$ 2.. P_aC1y
4	d	1	* p2mg d	.m. P_a2xy
8	***p*2*gg***			
2	a	2..	c2mm a	C
2	b			$\frac{1}{2}0$ C
4	c	1	* p2gg c	.g. C2xy
9	***c*2*mm***			
2	a	2mm	* c2mm a	C
2	b			$0\frac{1}{2}$ C
4	c	2..	p2mm a	$\frac{1}{4}\frac{1}{4}$ P_{ab}
4	d	..m	* c2mm d	C2x
4	e	.m.		C2y
8	f	1	* c2mm f	C2x2y
10	***p*4**			
1	a	4..	p4mm a	P
1	b			$\frac{1}{2}\frac{1}{2}$ P
2	c	2..	p4mm a	$0\frac{1}{2}$ C
4	d	1	* p4 d	P4xy
11	***p*4*mm***			
1	a	4mm	* p4mm a	P
1	b			$\frac{1}{2}\frac{1}{2}$ P
2	c	2mm.	p4mm a	$0\frac{1}{2}$ C
4	d	.m.	* p4mm d	P4x
4	e			$\frac{1}{2}\frac{1}{2}$ P4x
4	f	..m	* p4mm f	P4xx
8	g	1	* p4mm g	P4x2y
12	***p*4*gm***			
2	a	4..	p4mm a	C
2	b	2.mm	p4mm a	$0\frac{1}{2}$ C
4	c	..m	* p4gm c	$0\frac{1}{2}$ .g. C2xx
8	d	1	* p4gm d	..m C4xy
13	***p*3**			
1	a	3..	p6mm a	P
1	b			$\frac{1}{3}\frac{2}{3}$ P
1	c			$\frac{2}{3}\frac{1}{3}$ P
3	d	1	* p3 d	P3xy
14	***p*3*m*1**			
1	a	3m.	p6mm a	P
1	b			$\frac{1}{3}\frac{2}{3}$ P
1	c			$\frac{2}{3}\frac{1}{3}$ P
3	d	.m.	* p3m1 d	$P3x\bar{x}$
6	e	1	* p3m1 e	$P3x\bar{x}2y$
15	***p*31*m***			
1	a	3.m	p6mm a	P
2	b	3..	p6mm b	G
3	c	..m	* p31m c	P3x
6	d	1	* p31m d	P3x2y
16	***p*6**			
1	a	6..	p6mm a	P
2	b	3..	p6mm b	G
3	c	2..	p6mm c	N
6	d	1	* p6 d	P6xy
17	***p*6*mm***			
1	a	6mm	* p6mm a	P
2	b	3m.	* p6mm b	G
3	c	2mm	* p6mm c	N
6	d	..m	* p6mm d	P6x
6	e	.m.	* p6mm e	$P6x\bar{x}$
12	f	1	* p6mm f	P6x2y

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes*

Wyckoff positions of the same Wyckoff set can be recognized by their consecutive listing without repetition of the reference symbol. Characteristic Wyckoff sets are marked by asterisks.

1 $P1$

1	*a*	1	$P\bar{1}$ *a*	$P[xyz]$

2 $P\bar{1}$

1	*a*	$\bar{1}$	* $P\bar{1}$ *a*	P
1	*b*			$00\frac{1}{2}\ P$
1	*c*			$0\frac{1}{2}0\ P$
1	*d*			$\frac{1}{2}00\ P$
1	*e*			$\frac{1}{2}\frac{1}{2}0\ P$
1	*f*			$\frac{1}{2}0\frac{1}{2}\ P$
1	*g*			$0\frac{1}{2}\frac{1}{2}\ P$
1	*h*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P$
2	*i*	1	* $P\bar{1}$ *i*	$P2xyz$

3 $P2$

1	*a*	2	$P2/m$ *a*	$P[y]$
1	*b*			$00\frac{1}{2}\ P[y]$
1	*c*			$\frac{1}{2}00\ P[y]$
1	*d*			$\frac{1}{2}0\frac{1}{2}\ P[y]$
2	*e*	1	$P2/m$ *m*	$P2xz[y]$

4 $P2_1$

2	*a*	1	$P2_1/m$ *e*	$2_1\ P_bACI1xz[y]$

5 $C2$

2	*a*	2	$C2/m$ *a*	$C[y]$
2	*b*			$00\frac{1}{2}\ C[y]$
4	*c*	1	$C2/m$ *i*	$C2xz[y]$

6 Pm

1	*a*	*m*	$P2/m$ *a*	$P[xz]$
1	*b*			$0\frac{1}{2}0\ P[xz]$
2	*c*	1	$P2/m$ *i*	$P2y[xz]$

7 Pc

2	*a*	1	$P2/c$ *e*	$c\ P_cA1y[xz]$

8 Cm

2	*a*	*m*	$C2/m$ *a*	$C[xz]$
4	*b*	1	$C2/m$ *g*	$C2y[xz]$

9 Cc

4	*a*	1	$C2/c$ *e*	$\bar{1}\ C_cF1y[xz]$

10 $P2/m$

1	*a*	$2/m$	* $P2/m$ *a*	P
1	*b*			$0\frac{1}{2}0\ P$
1	*c*			$00\frac{1}{2}\ P$
1	*d*			$\frac{1}{2}00\ P$
1	*e*			$\frac{1}{2}\frac{1}{2}0\ P$
1	*f*			$0\frac{1}{2}\frac{1}{2}\ P$
1	*g*			$\frac{1}{2}0\frac{1}{2}\ P$
1	*h*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P$
2	*i*	2	* $P2/m$ *i*	$P2y$
2	*j*			$\frac{1}{2}00\ P2y$
2	*k*			$00\frac{1}{2}\ P2y$
2	*l*			$\frac{1}{2}0\frac{1}{2}\ P2y$
2	*m*	*m*	* $P2/m$ *m*	$P2xz$
2	*n*			$0\frac{1}{2}0\ P2xz$
4	*o*	1	* $P2/m$ *o*	$P2xz2y$

11 $P2_1/m$

2	*a*	$\bar{1}$	$P2/m$ *a*	P_b
2	*b*			$\frac{1}{2}00\ P_b$
2	*c*			$00\frac{1}{2}\ P_b$
2	*d*			$\frac{1}{2}0\frac{1}{2}\ P_b$
2	*e*	*m*	* $P2_1/m$ *e*	$0\frac{1}{4}0\ 2_1P_bACI1xz$
4	*f*	1	* $P2_1/m$ *f*	$m\ P_b2xyz$

12 $C2/m$

2	*a*	$2/m$	* $C2/m$ *a*	C
2	*b*			$0\frac{1}{2}0\ C$
2	*c*			$00\frac{1}{2}\ C$
2	*d*			$0\frac{1}{2}\frac{1}{2}\ C$
4	*e*	$\bar{1}$	$P2/m$ *a*	$\frac{1}{4}\frac{1}{4}0\ P_{ab}$
4	*f*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}\ P_{ab}$
4	*g*	2	* $C2/m$ *g*	$C2y$
4	*h*			$00\frac{1}{2}\ C2y$
4	*i*	*m*	* $C2/m$ *i*	$C2xz$
8	*j*	1	* $C2/m$ *j*	$C2xz2y$

13 $P2/c$

2	*a*	$\bar{1}$	$P2/m$ *a*	P_c
2	*b*			$\frac{1}{2}\frac{1}{2}0\ P_c$
2	*c*			$0\frac{1}{2}0\ P_c$
2	*d*			$\frac{1}{2}00\ P_c$
2	*e*	2	* $P2/c$ *e*	$00\frac{1}{4}\ c\ P_cA1y$
2	*f*			$\frac{1}{2}0\frac{1}{4}\ c\ P_cA1y$
4	*g*	1	* $P2/c$ *g*	$2\ P_c2xyz$

14 $P2_1/c$

2	*a*	$\bar{1}$	$C2/m$ *a*	A
2	*b*			$\frac{1}{2}00\ A$
2	*c*			$00\frac{1}{2}\ A$
2	*d*			$\frac{1}{2}0\frac{1}{2}\ A$
4	*e*	1	* $P2_1/c$ *e*	$c\ A2xyz$

15 $C2/c$

4	*a*	$\bar{1}$	$C2/m$ *a*	C_c
4	*b*			$0\frac{1}{2}0\ C_c$
4	*c*			$\frac{1}{4}\frac{1}{4}0\ F$
4	*d*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}\ F$
4	*e*	2	* $C2/c$ *e*	$00\frac{1}{4}\ \bar{1}\ C_cF1y$
8	*f*	1	* $C2/c$ *f*	$2_1\ C_c2xyz$

16 $P222$

1	*a*	222	$Pmmm$ *a*	P
1	*b*			$\frac{1}{2}00\ P$
1	*c*			$0\frac{1}{2}0\ P$
1	*d*			$00\frac{1}{2}\ P$
1	*e*			$\frac{1}{2}\frac{1}{2}0\ P$
1	*f*			$\frac{1}{2}0\frac{1}{2}\ P$
1	*g*			$0\frac{1}{2}\frac{1}{2}\ P$
1	*h*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P$

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

2	*i*	2..		*Pmmm i*	$P2x$
2	*j*				$00\frac{1}{2}\ P2x$
2	*k*				$0\frac{1}{2}0\ P2x$
2	*l*				$0\frac{1}{2}\frac{1}{2}\ P2x$
2	*m*	.2.			$P2y$
2	*n*				$00\frac{1}{2}\ P2y$
2	*o*				$\frac{1}{2}00\ P2y$
2	*p*				$\frac{1}{2}0\frac{1}{2}\ P2y$
2	*q*	..2			$P2z$
2	*r*				$\frac{1}{2}00\ P2z$
2	*s*				$0\frac{1}{2}0\ P2z$
2	*t*				$\frac{1}{2}\frac{1}{2}0\ P2z$
4	*u*	1	*	*P*222 *u*	$P2x2yz$
17	$\boldsymbol{P222_1}$				
2	*a*	2..		*Pmma e*	$.2.\ P_cB1x$
2	*b*				$0\frac{1}{2}0\ .2.\ P_cB1x$
2	*c*	.2.			$00\frac{1}{4}\ 2..\ P_cA1y$
2	*d*				$\frac{1}{2}0\frac{1}{4}\ 2..\ P_cA1y$
4	*e*	1	*	$P222_1$ *e*	$.2.\ P_cB1x2yz$
18	$\boldsymbol{P2_12_12}$				
2	*a*	..2		*Pmmn a*	$2_1..\ CI1z$
2	*b*				$0\frac{1}{2}0\ 2_1..\ CI1z$
4	*c*	1	*	$P2_12_12$ *c*	$2_1..\ CI1z2xy$
19	$\boldsymbol{P2_12_12_1}$				
4	*a*	1	*	$P2_12_12_1$ *a*	$2_12_1.\ FA_aB_bC_cI_aI_bI_c1xyz$
20	$\boldsymbol{C222_1}$				
4	*a*	2..		*Cmcm c*	$.2_1.\ C_cF1x$
4	*b*	.2.			$00\frac{1}{4}\ 2_1..\ C_cF1y$
8	*c*	1	*	$C222_1$ *c*	$.2_1.\ C_cF1x2yz$
21	***C*222**				
2	*a*	222		*Cmmm a*	C
2	*b*				$0\frac{1}{2}0\ C$
2	*c*				$\frac{1}{2}0\frac{1}{2}\ C$
2	*d*				$00\frac{1}{2}\ C$
4	*e*	2..		*Cmmm g*	$C2x$
4	*f*				$00\frac{1}{2}\ C2x$
4	*g*	.2.			$C2y$
4	*h*				$00\frac{1}{2}\ C2y$
4	*i*	..2		*Cmmm k*	$C2z$
4	*j*				$0\frac{1}{2}0\ C2z$
4	*k*	..2		*Cmme g*	$\frac{1}{4}\frac{1}{4}0\ 2..\ P_{ab}F1z$
8	*l*	1	*	*C*222 *l*	$C2x2yz$
22	***F*222**				
4	*a*	222		*Fmmm a*	F
4	*b*				$00\frac{1}{2}\ F$
4	*c*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F$
4	*d*				$\frac{1}{4}\frac{1}{4}\frac{3}{4}\ F$
8	*e*	2..		*Fmmm g*	$F2x$
8	*j*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F2x$
8	*f*	.2.			$F2y$
8	*i*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F2y$
8	*g*	..2			$F2z$
8	*h*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F2z$
16	*k*	1	*	*F*222 *k*	$F2x2yz$
23	***I*222**				
2	*a*	222		*Immm a*	I
2	*b*				$\frac{1}{2}00\ I$
2	*c*				$00\frac{1}{2}\ I$
2	*d*				$0\frac{1}{2}0\ I$
4	*e*	2..		*Immm e*	$I2x$
4	*f*				$00\frac{1}{2}\ I2x$
4	*g*	.2.			$I2y$
4	*h*				$\frac{1}{2}00\ I2y$
4	*i*	..2			$I2z$
4	*j*				$0\frac{1}{2}0\ I2z$
8	*k*	1	*	*I*222 *k*	$I2x2yz$
24	$\boldsymbol{I2_12_12_1}$				
4	*a*	2..		*Imma e*	$\frac{1}{4}0\frac{1}{4}\ ..2\ C_cB_b1x$
4	*b*	.2.			$\frac{1}{4}\frac{1}{4}0\ 2..\ A_aC_c1y$
4	*c*	..2			$0\frac{1}{4}\frac{1}{4}\ .2.\ B_bA_a1z$
8	*d*	1	*	$I2_12_12_1$ *d*	$\frac{1}{4}0\frac{1}{4}\ ..2\ C_cB_b1x2yz$
25	***Pmm*2**				
1	*a*	*mm*2		*Pmmm a*	$P[z]$
1	*b*				$0\frac{1}{2}0\ P[z]$
1	*c*				$\frac{1}{2}00\ P[z]$
1	*d*				$\frac{1}{2}\frac{1}{2}0\ P[z]$
2	*e*	.*m*.		*Pmmm i*	$P2x[z]$
2	*f*				$0\frac{1}{2}0\ P2x[z]$
2	*g*	*m*..			$P2y[z]$
2	*h*				$\frac{1}{2}00\ P2y[z]$
4	*i*	1		*Pmmm u*	$P2x2y[z]$
26	$\boldsymbol{Pmc2_1}$				
2	*a*	*m*..		*Pmma e*	$2..\ P_cA1y[z]$
2	*b*				$\frac{1}{2}00\ 2..\ P_cA1y[z]$
4	*c*	1		*Pmma k*	$2..\ P_cA1y2x[z]$
27	***Pcc*2**				
2	*a*	..2		*Pmmm a*	$P_c[z]$
2	*b*				$0\frac{1}{2}0\ P_c[z]$
2	*c*				$\frac{1}{2}00\ P_c[z]$
2	*d*				$\frac{1}{2}\frac{1}{2}0\ P_c[z]$
4	*e*	1		*Pccm q*	$2..\ P_c2xy[z]$
28	***Pma*2**				
2	*a*	..2		*Pmmm a*	$P_a[z]$
2	*b*				$0\frac{1}{2}0\ P_a[z]$
2	*c*	*m*..		*Pmma e*	$\frac{1}{4}00\ ..2\ P_aC1y[z]$
4	*d*	1		*Pmma i*	$m..\ P_a2xy[z]$
29	$\boldsymbol{Pca2_1}$				
4	*a*	1		*Pbcm d*	$.2\bar{1}\ P_{ac}B_aC_cF1xy[z]$
30	***Pnc*2**				
2	*a*	..2		*Cmmm a*	$A[z]$
2	*b*				$\frac{1}{2}00\ A[z]$
4	*c*	1		*Pmna h*	$2..\ A2xy[z]$

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

31	***Pmn*2$_1$**			
2	*a*	*m..*	*Pmmn a*	$..2_1$ $BI1y[z]$
4	*b*	1	*Pmmn e*	$..2_1$ $BI1y2x[z]$
32	***Pba*2**			
2	*a*	..2	*Cmmm a*	$C[z]$
2	*b*			$0\frac{1}{2}0$ $C[z]$
4	*c*	1	*Pbam g*	*b..* $C2xy[z]$
33	***Pna*2$_1$**			
4	*a*	1	*Pnma c*	$\bar{1}2_1.$ $C_cA_aFI_a1xy[z]$
34	***Pnn*2**			
2	*a*	..2	*Immm a*	$I[z]$
2	*b*			$0\frac{1}{2}0$ $I[z]$
4	*c*	1	*Pnnm g*	*n..* $I2xy[z]$
35	***Cmm*2**			
2	*a*	*mm*2	*Cmmm a*	$C[z]$
2	*b*			$0\frac{1}{2}0$ $C[z]$
4	*c*	..2	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0$ $P_{ab}[z]$
4	*d*	*.m.*	*Cmmm g*	$C2x[z]$
4	*e*	*m..*		$C2y[z]$
8	*f*	1	*Cmmm p*	$C2x2y[z]$
36	***Cmc*2$_1$**			
4	*a*	*m..*	*Cmcm c*	$2_1..$ $C_cF1y[z]$
8	*b*	1	*Cmcm g*	$2_1..$ $C_cF1y2x[z]$
37	***Ccc*2**			
4	*a*	..2	*Cmmm a*	$C_c[z]$
4	*b*			$0\frac{1}{2}0$ $C_c[z]$
4	*c*	..2	*Fmmm a*	$\frac{1}{4}\frac{1}{4}0$ $F[z]$
8	*d*	1	*Cccm l*	*n..* $C_c2xy[z]$
38	***Amm*2**			
2	*a*	*mm*2	*Cmmm a*	$A[z]$
2	*b*			$\frac{1}{2}00$ $A[z]$
4	*c*	*.m.*	*Cmmm k*	$A2x[z]$
4	*d*	*m..*	*Cmmm g*	$A2y[z]$
4	*e*			$\frac{1}{2}00$ $A2y[z]$
8	*f*	1	*Cmmm n*	$A2x2y[z]$
39	***Aem*2**			
4	*a*	..2	*Pmmm a*	$P_{bc}[z]$
4	*b*			$\frac{1}{2}00$ $P_{bc}[z]$
4	*c*	*.m.*	*Cmme g*	$0\frac{1}{4}0$ ..2 $P_{bc}F1x[z]$
8	*d*	1	*Cmme m*	*.m.* $P_{bc}2xy[z]$
40	***Ama*2**			
4	*a*	..2	*Cmmm a*	$A_a[z]$
4	*b*	*m..*	*Cmcm c*	$\frac{1}{4}00$ $..2_1$ $A_aF1y[z]$
8	*c*	1	*Cmcm f*	*.n.* $A_a2xy[z]$
41	***Aea*2**			
4	*a*	..2	*Fmmm a*	$F[z]$
8	*b*	1	*Cmce f*	.2. $F2xy[z]$

42	***Fmm*2**			
4	*a*	*mm*2	*Fmmm a*	$F[z]$
8	*b*	..2	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0$ $P_2[z]$
8	*c*	*m..*	*Fmmm g*	$F2y[z]$
8	*d*	*.m.*		$F2x[z]$
16	*e*	1	*Fmmm m*	$F2x2y[z]$
43	***Fdd*2**			
8	*a*	..2	*Fddd a*	$D[z]$
16	*b*	1	* *Fdd*2 *b*	*d..* $D2xy[z]$
44	***Imm*2**			
2	*a*	*mm*2	*Immm a*	$I[z]$
2	*b*			$0\frac{1}{2}0$ $I[z]$
4	*c*	*.m.*	*Immm e*	$I2x[z]$
4	*d*	*m..*		$I2y[z]$
8	*e*	1	*Immm l*	$I2x2y[z]$
45	***Iba*2**			
4	*a*	..2	*Cmmm a*	$C_c[z]$
4	*b*			$0\frac{1}{2}0$ $C_c[z]$
8	*c*	1	*Ibam j*	*b..* $C_c2xy[z]$
46	***Ima*2**			
4	*a*	..2	*Cmmm a*	$A_a[z]$
4	*b*	*m..*	*Imma e*	$\frac{1}{4}00$ 2.. $A_aC_c1y[z]$
8	*c*	1	*Imma h*	2.. $A_a2xy[z]$
47	***Pmmm***			
1	*a*	*mmm*	* *Pmmm a*	P
1	*b*			$\frac{1}{2}00$ P
1	*c*			$00\frac{1}{2}$ P
1	*d*			$\frac{1}{2}0\frac{1}{2}$ P
1	*e*			$0\frac{1}{2}0$ P
1	*f*			$\frac{1}{2}\frac{1}{2}0$ P
1	*g*			$0\frac{1}{2}\frac{1}{2}$ P
1	*h*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$
2	*i*	2*mm*	* *Pmmm i*	$P2x$
2	*j*			$00\frac{1}{2}$ $P2x$
2	*k*			$0\frac{1}{2}0$ $P2x$
2	*l*			$0\frac{1}{2}\frac{1}{2}$ $P2x$
2	*m*	*m*2*m*		$P2y$
2	*n*			$00\frac{1}{2}$ $P2y$
2	*o*			$\frac{1}{2}00$ $P2y$
2	*p*			$\frac{1}{2}0\frac{1}{2}$ $P2y$
2	*q*	*mm*2		$P2z$
2	*r*			$0\frac{1}{2}0$ $P2z$
2	*s*			$\frac{1}{2}00$ $P2z$
2	*t*			$\frac{1}{2}\frac{1}{2}0$ $P2z$
4	*u*	*m..*	* *Pmmm u*	$P2y2z$
4	*v*			$\frac{1}{2}00$ $P2y2z$
4	*w*	*.m.*		$P2x2z$
4	*x*			$0\frac{1}{2}0$ $P2x2z$
4	*y*	*..m*		$P2x2y$
4	*z*			$00\frac{1}{2}$ $P2x2y$
8	α	1	* *Pmmm* α	$P2x2y2z$

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

48 *Pnnn*

2	*a*	222	*Immm a*	*I*
2	*b*			$\frac{1}{2}00\ I$
2	*c*			$00\frac{1}{2}\ I$
2	*d*			$0\frac{1}{2}0\ I$
4	*e*	$\bar{1}$	*Fmmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F$
4	*f*			$\frac{3}{4}\frac{3}{4}\frac{3}{4}\ F$
4	*g*	2..	*Immm e*	*I*2*x*
4	*h*			$00\frac{1}{2}\ I2x$
4	*i*	.2.		*I*2*y*
4	*j*			$\frac{1}{2}00\ I2y$
4	*k*	..2		*I*2*z*
4	*l*			$0\frac{1}{2}0\ I2z$
8	*m*	1	* *Pnnn m*	*n*.. *I*2*x*2*yz*

49 *Pccm*

2	*a*	..2/*m*	*Pmmm a*	P_c
2	*b*			$\frac{1}{2}\frac{1}{2}0\ P_c$
2	*c*			$0\frac{1}{2}0\ P_c$
2	*d*			$\frac{1}{2}00\ P_c$
2	*e*	222	*Pmmm a*	$00\frac{1}{4}\ P_c$
2	*f*			$\frac{1}{2}0\frac{1}{4}\ P_c$
2	*g*			$0\frac{1}{2}\frac{1}{4}\ P_c$
2	*h*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}\ P_c$
4	*i*	2..	*Pmmm i*	$00\frac{1}{4}\ P_c2x$
4	*j*			$0\frac{1}{2}\frac{1}{4}\ P_c2x$
4	*k*	.2.		$00\frac{1}{4}\ P_c2y$
4	*l*			$\frac{1}{2}0\frac{1}{4}\ P_c2y$
4	*m*	..2	*Pmmm i*	P_c2z
4	*n*			$\frac{1}{2}\frac{1}{2}0\ P_c2z$
4	*o*			$0\frac{1}{2}0\ P_c2z$
4	*p*			$\frac{1}{2}00\ P_c2z$
4	*q*	..*m*	* *Pccm q*	2.. P_c2xy
8	*r*	1	* *Pccm r*	*c*.. P_c2xy2z

50 *Pban*

2	*a*	222	*Cmmm a*	*C*
2	*b*			$\frac{1}{2}00\ C$
2	*c*			$\frac{1}{2}0\frac{1}{2}\ C$
2	*d*			$00\frac{1}{2}\ C$
4	*e*	$\bar{1}$	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0\ P_{ab}$
4	*f*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}\ P_{ab}$
4	*g*	2..	*Cmmm g*	*C*2*x*
4	*h*			$00\frac{1}{2}\ C2x$
4	*i*	.2.		*C*2*y*
4	*j*			$00\frac{1}{2}\ C2y$
4	*k*	..2	*Cmmm k*	*C*2*z*
4	*l*			$0\frac{1}{2}0\ C2z$
8	*m*	1	* *Pban m*	*b*.. *C*2*x*2*yz*

51 *Pmma*

2	*a*	.2/*m*.	*Pmmm a*	P_a
2	*b*			$0\frac{1}{2}0\ P_a$
2	*c*			$00\frac{1}{2}\ P_a$
2	*d*			$0\frac{1}{2}\frac{1}{2}\ P_a$
2	*e*	*mm*2	* *Pmma e*	$\frac{1}{4}00$ .2. P_aB1z
2	*f*			$\frac{1}{4}\frac{1}{2}0$ .2. P_aB1z
4	*g*	.2.	*Pmmm i*	P_a2y
4	*h*			$00\frac{1}{2}\ P_a2y$
4	*i*	.*m*.	* *Pmma i*	*m*.. P_a2xz
4	*j*			$0\frac{1}{2}0$ *m*.. P_a2xz
4	*k*	*m*..	* *Pmma k*	$\frac{1}{4}00$ .2. P_aB1z2y
8	*l*	1	* *Pmma l*	*m*.. P_a2xz2y

52 *Pnna*

4	*a*	$\bar{1}$	*Cmmm a*	A_a
4	*b*			$00\frac{1}{2}\ A_a$
4	*c*	..2	*Imma e*	$\frac{1}{4}0\frac{1}{4}$ .2. B_bA_a1z
4	*d*	2..	*Cmcm c*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $..2_1$ B_bF1x
8	*e*	1	* *Pnna e*	2.2 A_a2xyz

53 *Pmna*

2	*a*	2/*m*..	*Cmmm a*	*B*
2	*b*			$\frac{1}{2}00\ B$
2	*c*			$\frac{1}{2}\frac{1}{2}0\ B$
2	*d*			$0\frac{1}{2}0\ B$
4	*e*	2..	*Cmmm g*	*B*2*x*
4	*f*			$0\frac{1}{2}0\ B2x$
4	*g*	.2.	*Pmma e*	$\frac{1}{4}0\frac{1}{4}$ $(2..\ P_cA1y)_a$
4	*h*	*m*..	* *Pmna h*	.2. *B*2*yz*
8	*i*	1	* *Pmna i*	.2. *B*2*yz*2*x*

54 *Pcca*

4	*a*	$\bar{1}$	*Pmmm a*	P_{ac}
4	*b*			$0\frac{1}{2}0\ P_{ac}$
4	*c*	.2.	*Cmme g*	$00\frac{1}{4}$ ..2 $P_{ac}F1y$
4	*d*	..2	*Pmma e*	$\frac{1}{4}00$ $(.2.\ P_aB1z)_c$
4	*e*			$\frac{1}{4}\frac{1}{2}0$ $(.2.\ P_aB1z)_c$
8	*f*	1	* *Pcca f*	.22 $P_{ac}2xyz$

55 *Pbam*

2	*a*	..2/*m*	*Cmmm a*	*C*
2	*b*			$00\frac{1}{2}\ C$
2	*c*			$0\frac{1}{2}0\ C$
2	*d*			$0\frac{1}{2}\frac{1}{2}\ C$
4	*e*	..2	*Cmmm k*	*C*2*z*
4	*f*			$0\frac{1}{2}0\ C2z$
4	*g*	..*m*	* *Pbam g*	*b*.. *C*2*xy*
4	*h*			$00\frac{1}{2}$ *b*.. *C*2*xy*
8	*i*	1	* *Pbam i*	*b*.. *C*2*xy*2*z*

56 *Pccn*

4	*a*	$\bar{1}$	*Fmmm a*	*F*
4	*b*			$00\frac{1}{2}\ F$
4	*c*	..2	*Pmmn a*	$\frac{1}{4}\frac{1}{4}0$ $(2_1..\ CI1z)_c$
4	*d*			$\frac{1}{4}\frac{3}{4}0$ $(2_1..\ CI1z)_c$
8	*e*	1	* *Pccn e*	*c*.2 *F*2*xyz*

57 *Pbcm*

4	*a*	$\bar{1}$	*Pmmm a*	P_{bc}
4	*b*			$\frac{1}{2}00\ P_{bc}$
4	*c*	2..	*Pmma e*	$0\frac{1}{4}0$ $(..2\ P_bC1x)_c$
4	*d*	..*m*	* *Pbcm d*	$00\frac{1}{4}$ $2.\bar{1}$ $P_{bc}A_bC_cF1xy$
8	*e*	1	* *Pbcm e*	2.*m* $P_{bc}2xyz$

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

58 *Pnnm*

2	*a*	..2/*m*	*Immm a*	I
2	*b*			$00\frac{1}{2}\ I$
2	*c*			$0\frac{1}{2}0\ I$
2	*d*			$0\frac{1}{2}\frac{1}{2}\ I$
4	*e*	..2	*Immm e*	$I2z$
4	*f*			$0\frac{1}{2}0\ I2z$
4	*g*	..*m*	* *Pnnm g*	$n..\ I2xy$
8	*h*	1	* *Pnnm h*	$n..\ I2xy2z$

59 *Pmmn*

2	*a*	*mm*2	* *Pmmn a*	$2_1..\ CI1z$
2	*b*			$0\frac{1}{2}0\ 2_1..\ CI1z$
4	*c*	$\bar{1}$	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0\ P_{ab}$
4	*d*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}\ P_{ab}$
4	*e*	*m*..	* *Pmmn e*	$2_1..\ CI1z2y$
4	*f*	.*m*.		$.2_1.\ CI1z2x$
8	*g*	1	* *Pmmn g*	$\frac{1}{4}\frac{1}{4}0\ mm.\ P_{ab}2xyz$

60 *Pbcn*

4	*a*	$\bar{1}$	*Cmmm a*	C_c
4	*b*			$0\frac{1}{2}0\ C_c$
4	*c*	.2.	*Cmcm c*	$00\frac{1}{4}\ 2_1..\ C_cF1y$
8	*d*	1	* *Pbcn d*	$b2.\ C_c2xyz$

61 *Pbca*

4	*a*	$\bar{1}$	*Fmmm a*	F
4	*b*			$00\frac{1}{2}\ F$
8	*c*	1	* *Pbca c*	$bc.\ F2xyz$

62 *Pnma*

4	*a*	$\bar{1}$	*Cmmm a*	B_b
4	*b*			$00\frac{1}{2}\ B_b$
4	*c*	.*m*.	* *Pnma c*	$0\frac{1}{4}0\ \bar{1}.2_1\ B_bA_aFI_a1xz$
8	*d*	1	* *Pnma d*	$.ma\ B_b2xyz$

63 *Cmcm*

4	*a*	2/*m*..	*Cmmm a*	C_c
4	*b*			$0\frac{1}{2}0\ C_c$
4	*c*	*m*2*m*	* *Cmcm c*	$00\frac{1}{4}\ 2_1..\ C_cF1y$
8	*d*	$\bar{1}$	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0\ P_2$
8	*e*	2..	*Cmmm g*	C_c2x
8	*f*	*m*..	* *Cmcm f*	$.n.\ C_c2yz$
8	*g*	..*m*	* *Cmcm g*	$00\frac{1}{4}\ 2_1..\ C_cF1y2x$
16	*h*	1	* *Cmcm h*	$.n.\ C_c2yz2x$

64 *Cmce*

4	*a*	2/*m*..	*Fmmm a*	F
4	*b*			$00\frac{1}{2}\ F$
8	*c*	$\bar{1}$	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0\ P_2$
8	*d*	2..	*Fmmm g*	$F2x$
8	*e*	.2.	*Pmma e*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ (2..\ P_cA1y)_{ab}$
8	*f*	*m*..	* *Cmce f*	$.2.\ F2yz$
16	*g*	1	* *Cmce g*	$.2.\ F2yz2x$

65 *Cmmm*

2	*a*	*mmm*	* *Cmmm a*	C
2	*b*			$\frac{1}{2}00\ C$
2	*c*			$\frac{1}{2}0\frac{1}{2}\ C$
2	*d*			$00\frac{1}{2}\ C$
4	*e*	..2/*m*	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0\ P_{ab}$
4	*f*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}\ P_{ab}$
4	*g*	2*mm*	* *Cmmm g*	$C2x$
4	*h*			$00\frac{1}{2}\ C2x$
4	*i*	*m*2*m*		$C2y$
4	*j*			$00\frac{1}{2}\ C2y$
4	*k*	*mm*2	* *Cmmm k*	$C2z$
4	*l*			$0\frac{1}{2}0\ C2z$
8	*m*	..2	*Pmmm i*	$\frac{1}{4}\frac{1}{4}0\ P_{ab}2z$
8	*n*	*m*..	* *Cmmm n*	$C2y2z$
8	*o*	.*m*.		$C2x2z$
8	*p*	..*m*	* *Cmmm p*	$C2x2y$
8	*q*			$00\frac{1}{2}\ C2x2y$
16	*r*	1	* *Cmmm r*	$C2x2y2z$

66 *Cccm*

4	*a*	222	*Cmmm a*	$00\frac{1}{4}\ C_c$
4	*b*			$0\frac{1}{2}\frac{1}{4}\ C_c$
4	*c*	..2/*m*	*Cmmm a*	C_c
4	*d*			$0\frac{1}{2}0\ C_c$
4	*e*	..2/*m*	*Fmmm a*	$\frac{1}{4}\frac{1}{4}0\ F$
4	*f*			$\frac{1}{4}\frac{3}{4}0\ F$
8	*g*	2..	*Cmmm g*	$00\frac{1}{4}\ C_c2x$
8	*h*	.2.		$00\frac{1}{4}\ C_c2y$
8	*i*	..2	*Cmmm k*	C_c2z
8	*j*			$0\frac{1}{2}0\ C_c2z$
8	*k*	..2	*Fmmm g*	$\frac{1}{4}\frac{1}{4}0\ F2z$
8	*l*	..*m*	* *Cccm l*	$c..\ C_c2xy$
16	*m*	1	* *Cccm m*	$c..\ C_c2xy2z$

67 *Cmme*

4	*a*	222	*Pmmm a*	$\frac{1}{4}00\ P_{ab}$
4	*b*			$\frac{1}{4}0\frac{1}{2}\ P_{ab}$
4	*c*	2/*m*..	*Pmmm a*	P_{ab}
4	*d*			$00\frac{1}{2}\ P_{ab}$
4	*e*	.2/*m*.		$\frac{1}{4}\frac{1}{4}0\ P_{ab}$
4	*f*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}\ P_{ab}$
4	*g*	*mm*2	* *Cmme g*	$0\frac{1}{4}0\ 2..\ P_{ab}F1z$
8	*h*	2..	*Pmmm i*	$P_{ab}2x$
8	*i*			$00\frac{1}{2}\ P_{ab}2x$
8	*j*	.2.		$\frac{1}{4}00\ P_{ab}2y$
8	*k*			$\frac{1}{4}0\frac{1}{2}\ P_{ab}2y$
8	*l*	..2	*Pmmm i*	$\frac{1}{4}00\ P_{ab}2z$
8	*m*	*m*..	* *Cmme m*	$.m.\ P_{ab}2yz$
8	*n*	.*m*.		$0\frac{1}{4}0\ m..\ P_{ab}2xz$
16	*o*	1	* *Cmme o*	$.m.\ P_{ab}2yz2x$

68 *Ccce*

4	*a*	222	*Fmmm a*	F
4	*b*			$00\frac{1}{2}\ F$
8	*c*	$\bar{1}$	*Pmmm a*	$\frac{1}{4}0\frac{1}{4}\ P_2$
8	*d*			$0\frac{1}{4}\frac{1}{4}\ P_2$
8	*e*	2..	*Fmmm g*	$F2x$
8	*f*	.2.		$F2y$
8	*g*	..2	*Fmmm g*	$F2z$
8	*h*	..2	*Cmme g*	$\frac{1}{4}\frac{1}{4}0\ (2..\ P_{ab}F1z)_c$

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

16	*i*	1	* *Ccce i*	$c..\ F2x2yz$
69	***Fmmm***			
4	*a*	*mmm*	* *Fmmm a*	F
4	*b*			$00\frac{1}{2}\ F$
8	*c*	$2/m..$	*Pmmm a*	$0\frac{1}{4}\frac{1}{4}\ P_2$
8	*d*	$.2/m.$		$\frac{1}{4}0\frac{1}{4}\ P_2$
8	*e*	$..2/m$		$\frac{1}{4}\frac{1}{4}0\ P_2$
8	*f*	222	*Pmmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*g*	2*mm*	* *Fmmm g*	$F2x$
8	*h*	*m*2*m*		$F2y$
8	*i*	*mm*2		$F2z$
16	*j*	..2	*Pmmm i*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_22z$
16	*k*	.2.		$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_22y$
16	*l*	2..		$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_22x$
16	*m*	*m*..	* *Fmmm m*	$F2y2z$
16	*n*	.*m*.		$F2x2z$
16	*o*	..*m*		$F2x2y$
32	*p*	1	* *Fmmm p*	$F2x2y2z$
70	***Fddd***			
8	*a*	222	* *Fddd a*	D
8	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ D$
16	*c*	$\bar{1}$	* *Fddd c*	T
16	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ T$
16	*e*	2..	* *Fddd e*	$D2x$
16	*f*	.2.		$D2y$
16	*g*	..2		$D2z$
32	*h*	1	* *Fddd h*	$d..\ D2x2yz$
71	***Immm***			
2	*a*	*mmm*	* *Immm a*	I
2	*b*			$0\frac{1}{2}\frac{1}{2}\ I$
2	*c*			$\frac{1}{2}\frac{1}{2}0\ I$
2	*d*			$\frac{1}{2}0\frac{1}{2}\ I$
4	*e*	2*mm*	* *Immm e*	$I2x$
4	*f*			$0\frac{1}{2}0\ I2x$
4	*g*	*m*2*m*		$I2y$
4	*h*			$00\frac{1}{2}\ I2y$
4	*i*	*mm*2		$I2z$
4	*j*			$\frac{1}{2}00\ I2z$
8	*k*	$\bar{1}$	*Pmmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*l*	*m*..	* *Immm l*	$I2y2z$
8	*m*	.*m*.		$I2x2z$
8	*n*	..*m*		$I2x2y$
16	*o*	1	* *Immm o*	$I2x2y2z$
72	***Ibam***			
4	*a*	222	*Cmmm a*	$00\frac{1}{4}\ C_c$
4	*b*			$\frac{1}{2}0\frac{1}{4}\ C_c$
4	*c*	$..2/m$	*Cmmm a*	C_c
4	*d*			$\frac{1}{2}00\ C_c$
8	*e*	$\bar{1}$	*Pmmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*f*	2..	*Cmmm g*	$00\frac{1}{4}\ C_c2x$
8	*g*	.2.		$00\frac{1}{4}\ C_c2y$
8	*h*	..2	*Cmmm k*	C_c2z
8	*i*			$0\frac{1}{2}0\ C_c2z$
8	*j*	..*m*	* *Ibam j*	$c..\ C_c2xy$
16	*k*	1	* *Ibam k*	$c..\ C_c2xy2z$
73	***Ibca***			
8	*a*	$\bar{1}$	*Pmmm a*	P_2
8	*b*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*c*	2..	*Cmme g*	$00\frac{1}{4}\ (.2.\ P_{bc}F1x)_a$
8	*d*	.2.		$\frac{1}{4}00\ (..2\ P_{ac}F1y)_b$
8	*e*	..2		$0\frac{1}{4}0\ (2..\ P_{ab}F1z)_c$
16	*f*	1	* *Ibca f*	$22.\ P_22xyz$
74	***Imma***			
4	*a*	$2/m..$	*Cmmm a*	B_b
4	*b*			$00\frac{1}{2}\ B_b$
4	*c*	$.2/m.$		$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ A_a$
4	*d*			$\frac{1}{4}\frac{1}{4}\frac{3}{4}\ A_a$
4	*e*	*mm*2	* *Imma e*	$0\frac{1}{4}0\ .2.\ B_bA_a1z$
8	*f*	2..	*Cmmm g*	B_b2x
8	*g*	.2.		$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ A_a2y$
8	*h*	*m*..	* *Imma h*	$.2.\ B_b2yz$
8	*i*	.*m*.		$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ 2..\ A_a2xz$
16	*j*	1	* *Imma j*	$.2.\ B_b2yz2x$
75	***P*4**			
1	*a*	4..	*P*4/*mmm a*	$P[z]$
1	*b*			$\frac{1}{2}\frac{1}{2}0\ P[z]$
2	*c*	2..	*P*4/*mmm a*	$0\frac{1}{2}0\ C[z]$
4	*d*	1	*P*4/*m j*	$P4xy[z]$
76	***P*4$_1$**			
4	*a*	1	* *P*4$_3$ *a*	$4_1..\ P_{cc}{}^{v}DI_c1xy[z]$
77	***P*4$_2$**			
2	*a*	2..	*P*4/*mmm a*	$P_c[z]$
2	*b*			$\frac{1}{2}\frac{1}{2}0\ P_c[z]$
2	*c*	2..	*I*4/*mmm a*	$0\frac{1}{2}0\ I[z]$
4	*d*	1	*P*4$_2$/*m j*	$\bar{4}..\ P_c2xy[z]$
78	***P*4$_3$**			
4	*a*	1	* *P*4$_3$ *a*	$4_3..\ P_{cc}{}^{v}DI_c1xy[z]$
79	***I*4**			
2	*a*	4..	*I*4/*mmm a*	$I[z]$
4	*b*	2..	*P*4/*mmm a*	$0\frac{1}{2}0\ C_c[z]$
8	*c*	1	*I*4/*m h*	$I4xy[z]$
80	***I*4$_1$**			
4	*a*	2..	*I*4$_1$/*amd a*	${}^{v}D[z]$
8	*b*	1	* *I*4$_1$ *b*	$4_1..\ {}^{v}D2xy[z]$
81	***P*$\bar{4}$**			
1	*a*	$\bar{4}..$	*P*4/*mmm a*	P
1	*b*			$00\frac{1}{2}\ P$
1	*c*			$\frac{1}{2}\frac{1}{2}0\ P$
1	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P$
2	*e*	2..	*P*4/*mmm g*	$P2z$
2	*f*			$\frac{1}{2}\frac{1}{2}0\ P2z$
2	*g*	2..	*P*4/*nmm c*	$0\frac{1}{2}0\ ..2\ CI1z$
4	*h*	1	* *P*$\bar{4}$ *h*	$P4xyz$

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

82 $I\bar{4}$

2	*a*	$\bar{4}$..	$I4/mmm\ a$	I
2	*b*			$00\frac{1}{2}\ I$
2	*c*			$0\frac{1}{2}\frac{1}{4}\ I$
2	*d*			$0\frac{1}{2}\frac{3}{4}\ I$
4	*e*	2..	$I4/mmm\ e$	$I2z$
4	*f*			$0\frac{1}{2}\frac{1}{4}\ I2z$
8	*g*	1	* $I\bar{4}\ g$	$I4xyz$

83 $P4/m$

1	*a*	$4/m$..	$P4/mmm\ a$	P
1	*b*			$00\frac{1}{2}\ P$
1	*c*			$\frac{1}{2}\frac{1}{2}0\ P$
1	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P$
2	*e*	$2/m$..	$P4/mmm\ a$	$0\frac{1}{2}0\ C$
2	*f*			$0\frac{1}{2}\frac{1}{2}\ C$
2	*g*	4..	$P4/mmm\ g$	$P2z$
2	*h*			$\frac{1}{2}\frac{1}{2}0\ P2z$
4	*i*	2..	$P4/mmm\ g$	$0\frac{1}{2}0\ C2z$
4	*j*	*m*..	* $P4/m\ j$	$P4xy$
4	*k*			$00\frac{1}{2}\ P4xy$
8	*l*	1	* $P4/m\ l$	$P4xy2z$

84 $P4_2/m$

2	*a*	$2/m$..	$P4/mmm\ a$	P_c
2	*b*			$\frac{1}{2}\frac{1}{2}0\ P_c$
2	*c*	$2/m$..	$I4/mmm\ a$	$0\frac{1}{2}0\ I$
2	*d*			$0\frac{1}{2}\frac{1}{2}\ I$
2	*e*	$\bar{4}$..	$P4/mmm\ a$	$00\frac{1}{4}\ P_c$
2	*f*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}\ P_c$
4	*g*	2..	$P4/mmm\ g$	P_c2z
4	*h*			$\frac{1}{2}\frac{1}{2}0\ P_c2z$
4	*i*	2..	$I4/mmm\ e$	$0\frac{1}{2}0\ I2z$
4	*j*	*m*..	* $P4_2/m\ j$	$\bar{4}..\ P_c2xy$
8	*k*	1	* $P4_2/m\ k$	$\bar{4}..\ P_c2xy2z$

85 $P4/n$

2	*a*	$\bar{4}$..	$P4/mmm\ a$	C
2	*b*			$00\frac{1}{2}\ C$
2	*c*	4..	$P4/nmm\ c$	$0\frac{1}{2}0\ ..2\ CI1z$
4	*d*	$\bar{1}$	$P4/mmm\ a$	$\frac{1}{4}\frac{1}{4}0\ P_{ab}$
4	*e*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}\ P_{ab}$
4	*f*	2..	$P4/mmm\ g$	$C2z$
8	*g*	1	* $P4/n\ g$	$\bar{1}\ C4xyz$

86 $P4_2/n$

2	*a*	$\bar{4}$..	$I4/mmm\ a$	I
2	*b*			$00\frac{1}{2}\ I$
4	*c*	$\bar{1}$	$I4/mmm\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F$
4	*d*			$\frac{1}{4}\frac{1}{4}\frac{3}{4}\ F$
4	*e*	2..	$P4/nmm\ c$	$0\frac{1}{2}0\ (..2\ CI1z)_c$
4	*f*	2..	$I4/mmm\ e$	$I2z$
8	*g*	1	* $P4_2/n\ g$	$n..\ I4xyz$

87 $I4/m$

2	*a*	$4/m$..	$I4/mmm\ a$	I
2	*b*			$00\frac{1}{2}\ I$
4	*c*	$2/m$..	$P4/mmm\ a$	$0\frac{1}{2}0\ C_c$
4	*d*	$\bar{4}$..	$P4/mmm\ a$	$0\frac{1}{2}\frac{1}{4}\ C_c$
4	*e*	4..	$I4/mmm\ e$	$I2z$
8	*f*	$\bar{1}$	$P4/mmm\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*g*	2..	$P4/mmm\ g$	$0\frac{1}{2}0\ C_c2z$
8	*h*	*m*..	* $I4/m\ h$	$I4xy$
16	*i*	1	* $I4/m\ i$	$I4xy2z$

88 $I4_1/a$

4	*a*	$\bar{4}$..	$I4_1/amd\ a$	${}^vD$
4	*b*			$00\frac{1}{2}\ {}^vD$
8	*c*	$\bar{1}$	$I4_1/amd\ c$	${}^vT$
8	*d*			$00\frac{1}{2}\ {}^vT$
8	*e*	2..	$I4_1/amd\ e$	${}^vD2z$
16	*f*	1	* $I4_1/a\ f$	$a..\ {}^vD4xyz$

89 $P422$

1	*a*	422	$P4/mmm\ a$	P
1	*b*			$00\frac{1}{2}\ P$
1	*c*			$\frac{1}{2}\frac{1}{2}0\ P$
1	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P$
2	*e*	222.	$P4/mmm\ a$	$\frac{1}{2}00\ C$
2	*f*			$\frac{1}{2}0\frac{1}{2}\ C$
2	*g*	4..	$P4/mmm\ g$	$P2z$
2	*h*			$\frac{1}{2}\frac{1}{2}0\ P2z$
4	*i*	2..	$P4/mmm\ g$	$0\frac{1}{2}0\ C2z$
4	*j*	..2	$P4/mmm\ j$	$P4xx$
4	*k*			$00\frac{1}{2}\ P4xx$
4	*l*	.2.	$P4/mmm\ l$	$P4x$
4	*m*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P4x$
4	*n*			$00\frac{1}{2}\ P4x$
4	*o*			$\frac{1}{2}\frac{1}{2}0\ P4x$
8	*p*	1	* $P422\ p$	$P4x2yz$

90 $P42_12$

2	*a*	2.22	$P4/mmm\ a$	C
2	*b*			$00\frac{1}{2}\ C$
2	*c*	4..	$P4/nmm\ c$	$0\frac{1}{2}0\ ..2\ CI1z$
4	*d*	2..	$P4/mmm\ g$	$C2z$
4	*e*	..2	$P4/mbm\ g$	$.b.\ C2xx$
4	*f*			$00\frac{1}{2}\ .b.\ C2xx$
8	*g*	1	* $P42_12\ g$	$.2_1.\ C2xx2yz$

91 $P4_122$

4	*a*	.2.	* $P4_322\ a$	$00\frac{3}{4}\ 4_1..\ P_{cc}I_c1x$
4	*b*			$\frac{1}{2}\frac{1}{2}\frac{3}{4}\ 4_1..\ P_{cc}I_c1x$
4	*c*	..2	* $P4_322\ c$	$00\frac{3}{8}\ 4_1..\ P_{cc}{}^vD1xx$
8	*d*	1	* $P4_322\ d$	$00\frac{3}{4}\ 4_1..\ P_{cc}I_c1x2yz$

92 $P4_12_12$

4	*a*	..2	* $P4_32_12\ a$	$4_1..\ I_c{}^vD1xx$
8	*b*	1	* $P4_32_12\ b$	$4_1..\ I_c{}^vD1xx2yz$

93 $P4_222$

2	*a*	222.	$P4/mmm\ a$	P_c
2	*b*			$\frac{1}{2}\frac{1}{2}0\ P_c$
2	*c*	222.	$I4/mmm\ a$	$0\frac{1}{2}0\ I$
2	*d*			$0\frac{1}{2}\frac{1}{2}\ I$
2	*e*	2.22	$P4/mmm\ a$	$00\frac{1}{4}\ P_c$

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

2	f			$\frac{1}{2}\frac{1}{2}\frac{1}{4}\ P_c$
4	g	2..	$P4/mmm\ g$	P_c2z
4	h			$\frac{1}{2}\frac{1}{2}0\ P_c2z$
4	i	2..	$I4/mmm\ e$	$0\frac{1}{2}0\ I2z$
4	j	.2.	$P4_2/mmc\ j$	$..2\ P_c2x$
4	k			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ ..2\ P_c2x$
4	l			$00\frac{1}{2}\ ..2\ P_c2x$
4	m			$\frac{1}{2}\frac{1}{2}0\ ..2\ P_c2x$
4	n	..2	$P4_2/mcm\ i$	$00\frac{1}{4}\ .2.\ P_c2xx$
4	o			$00\frac{3}{4}\ .2.\ P_c2xx$
8	p	1	* $P4_222\ p$	$..2\ P_c2x2yz$
94	**$P4_22_12$**			
2	a	2.22	$I4/mmm\ a$	I
2	b			$00\frac{1}{2}\ I$
4	c	2..	$I4/mmm\ e$	$I2z$
4	d	2..	$P4/nmm\ c$	$0\frac{1}{2}0\ (..2\ CI1z)_c$
4	e	..2	$P4_2/mnm\ f$	$.n.\ I2xx$
4	f			$00\frac{1}{2}\ .n.\ I2xx$
8	g	1	* $P4_22_12\ g$	$.2_1.\ I2xx2yz$
95	**$P4_322$**			
4	a	.2.	* $P4_322\ a$	$00\frac{1}{4}\ 4_3..\ P_{cc}I_c1x$
4	b			$\frac{1}{2}\frac{1}{2}\frac{1}{4}\ 4_3..\ P_{cc}I_c1x$
4	c	..2	* $P4_322\ c$	$00\frac{5}{8}\ 4_3..\ P_{cc}{}^vD1xx$
8	d	1	* $P4_322\ d$	$00\frac{1}{4}\ 4_3..\ P_{cc}I_c1x2yz$
96	**$P4_32_12$**			
4	a	..2	* $P4_32_12\ a$	$4_3..\ I_c{}^vD1xx$
8	b	1	* $P4_32_12\ b$	$4_3..\ I_c{}^vD1xx2yz$
97	**$I422$**			
2	a	422	$I4/mmm\ a$	I
2	b			$00\frac{1}{2}\ I$
4	c	222.	$P4/mmm\ a$	$0\frac{1}{2}0\ C_c$
4	d	2.22	$P4/mmm\ a$	$0\frac{1}{2}\frac{1}{4}\ C_c$
4	e	4..	$I4/mmm\ e$	$I2z$
8	f	2..	$P4/mmm\ g$	$0\frac{1}{2}0\ C_c2z$
8	g	..2	$I4/mmm\ h$	$I4xx$
8	h	.2.	$I4/mmm\ i$	$I4x$
8	i			$00\frac{1}{2}\ I4x$
8	j	..2	$I4/mcm\ h$	$0\frac{1}{2}\frac{1}{4}\ .b.\ C_c2xx$
16	k	1	* $I422\ k$	$I4x2yz$
98	**$I4_122$**			
4	a	2.22	$I4_1/amd\ a$	${}^vD$
4	b			$00\frac{1}{2}\ {}^vD$
8	c	2..	$I4_1/amd\ e$	${}^vD2z$
8	d	..2	* $I4_122\ d$	$.2.\ {}^vD2xx$
8	e			$.2.\ {}^vD2x\bar{x}$
8	f	.2.	* $I4_122\ f$	$..22\ {}^vTC_{cc}1x$
16	g	1	* $I4_122\ g$	$.2.\ {}^vD2xx2yz$
99	**$P4mm$**			
1	a	4mm	$P4/mmm\ a$	$P[z]$
1	b			$\frac{1}{2}\frac{1}{2}0\ P[z]$
2	c	2mm.	$P4/mmm\ a$	$\frac{1}{2}00\ C[z]$
4	d	..m	$P4/mmm\ j$	$P4xx[z]$
4	e	.m.	$P4/mmm\ l$	$P4x[z]$
4	f			$\frac{1}{2}\frac{1}{2}0\ P4x[z]$
8	g	1	$P4/mmm\ p$	$P4x2y[z]$
100	**$P4bm$**			
2	a	4..	$P4/mmm\ a$	$C[z]$
2	b	2.mm	$P4/mmm\ a$	$\frac{1}{2}00\ C[z]$
4	c	..m	$P4/mbm\ g$	$0\frac{1}{2}0\ .b.\ C2xx[z]$
8	d	1	$P4/mbm\ i$	$..m\ C4xy[z]$
101	**$P4_2cm$**			
2	a	2.mm	$P4/mmm\ a$	$P_c[z]$
2	b			$\frac{1}{2}\frac{1}{2}0\ P_c[z]$
4	c	2..	$P4/mmm\ a$	$0\frac{1}{2}0\ C_c[z]$
4	d	..m	$P4_2/mcm\ i$	$.2.\ P_c2xx[z]$
8	e	1	$P4_2/mcm\ n$	$.2.\ P_c2xx2y[z]$
102	**$P4_2nm$**			
2	a	2.mm	$I4/mmm\ a$	$I[z]$
4	b	2..	$P4/mmm\ a$	$0\frac{1}{2}0\ C_c[z]$
4	c	..m	$P4_2/mnm\ f$	$.n.\ I2xx[z]$
8	d	1	$P4_2/mnm\ i$	$.n.\ I2xx2y[z]$
103	**$P4cc$**			
2	a	4..	$P4/mmm\ a$	$P_c[z]$
2	b			$\frac{1}{2}\frac{1}{2}0\ P_c[z]$
4	c	2..	$P4/mmm\ a$	$0\frac{1}{2}0\ C_c[z]$
8	d	1	$P4/mcc\ m$	$.c.\ P_c4xy[z]$
104	**$P4nc$**			
2	a	4..	$I4/mmm\ a$	$I[z]$
4	b	2..	$P4/mmm\ a$	$0\frac{1}{2}0\ C_c[z]$
8	c	1	$P4/mnc\ h$	$..2\ I4xy[z]$
105	**$P4_2mc$**			
2	a	2mm.	$P4/mmm\ a$	$P_c[z]$
2	b			$\frac{1}{2}\frac{1}{2}0\ P_c[z]$
2	c	2mm.	$I4/mmm\ a$	$0\frac{1}{2}0\ I[z]$
4	d	.m.	$P4_2/mmc\ j$	$..2\ P_c2x[z]$
4	e			$\frac{1}{2}\frac{1}{2}0\ ..2\ P_c2x[z]$
8	f	1	$P4_2/mmc\ q$	$..2\ P_c2x2y[z]$
106	**$P4_2bc$**			
4	a	2..	$P4/mmm\ a$	$C_c[z]$
4	b	2..	$P4/mmm\ a$	$0\frac{1}{2}0\ C_c[z]$
8	c	1	$P4_2/mbc\ h$	$.b2\ C_c2xy[z]$
107	**$I4mm$**			
2	a	4mm	$I4/mmm\ a$	$I[z]$
4	b	2mm.	$P4/mmm\ a$	$0\frac{1}{2}0\ C_c[z]$
8	c	..m	$I4/mmm\ h$	$I4xx[z]$
8	d	.m.	$I4/mmm\ i$	$I4x[z]$
16	e	1	$I4/mmm\ l$	$I4x2y[z]$
108	**$I4cm$**			
4	a	4..	$P4/mmm\ a$	$C_c[z]$
4	b	2.mm	$P4/mmm\ a$	$\frac{1}{2}00\ C_c[z]$

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

8	*c*	..*m*	*I*4/*mcm h*	$\frac{1}{2}00$.*b*. $C_c2xx[z]$
16	*d*	1	*I*4/*mcm k*	..*m* $C_c4xy[z]$

109 $I4_1md$

4	*a*	2*mm*.	$I4_1/amd$ *a*	$^vD[z]$
8	*b*	.*m*.	* $I4_1md$ *b*	..*d* $^vD2x[z]$
16	*c*	1	* $I4_1md$ *c*	..*d* $^vD2x2y[z]$

110 $I4_1cd$

8	*a*	2..	*I*4/*mmm a*	$F_c[z]$
16	*b*	1	* $I4_1cd$ *b*	.*bd* $F_c2xy[z]$

111 $P\bar{4}2m$

1	*a*	$\bar{4}2m$	*P*4/*mmm a*	*P*
1	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
1	*c*			$00\frac{1}{2}$ *P*
1	*d*			$\frac{1}{2}\frac{1}{2}0$ *P*
2	*e*	222.	*P*4/*mmm a*	$\frac{1}{2}00$ *C*
2	*f*			$\frac{1}{2}0\frac{1}{2}$ *C*
2	*g*	2.*mm*	*P*4/*mmm g*	*P*2*z*
2	*h*			$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
4	*i*	.2.	*P*4/*mmm l*	*P*4*x*
4	*j*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*4*x*
4	*k*			$00\frac{1}{2}$ *P*4*x*
4	*l*			$\frac{1}{2}\frac{1}{2}0$ *P*4*x*
4	*m*	2..	*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
4	*n*	..*m*	* $P\bar{4}2m$ *n*	*P*4*xxz*
8	*o*	1	* $P\bar{4}2m$ *o*	*P*4*xxz*2*y*

112 $P\bar{4}2c$

2	*a*	222.	*P*4/*mmm a*	$00\frac{1}{4}$ P_c
2	*c*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
2	*b*	222.	*I*4/*mmm a*	$\frac{1}{2}0\frac{1}{4}$ *I*
2	*d*			$0\frac{1}{2}\frac{1}{4}$ *I*
2	*e*	$\bar{4}$..	*P*4/*mmm a*	P_c
2	*f*			$\frac{1}{2}\frac{1}{2}0$ P_c
4	*g*	.2.	$P4_2/mmc$ *j*	$00\frac{1}{4}$ ..2 P_c2x
4	*h*			$\frac{1}{2}\frac{1}{2}\frac{3}{4}$ ..2 P_c2x
4	*i*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ ..2 P_c2x
4	*j*			$00\frac{3}{4}$ ..2 P_c2x
4	*k*	2..	*P*4/*mmm g*	P_c2z
4	*l*			$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*m*	2..	*I*4/*mmm e*	$0\frac{1}{2}\frac{1}{4}$ *I*2*z*
8	*n*	1	* $P\bar{4}2c$ *n*	.2. P_c4xyz

113 $P\bar{4}2_1m$

2	*a*	$\bar{4}$..	*P*4/*mmm a*	*C*
2	*b*			$00\frac{1}{2}$ *C*
2	*c*	2.*mm*	*P*4/*nmm c*	$0\frac{1}{2}0$ ..2 *CI*1*z*
4	*d*	2..	*P*4/*mmm g*	*C*2*z*
4	*e*	..*m*	* $P\bar{4}2_1m$ *e*	$0\frac{1}{2}0$ .2_1. *CI*1*z*2*xx*
8	*f*	1	* $P\bar{4}2_1m$ *f*	..*m* *C*4*xyz*

114 $P\bar{4}2_1c$

2	*a*	$\bar{4}$..	*I*4/*mmm a*	*I*
2	*b*			$00\frac{1}{2}$ *I*
4	*c*	2..	*I*4/*mmm e*	*I*2*z*
4	*d*	2..	*P*4/*nmm c*	$0\frac{1}{2}0$ $(..2\ CI1z)_c$
8	*e*	1	* $P\bar{4}2_1c$ *e*	..*c* *I*4*xyz*

115 $P\bar{4}m2$

1	*a*	$\bar{4}m2$	*P*4/*mmm a*	*P*
1	*b*			$\frac{1}{2}\frac{1}{2}0$ *P*
1	*c*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
1	*d*			$00\frac{1}{2}$ *P*
2	*e*	2*mm*.	*P*4/*mmm g*	*P*2*z*
2	*f*			$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
2	*g*	2*mm*.	*P*4/*nmm c*	$0\frac{1}{2}0$ ..2 *CI*1*z*
4	*h*	..2	*P*4/*mmm j*	*P*4*xx*
4	*i*			$00\frac{1}{2}$ *P*4*xx*
4	*j*	.*m*.	* $P\bar{4}m2$ *j*	*P*4*xz*
4	*k*			$\frac{1}{2}\frac{1}{2}0$ *P*4*xz*
8	*l*	1	* $P\bar{4}m2$ *l*	*P*4*xz*2*y*

116 $P\bar{4}c2$

2	*a*	2.22	*P*4/*mmm a*	$00\frac{1}{4}$ P_c
2	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
2	*c*	$\bar{4}$..	*P*4/*mmm a*	P_c
2	*d*			$\frac{1}{2}\frac{1}{2}0$ P_c
4	*e*	..2	$P4_2/mcm$ *i*	$00\frac{1}{4}$ .2. P_c2xx
4	*f*			$00\frac{3}{4}$ .2. P_c2xx
4	*g*	2..	*P*4/*mmm g*	P_c2z
4	*h*			$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*i*	2..	*P*4/*nmm c*	$0\frac{1}{2}0$ $(..2\ CI1z)_c$
8	*j*	1	* $P\bar{4}c2$ *j*	..2 P_c4xyz

117 $P\bar{4}b2$

2	*a*	$\bar{4}$..	*P*4/*mmm a*	*C*
2	*b*			$00\frac{1}{2}$ *C*
2	*c*	2.22	*P*4/*mmm a*	$0\frac{1}{2}0$ *C*
2	*d*			$0\frac{1}{2}\frac{1}{2}$ *C*
4	*e*	2..	*P*4/*mmm g*	*C*2*z*
4	*f*	2..	*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
4	*g*	..2	*P*4/*mbm g*	$0\frac{1}{2}0$.*b*. *C*2*xx*
4	*h*			$0\frac{1}{2}\frac{1}{2}$.*b*. *C*2*xx*
8	*i*	1	* $P\bar{4}b2$ *i*	..2 *C*4*xyz*

118 $P\bar{4}n2$

2	*a*	$\bar{4}$..	*I*4/*mmm a*	*I*
2	*b*			$00\frac{1}{2}$ *I*
2	*c*	2.22	*I*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ *I*
2	*d*			$0\frac{1}{2}\frac{3}{4}$ *I*
4	*e*	2..	*I*4/*mmm e*	*I*2*z*
4	*f*	..2	$P4_2/mnm$ *f*	$\frac{1}{2}0\frac{3}{4}$.*n*. *I*2*xx*
4	*g*			$0\frac{1}{2}\frac{1}{4}$.*n*. *I*2*xx*
4	*h*	2..	*I*4/*mmm e*	$0\frac{1}{2}\frac{1}{4}$ *I*2*z*
8	*i*	1	* $P\bar{4}n2$ *i*	..2 *I*4*xyz*

119 $I\bar{4}m2$

2	*a*	$\bar{4}m2$	*I*4/*mmm a*	*I*
2	*b*			$00\frac{1}{2}$ *I*
2	*c*			$0\frac{1}{2}\frac{1}{4}$ *I*
2	*d*			$0\frac{1}{2}\frac{3}{4}$ *I*
4	*e*	2*mm*.	*I*4/*mmm e*	*I*2*z*
4	*f*			$0\frac{1}{2}\frac{1}{4}$ *I*2*z*
8	*g*	..2	*I*4/*mmm h*	*I*4*xx*

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

8	*h*			$0\frac{1}{2}\frac{1}{4}$ $I4xx$
8	*i*	.*m*.	* $I\bar{4}m2$ *i*	$I4xz$
16	*j*	1	* $I\bar{4}m2$ *j*	$I4xz2y$
120	**$I\bar{4}c2$**			
4	*a*	2.22	$P4/mmm$ *a*	$00\frac{1}{4}$ C_c
4	*d*			$0\frac{1}{2}0$ C_c
4	*b*	$\bar{4}$..	$P4/mmm$ *a*	C_c
4	*c*			$0\frac{1}{2}\frac{1}{4}$ C_c
8	*e*	..2	$I4/mcm$ *h*	$00\frac{1}{4}$.*b*. C_c2xx
8	*h*			$0\frac{1}{2}0$.*b*. C_c2xx
8	*f*	2..	$P4/mmm$ *g*	C_c2z
8	*g*			$0\frac{1}{2}0$ C_c2z
16	*i*	1	* $I\bar{4}c2$ *i*	..2 C_c4xyz
121	**$I\bar{4}2m$**			
2	*a*	$\bar{4}2m$	$I4/mmm$ *a*	I
2	*b*			$00\frac{1}{2}$ I
4	*c*	222.	$P4/mmm$ *a*	$0\frac{1}{2}0$ C_c
4	*d*	$\bar{4}$..	$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	2.*mm*	$I4/mmm$ *e*	$I2z$
8	*f*	.2.	$I4/mmm$ *i*	$I4x$
8	*g*			$00\frac{1}{2}$ $I4x$
8	*h*	2..	$P4/mmm$ *g*	$0\frac{1}{2}0$ C_c2z
8	*i*	..*m*	* $I\bar{4}2m$ *i*	$I4xxz$
16	*j*	1	* $I\bar{4}2m$ *j*	$I4xxz2y$
122	**$I\bar{4}2d$**			
4	*a*	$\bar{4}$..	$I4_1/amd$ *a*	${}^vD$
4	*b*			$00\frac{1}{2}$ ${}^vD$
8	*c*	2..	$I4_1/amd$ *e*	${}^vD2z$
8	*d*	.2.	* $I\bar{4}2d$ *d*	$\bar{4}$.. ${}^vTF_c1x$
16	*e*	1	* $I\bar{4}2d$ *e*	.2. ${}^vD4xyz$
123	**$P4/mmm$**			
1	*a*	$4/mmm$	* $P4/mmm$ *a*	P
1	*b*			$00\frac{1}{2}$ P
1	*c*			$\frac{1}{2}\frac{1}{2}0$ P
1	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ P
2	*e*	*mmm*.	$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{2}$ C
2	*f*			$0\frac{1}{2}0$ C
2	*g*	4*mm*	* $P4/mmm$ *g*	$P2z$
2	*h*			$\frac{1}{2}\frac{1}{2}0$ $P2z$
4	*i*	2*mm*.	$P4/mmm$ *g*	$0\frac{1}{2}0$ $C2z$
4	*j*	*m*.2*m*	* $P4/mmm$ *j*	$P4xx$
4	*k*			$00\frac{1}{2}$ $P4xx$
4	*l*	*m*2*m*.	* $P4/mmm$ *l*	$P4x$
4	*m*			$00\frac{1}{2}$ $P4x$
4	*n*			$\frac{1}{2}\frac{1}{2}0$ $P4x$
4	*o*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ $P4x$
8	*p*	*m*..	* $P4/mmm$ *p*	$P4x2y$
8	*q*			$00\frac{1}{2}$ $P4x2y$
8	*r*	..*m*	* $P4/mmm$ *r*	$P4xx2z$
8	*s*	.*m*.	* $P4/mmm$ *s*	$P4x2z$
8	*t*			$\frac{1}{2}\frac{1}{2}0$ $P4x2z$
16	*u*	1	* $P4/mmm$ *u*	$P4x2y2z$
124	**$P4/mcc$**			
2	*a*	422	$P4/mmm$ *a*	$00\frac{1}{4}$ P_c
2	*c*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
2	*b*	$4/m$..	$P4/mmm$ *a*	P_c
2	*d*			$\frac{1}{2}\frac{1}{2}0$ P_c
4	*e*	$2/m$..	$P4/mmm$ *a*	$0\frac{1}{2}0$ C_c
4	*f*	222.	$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*g*	4..	$P4/mmm$ *g*	P_c2z
4	*h*			$\frac{1}{2}\frac{1}{2}0$ P_c2z
8	*i*	2..	$P4/mmm$ *g*	$0\frac{1}{2}0$ C_c2z
8	*j*	..2	$P4/mmm$ *j*	$00\frac{1}{4}$ P_c4xx
8	*k*	.2.	$P4/mmm$ *l*	$00\frac{1}{4}$ P_c4x
8	*l*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c4x
8	*m*	*m*..	* $P4/mcc$ *m*	.*c*. P_c4xy
16	*n*	1	* $P4/mcc$ *n*	.*c*. P_c4xy2z
125	**$P4/nbm$**			
2	*a*	422	$P4/mmm$ *a*	C
2	*b*			$00\frac{1}{2}$ C
2	*c*	$\bar{4}2m$	$P4/mmm$ *a*	$0\frac{1}{2}0$ C
2	*d*			$0\frac{1}{2}\frac{1}{2}$ C
4	*e*	..$2/m$	$P4/mmm$ *a*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*f*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*g*	4..	$P4/mmm$ *g*	$C2z$
4	*h*	2.*mm*	$P4/mmm$ *g*	$0\frac{1}{2}0$ $C2z$
8	*i*	..2	$P4/mmm$ *l*	$C4xx$
8	*j*			$00\frac{1}{2}$ $C4xx$
8	*k*	.2.	$P4/mmm$ *j*	$C4x$
8	*l*			$00\frac{1}{2}$ $C4x$
8	*m*	..*m*	* $P4/nbm$ *m*	$0\frac{1}{2}0$ ..2 $C4xxz$
16	*n*	1	* $P4/nbm$ *n*	..*m* $C4x2yz$
126	**$P4/nnc$**			
2	*a*	422	$I4/mmm$ *a*	I
2	*b*			$00\frac{1}{2}$ I
4	*c*	222.	$P4/mmm$ *a*	$\frac{1}{2}00$ C_c
4	*d*	$\bar{4}$..	$P4/mmm$ *a*	$\frac{1}{2}0\frac{1}{4}$ C_c
4	*e*	4..	$I4/mmm$ *e*	$I2z$
8	*f*	$\bar{1}$	$P4/mmm$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*g*	2..	$P4/mmm$ *g*	$\frac{1}{2}00$ C_c2z
8	*h*	..2	$I4/mmm$ *h*	$I4xx$
8	*i*	.2.	$I4/mmm$ *i*	$I4x$
8	*j*			$00\frac{1}{2}$ $I4x$
16	*k*	1	* $P4/nnc$ *k*	..*c* $I4x2yz$
127	**$P4/mbm$**			
2	*a*	$4/m$..	$P4/mmm$ *a*	C
2	*b*			$00\frac{1}{2}$ C
2	*c*	*m*.*mm*	$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{2}$ C
2	*d*			$0\frac{1}{2}0$ C
4	*e*	4..	$P4/mmm$ *g*	$C2z$
4	*f*	2.*mm*	$P4/mmm$ *g*	$0\frac{1}{2}0$ $C2z$
4	*g*	*m*.2*m*	* $P4/mbm$ *g*	$0\frac{1}{2}0$.*b*. $C2xx$
4	*h*			$0\frac{1}{2}\frac{1}{2}$.*b*. $C2xx$
8	*i*	*m*..	* $P4/mbm$ *i*	..*m* $C4xy$
8	*j*			$00\frac{1}{2}$ ..*m* $C4xy$
8	*k*	..*m*	* $P4/mbm$ *k*	$0\frac{1}{2}0$.*b*. $C2xx2z$
16	*l*	1	* $P4/mbm$ *l*	..*m* $C4xy2z$

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

128 $P4/mnc$

2	*a*	$4/m..$	$I4/mmm$ *a*	I
2	*b*			$00\frac{1}{2}$ I
4	*c*	$2/m..$	$P4/mmm$ *a*	$0\frac{1}{2}0$ C_c
4	*d*	2.22	$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	$4..$	$I4/mmm$ *e*	$I2z$
8	*f*	$2..$	$P4/mmm$ *g*	$0\frac{1}{2}0$ C_c2z
8	*g*	$..2$	$P4/mbm$ *g*	$0\frac{1}{2}\frac{1}{4}$ $(.b.\ C2xx)_c$
8	*h*	$m..$	* $P4/mnc$ *h*	$..2$ $I4xy$
16	*i*	1	* $P4/mnc$ *i*	$..2$ $I4xy2z$

129 $P4/nmm$

2	*a*	$\bar{4}m2$	$P4/mmm$ *a*	C
2	*b*			$00\frac{1}{2}$ C
2	*c*	$4mm$	* $P4/nmm$ *c*	$0\frac{1}{2}0$ $..2$ $CI1z$
4	*d*	$..2/m$	$P4/mmm$ *a*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*e*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*f*	$2mm.$	$P4/mmm$ *g*	$C2z$
8	*g*	$..2$	$P4/mmm$ *l*	$C4xx$
8	*h*			$00\frac{1}{2}$ $C4xx$
8	*i*	$.m.$	* $P4/nmm$ *i*	$..m$ $C4xz$
8	*j*	$..m$	* $P4/nmm$ *j*	$0\frac{1}{2}0$ $..2$ $CI1z4xx$
16	*k*	1	* $P4/nmm$ *k*	$..m$ $C4xz2y$

130 $P4/ncc$

4	*a*	2.22	$P4/mmm$ *a*	$00\frac{1}{4}$ C_c
4	*b*	$\bar{4}..$	$P4/mmm$ *a*	C_c
4	*c*	$4..$	$P4/nmm$ *c*	$0\frac{1}{2}0$ $(..2\ CI1z)_c$
8	*d*	$\bar{1}$	$P4/mmm$ *a*	$\frac{1}{4}\frac{1}{4}0$ P_2
8	*e*	$2..$	$P4/mmm$ *g*	C_c2z
8	*f*	$..2$	$I4/mcm$ *h*	$00\frac{1}{4}$ $.b.$ C_c2xx
16	*g*	1	* $P4/ncc$ *g*	$..c2$ C_c4xyz

131 $P4_2/mmc$

2	*a*	$mmm.$	$P4/mmm$ *a*	P_c
2	*b*			$\frac{1}{2}\frac{1}{2}0$ P_c
2	*c*	$mmm.$	$I4/mmm$ *a*	$0\frac{1}{2}0$ I
2	*d*			$0\frac{1}{2}\frac{1}{2}$ I
2	*e*	$\bar{4}m2$	$P4/mmm$ *a*	$00\frac{1}{4}$ P_c
2	*f*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
4	*g*	$2mm.$	$P4/mmm$ *g*	P_c2z
4	*h*			$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*i*	$2mm.$	$I4/mmm$ *e*	$0\frac{1}{2}0$ $I2z$
4	*j*	$m2m.$	* $P4_2/mmc$ *j*	$..2$ P_c2x
4	*k*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ $..2$ P_c2x
4	*l*			$00\frac{1}{2}$ $..2$ P_c2x
4	*m*			$\frac{1}{2}\frac{1}{2}0$ $..2$ P_c2x
8	*n*	$..2$	$P4/mmm$ *j*	$00\frac{1}{4}$ P_c4xx
8	*o*	$.m.$	* $P4_2/mmc$ *o*	$..c$ P_c2x2z
8	*p*			$\frac{1}{2}\frac{1}{2}0$ $..c$ P_c2x2z
8	*q*	$m..$	* $P4_2/mmc$ *q*	$..2$ P_c2x2y
16	*r*	1	* $P4_2/mmc$ *r*	$..c$ $P_c2x2y2z$

132 $P4_2/mcm$

2	*a*	$m.mm$	$P4/mmm$ *a*	P_c
2	*c*			$\frac{1}{2}\frac{1}{2}0$ P_c
2	*b*	$\bar{4}2m$	$P4/mmm$ *a*	$00\frac{1}{4}$ P_c
2	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
4	*e*	$222.$	$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*f*	$2/m..$	$P4/mmm$ *a*	$0\frac{1}{2}0$ C_c
4	*g*	$2.mm$	$P4/mmm$ *g*	P_c2z
4	*h*			$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*i*	$m.2m$	* $P4_2/mcm$ *i*	$.2.$ P_c2xx
4	*j*			$00\frac{1}{2}$ $.2.$ P_c2xx
8	*k*	$2..$	$P4/mmm$ *g*	$0\frac{1}{2}0$ C_c2z
8	*l*	$.2.$	$P4/mmm$ *l*	$00\frac{1}{4}$ P_c4x
8	*m*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c4x
8	*n*	$m..$	* $P4_2/mcm$ *n*	$.2.$ P_c2xx2y
8	*o*	$..m$	* $P4_2/mcm$ *o*	$.c.$ P_c2xx2z
16	*p*	1	* $P4_2/mcm$ *p*	$.c.$ $P_c2xx2y2z$

133 $P4_2/nbc$

4	*a*	$222.$	$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*b*	$222.$	$P4/mmm$ *a*	$00\frac{1}{4}$ C_c
4	*c*	2.22	$P4/mmm$ *a*	$0\frac{1}{2}0$ C_c
4	*d*	$\bar{4}..$	$P4/mmm$ *a*	C_c
8	*e*	$\bar{1}$	$P4/mmm$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*f*	$2..$	$P4/mmm$ *g*	$0\frac{1}{2}0$ C_c2z
8	*g*	$2..$	$P4/mmm$ *g*	C_c2z
8	*h*	$.2.$	$P4_2/mcm$ *i*	$00\frac{1}{4}$ $..2$ C_c2x
8	*i*			$00\frac{3}{4}$ $..2$ C_c2x
8	*j*	$..2$	$I4/mcm$ *h*	$0\frac{1}{2}0$ $.b.$ C_c2xx
16	*k*	1	* $P4_2/nbc$ *k*	$.22$ C_c4xyz

134 $P4_2/nnm$

2	*a*	$\bar{4}2m$	$I4/mmm$ *a*	I
2	*b*			$00\frac{1}{2}$ I
4	*c*	$222.$	$P4/mmm$ *a*	$0\frac{1}{2}0$ C_c
4	*d*	2.22	$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	$..2/m$	$I4/mmm$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ F
4	*f*			$\frac{1}{4}\frac{1}{4}\frac{3}{4}$ F
4	*g*	$2.mm$	$I4/mmm$ *e*	$I2z$
8	*h*	$2..$	$P4/mmm$ *g*	$0\frac{1}{2}0$ C_c2z
8	*i*	$.2.$	$I4/mmm$ *i*	$I4x$
8	*j*			$00\frac{1}{2}$ $I4x$
8	*k*	$..2$	$P4_2/mmc$ *j*	$0\frac{1}{2}\frac{1}{4}$ $.2.$ C_c2xx
8	*l*			$0\frac{1}{2}\frac{3}{4}$ $.2.$ C_c2xx
8	*m*	$..m$	* $P4_2/nnm$ *m*	$..2$ $I4xxz$
16	*n*	1	* $P4_2/nnm$ *n*	$..2$ $I4xxz2y$

135 $P4_2/mbc$

4	*a*	$2/m..$	$P4/mmm$ *a*	C_c
4	*b*	$\bar{4}..$	$P4/mmm$ *a*	$00\frac{1}{4}$ C_c
4	*c*	$2/m..$	$P4/mmm$ *a*	$0\frac{1}{2}0$ C_c
4	*d*	2.22	$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{4}$ C_c
8	*e*	$2..$	$P4/mmm$ *g*	C_c2z
8	*f*	$2..$	$P4/mmm$ *g*	$0\frac{1}{2}0$ C_c2z
8	*g*	$..2$	$P4/mbm$ *g*	$0\frac{1}{2}\frac{1}{4}$ $(.b.\ C2xx)_c$
8	*h*	$m..$	* $P4_2/mbc$ *h*	$.b2$ C_c2xy
16	*i*	1	* $P4_2/mbc$ *i*	$.b2$ C_c2xy2z

136 $P4_2/mnm$

2	*a*	$m.mm$	$I4/mmm$ *a*	I
2	*b*			$00\frac{1}{2}$ I
4	*c*	$2/m..$	$P4/mmm$ *a*	$0\frac{1}{2}0$ C_c
4	*d*	$\bar{4}..$	$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{4}$ C_c

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

4	*e*	$2.mm$	$I4/mmm\ e$	$I2z$
4	*f*	$m.2m$	* $P4_2/mnm\ f$	$.n.\ I2xx$
4	*g*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ .n.\ I2xx$
8	*h*	$2..$	$P4/mmm\ g$	$0\frac{1}{2}0\ C_c2z$
8	*i*	$m..$	* $P4_2/mnm\ i$	$.n.\ I2xx2y$
8	*j*	$..m$	* $P4_2/mnm\ j$	$.n.\ I2xx2z$
16	*k*	1	* $P4_2/mnm\ k$	$.n.\ I2xx2y2z$

137 $P4_2/nmc$

2	*a*	$\bar{4}m2$	$I4/mmm\ a$	I
2	*b*			$00\frac{1}{2}\ I$
4	*c*	$2mm.$	$I4/mmm\ e$	$I2z$
4	*d*	$2mm.$	$P4/nmm\ c$	$0\frac{1}{2}0\ (..2\ CI1z)_c$
8	*e*	$\bar{1}$	$P4/mmm\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*f*	$..2$	$I4/mmm\ h$	$I4xx$
8	*g*	$.m.$	* $P4_2/nmc\ g$	$..c\ I4xz$
16	*h*	1	* $P4_2/nmc\ h$	$..c\ I4xz2y$

138 $P4_2/ncm$

4	*a*	2.22	$P4/mmm\ a$	$00\frac{1}{4}\ C_c$
4	*b*	$\bar{4}..$	$P4/mmm\ a$	C_c
4	*c*	$..2/m$	$I4/mmm\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F$
4	*d*			$\frac{1}{4}\frac{1}{4}\frac{3}{4}\ F$
4	*e*	$2.mm$	$P4/nmm\ c$	$0\frac{1}{2}0\ (..2\ CI1z)_c$
8	*f*	$2..$	$P4/mmm\ g$	C_c2z
8	*g*	$..2$	$P4_2/mmc\ j$	$00\frac{1}{4}\ .2.\ C_c2xx$
8	*h*			$00\frac{3}{4}\ .2.\ C_c2xx$
8	*i*	$..m$	* $P4_2/ncm\ i$	$\frac{1}{4}\frac{3}{4}\frac{1}{4}\ \bar{4}..\ F2xxz$
16	*j*	1	* $P4_2/ncm\ j$	$..m2\ C_c4xyz$

139 $I4/mmm$

2	*a*	$4/mmm$	* $I4/mmm\ a$	I
2	*b*			$00\frac{1}{2}\ I$
4	*c*	$mmm.$	$P4/mmm\ a$	$0\frac{1}{2}0\ C_c$
4	*d*	$\bar{4}m2$	$P4/mmm\ a$	$0\frac{1}{2}\frac{1}{4}\ C_c$
4	*e*	$4mm$	* $I4/mmm\ e$	$I2z$
8	*f*	$..2/m$	$P4/mmm\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*g*	$2mm.$	$P4/mmm\ g$	$0\frac{1}{2}0\ C_c2z$
8	*h*	$m.2m$	* $I4/mmm\ h$	$I4xx$
8	*i*	$m2m.$	* $I4/mmm\ i$	$I4x$
8	*j*			$\frac{1}{2}\frac{1}{2}0\ I4x$
16	*k*	$..2$	$P4/mmm\ l$	$0\frac{1}{2}\frac{1}{4}\ C_c4xx$
16	*l*	$m..$	* $I4/mmm\ l$	$I4x2y$
16	*m*	$..m$	* $I4/mmm\ m$	$I4xx2z$
16	*n*	$.m.$	* $I4/mmm\ n$	$I4x2z$
32	*o*	1	* $I4/mmm\ o$	$I4x2y2z$

140 $I4/mcm$

4	*a*	422	$P4/mmm\ a$	$00\frac{1}{4}\ C_c$
4	*b*	$\bar{4}2m$	$P4/mmm\ a$	$0\frac{1}{2}\frac{1}{4}\ C_c$
4	*c*	$4/m..$	$P4/mmm\ a$	C_c
4	*d*	$m.mm$	$P4/mmm\ a$	$0\frac{1}{2}0\ C_c$
8	*e*	$..2/m$	$P4/mmm\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*f*	$4..$	$P4/mmm\ g$	C_c2z
8	*g*	$2.mm$	$P4/mmm\ g$	$0\frac{1}{2}0\ C_c2z$
8	*h*	$m.2m$	* $I4/mcm\ h$	$0\frac{1}{2}0\ .b.\ C_c2xx$
16	*i*	$..2$	$P4/mmm\ l$	$00\frac{1}{4}\ C_c4xx$
16	*j*	$.2.$	$P4/mmm\ j$	$00\frac{1}{4}\ C_c4x$
16	*k*	$m..$	* $I4/mcm\ k$	$..m\ C_c4xy$
16	*l*	$..m$	* $I4/mcm\ l$	$0\frac{1}{2}\frac{1}{4}\ .b.\ C_c4xxz$
32	*m*	1	* $I4/mcm\ m$	$.c.\ C_c4xy2z$

141 $I4_1/amd$

4	*a*	$\bar{4}m2$	* $I4_1/amd\ a$	^vD
4	*b*			$00\frac{1}{2}\ ^vD$
8	*c*	$.2/m.$	* $I4_1/amd\ c$	^vT
8	*d*			$00\frac{1}{2}\ ^vT$
8	*e*	$2mm.$	* $I4_1/amd\ e$	^vD2z
16	*f*	$.2.$	* $I4_1/amd\ f$	$..2\ ^vT2x$
16	*g*	$..2$	* $I4_1/amd\ g$	^vD4xx
16	*h*	$.m.$	* $I4_1/amd\ h$	$.2.\ ^vD4xz$
32	*i*	1	* $I4_1/amd\ i$	$.2.\ ^vD4xz2y$

142 $I4_1/acd$

8	*a*	$\bar{4}..$	$I4/mmm\ a$	F_c
8	*b*	2.22	$I4/mmm\ a$	$00\frac{1}{4}\ F_c$
16	*c*	$\bar{1}$	$I4/mmm\ a$	$0\frac{1}{4}\frac{1}{8}\ I_2$
16	*d*	$2..$	$I4/mmm\ e$	F_c2z
16	*e*	$.2.$	* $I4_1/acd\ e$	$0\frac{1}{4}\frac{3}{8}\ \bar{4}..\ I_2P_{c2}1x$
16	*f*	$..2$	* $I4_1/acd\ f$	$00\frac{1}{4}\ .2.\ F_c2xx$
32	*g*	1	* $I4_1/acd\ g$	$.22\ F_c4xyz$

143 $P3$

1	*a*	$3..$	$P6/mmm\ a$	$P[z]$
1	*b*			$\frac{1}{3}\frac{2}{3}0\ P[z]$
1	*c*			$\frac{2}{3}\frac{1}{3}0\ P[z]$
3	*d*	1	$P\bar{6}\ j$	$P3xy[z]$

144 $P3_1$

3	*a*	1	* $P3_2\ a$	$3_1..\ P_CR^-Q1xy[z]$

145 $P3_2$

3	*a*	1	* $P3_2\ a$	$3_2..\ P_CR^+Q1xy[z]$

146 $R3$ (Hexagonal axes)

3	*a*	$3.$	$R\bar{3}m\ a$	$R[z]$
9	*b*	1	* $R3\ b$	$R3xy[z]$

146 $R3$ (Rhombohedral axes)

1	*a*	$3.$	$R\bar{3}m\ a$	$P[xxx]$
3	*b*	1	* $R3\ b$	$P3yz[xxx]$

147 $P\bar{3}$

1	*a*	$\bar{3}..$	$P6/mmm\ a$	P
1	*b*			$00\frac{1}{2}\ P$
2	*c*	$3..$	$P6/mmm\ e$	$P2z$
2	*d*	$3..$	$P\bar{3}m1\ d$	$.2.\ GE1z$
3	*e*	$\bar{1}$	$P6/mmm\ f$	N
3	*f*			$00\frac{1}{2}\ N$
6	*g*	1	* $P\bar{3}\ g$	$P6xyz$

148 $R\bar{3}$ (Hexagonal axes)

3	*a*	$\bar{3}.$	$R\bar{3}m\ a$	R
3	*b*			$00\frac{1}{2}\ R$
6	*c*	$3.$	$R\bar{3}m\ c$	$R2z$
9	*d*	$\bar{1}$	$R\bar{3}m\ e$	$00\frac{1}{2}\ M$

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

9	*e*				*M*
18	*f*	1	*	$R\bar{3}\,f$	*R6xyz*
148	$\boldsymbol{R\bar{3}}$	(Rhombohedral axes)			
1	*a*	$\bar{3}.$		$R\bar{3}m\ a$	*P*
1	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P$
2	*c*	3.		$R\bar{3}m\ c$	*P2xxx*
3	*d*	$\bar{1}$		$R\bar{3}m\ e$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ J$
3	*e*				*J*
6	*f*	1	*	$R\bar{3}\,f$	*P6xyz*
149	***P*312**				
1	*a*	3.2		$P6/mmm\ a$	*P*
1	*b*				$00\frac{1}{2}\ P$
1	*c*				$\frac{1}{3}\frac{2}{3}0\ P$
1	*d*				$\frac{1}{3}\frac{2}{3}\frac{1}{2}\ P$
1	*e*				$\frac{2}{3}\frac{1}{3}0\ P$
1	*f*				$\frac{2}{3}\frac{1}{3}\frac{1}{2}\ P$
2	*g*	3..		$P6/mmm\ e$	*P2z*
2	*h*				$\frac{1}{3}\frac{2}{3}0\ P2z$
2	*i*				$\frac{2}{3}\frac{1}{3}0\ P2z$
3	*j*	..2		$P\bar{6}m2\ j$	$P3x\bar{x}$
3	*k*				$00\frac{1}{2}\ P3x\bar{x}$
6	*l*	1	*	$P312\ l$	$P3x\bar{x}2yz$
150	***P*321**				
1	*a*	32.		$P6/mmm\ a$	*P*
1	*b*				$00\frac{1}{2}\ P$
2	*c*	3..		$P6/mmm\ e$	*P2z*
2	*d*	3..		$P\bar{3}m1\ d$	*.2. GE1z*
3	*e*	.2.		$P\bar{6}2m\,f$	*P3x*
3	*f*				$00\frac{1}{2}\ P3x$
6	*g*	1	*	$P321\ g$	*P3x2yz*
151	$\boldsymbol{P3_112}$				
3	*a*	..2	*	$P3_212\ a$	$00\frac{1}{3}\ 3_1..\ P_C{}^-Q1x\bar{x}$
3	*b*				$00\frac{5}{6}\ 3_1..\ P_C{}^-Q1x\bar{x}$
6	*c*	1	*	$P3_212\ c$	$00\frac{1}{3}\ 3_1..\ P_C{}^-Q1x\bar{x}2yz$
152	$\boldsymbol{P3_121}$				
3	*a*	.2.	*	$P3_221\ a$	$00\frac{1}{3}\ 3_1..\ P_CR^-Q1x$
3	*b*				$00\frac{5}{6}\ 3_1..\ P_CR^-Q1x$
6	*c*	1	*	$P3_221\ c$	$00\frac{1}{3}\ 3_1..\ P_CR^-Q1x2yz$
153	$\boldsymbol{P3_212}$				
3	*a*	..2	*	$P3_212\ a$	$00\frac{2}{3}\ 3_2..\ P_C{}^+Q1x\bar{x}$
3	*b*				$00\frac{1}{6}\ 3_2..\ P_C{}^+Q1x\bar{x}$
6	*c*	1	*	$P3_212\ c$	$00\frac{2}{3}\ 3_2..\ P_C{}^+Q1x\bar{x}2yz$
154	$\boldsymbol{P3_221}$				
3	*a*	.2.	*	$P3_221\ a$	$00\frac{2}{3}\ 3_2..\ P_CR^+Q1x$
3	*b*				$00\frac{1}{6}\ 3_2..\ P_CR^+Q1x$
6	*c*	1	*	$P3_221\ c$	$00\frac{2}{3}\ 3_2..\ P_CR^+Q1x2yz$
155	***R*32**	(Hexagonal axes)			
3	*a*	32		$R\bar{3}m\ a$	*R*
3	*b*				$00\frac{1}{2}\ R$
6	*c*	3.		$R\bar{3}m\ c$	*R2z*
9	*d*	.2	*	$R32\ d$	*R3x*
9	*e*				$00\frac{1}{2}\ R3x$
18	*f*	1	*	$R32\,f$	*R3x2yz*
155	***R*32**	(Rhombohedral axes)			
1	*a*	32		$R\bar{3}m\ a$	*P*
1	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P$
2	*c*	3.		$R\bar{3}m\ c$	*P2xxx*
3	*d*	.2	*	$R32\ d$	$P3x\bar{x}$
3	*e*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P3x\bar{x}$
6	*f*	1	*	$R32\,f$	$P3x\bar{x}2yz$
156	***P*3*m*1**				
1	*a*	3*m*.		$P6/mmm\ a$	*P*[*z*]
1	*b*				$\frac{1}{3}\frac{2}{3}0\ P[z]$
1	*c*				$\frac{2}{3}\frac{1}{3}0\ P[z]$
3	*d*	.*m*.		$P\bar{6}m2\ j$	$P3x\bar{x}[z]$
6	*e*	1		$P\bar{6}m2\ l$	$P3x\bar{x}2y[z]$
157	***P*31*m***				
1	*a*	3.*m*		$P6/mmm\ a$	*P*[*z*]
2	*b*	3..		$P6/mmm\ c$	*G*[*z*]
3	*c*	..*m*		$P\bar{6}2m\,f$	*P3x*[*z*]
6	*d*	1		$P\bar{6}2m\ j$	*P3x2y*[*z*]
158	***P*3*c*1**				
2	*a*	3..		$P6/mmm\ a$	$P_c[z]$
2	*b*				$\frac{1}{3}\frac{2}{3}0\ P_c[z]$
2	*c*				$\frac{2}{3}\frac{1}{3}0\ P_c[z]$
6	*d*	1		$P\bar{6}c2\ k$	$..2\ P_c3xy[z]$
159	***P*31*c***				
2	*a*	3..		$P6/mmm\ a$	$P_c[z]$
2	*b*	3..		$P6_3/mmc\ c$	*E*[*z*]
6	*c*	1		$P\bar{6}2c\ h$	$.2.\ P_c3xy[z]$
160	***R*3*m***	(Hexagonal axes)			
3	*a*	3*m*		$R\bar{3}m\ a$	*R*[*z*]
9	*b*	.*m*	*	$R3m\ b$	$R3x\bar{x}[z]$
18	*c*	1	*	$R3m\ c$	$R3x\bar{x}2y[z]$
160	***R*3*m***	(Rhombohedral axes)			
1	*a*	3*m*		$R\bar{3}m\ a$	*P*[*xxx*]
3	*b*	.*m*	*	$R3m\ b$	*P3z*[*xxx*]
6	*c*	1	*	$R3m\ c$	*P3z2y*[*xxx*]
161	***R*3*c***	(Hexagonal axes)			
6	*a*	3.		$R\bar{3}m\ a$	$'R_c[z]$
18	*b*	1	*	$R3c\ b$	$.c\ 'R_c3xy[z]$
161	***R*3*c***	(Rhombohedral axes)			
2	*a*	3.		$R\bar{3}m\ a$	*I*[*xxx*]
6	*b*	1	*	$R3c\ b$	*.n I3yz*[*xxx*]
162	$\boldsymbol{P\bar{3}1m}$				
1	*a*	$\bar{3}.m$		$P6/mmm\ a$	*P*
1	*b*				$00\frac{1}{2}\ P$
2	*c*	3.2		$P6/mmm\ c$	*G*

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

2	*d*			$00\frac{1}{2}\ G$
2	*e*	$3.m$	$P6/mmm\ e$	$P2z$
3	*f*	$..2/m$	$P6/mmm\ f$	N
3	*g*			$00\frac{1}{2}\ N$
4	*h*	$3..$	$P6/mmm\ h$	$G2z$
6	*i*	$..2$	$P6/mmm\ l$	$P6x\bar{x}$
6	*j*			$00\frac{1}{2}\ P6x\bar{x}$
6	*k*	$..m$	$^*\ P\bar{3}1m\ k$	$P6xz$
12	*l*	1	$^*\ P\bar{3}1m\ l$	$P6xz2y$
163	**$P\bar{3}1c$**			
2	*a*	3.2	$P6/mmm\ a$	$00\frac{1}{4}\ P_c$
2	*b*	$\bar{3}..$	$P6/mmm\ a$	P_c
2	*c*	3.2	$P6_3/mmc\ c$	E
2	*d*			$00\frac{1}{2}\ E$
4	*e*	$3..$	$P6/mmm\ e$	P_c2z
4	*f*	$3..$	$P6_3/mmc\ f$	$E2z$
6	*g*	$\bar{1}$	$P6/mmm\ f$	N_c
6	*h*	$..2$	$P6_3/mmc\ h$	$00\frac{1}{4}\ .2.\ P_c3x\bar{x}$
12	*i*	1	$^*\ P\bar{3}1c\ i$	$..c\ P_c6xyz$
164	**$P\bar{3}m1$**			
1	*a*	$\bar{3}m.$	$P6/mmm\ a$	P
1	*b*			$00\frac{1}{2}\ P$
2	*c*	$3m.$	$P6/mmm\ e$	$P2z$
2	*d*	$3m.$	$^*\ P\bar{3}m1\ d$	$.2.\ GE1z$
3	*e*	$.2/m.$	$P6/mmm\ f$	N
3	*f*			$00\frac{1}{2}\ N$
6	*g*	$.2.$	$P6/mmm\ j$	$P6x$
6	*h*			$00\frac{1}{2}\ P6x$
6	*i*	$.m.$	$^*\ P\bar{3}m1\ i$	$P6x\bar{x}z$
12	*j*	1	$^*\ P\bar{3}m1\ j$	$P6x\bar{x}z2y$
165	**$P\bar{3}c1$**			
2	*a*	$32.$	$P6/mmm\ a$	$00\frac{1}{4}\ P_c$
2	*b*	$\bar{3}..$	$P6/mmm\ a$	P_c
4	*c*	$3..$	$P6/mmm\ e$	P_c2z
4	*d*	$3..$	$P\bar{3}m1\ d$	$(.2.\ GE1z)_c$
6	*e*	$\bar{1}$	$P6/mmm\ f$	N_c
6	*f*	$.2.$	$P6_3/mcm\ g$	$00\frac{1}{4}\ ..2\ P_c3x$
12	*g*	1	$^*\ P\bar{3}c1\ g$	$.c.\ P_c6xyz$
166	**$R\bar{3}m$**	(Hexagonal axes)		
3	*a*	$\bar{3}m$	$^*\ R\bar{3}m\ a$	R
3	*b*			$00\frac{1}{2}\ R$
6	*c*	$3m$	$^*\ R\bar{3}m\ c$	$R2z$
9	*e*	$.2/m$	$^*\ R\bar{3}m\ e$	M
9	*d*			$00\frac{1}{2}\ M$
18	*f*	$.2$	$^*\ R\bar{3}m\ f$	$R6x$
18	*g*			$00\frac{1}{2}\ R6x$
18	*h*	$.m$	$^*\ R\bar{3}m\ h$	$R6x\bar{x}z$
36	*i*	1	$^*\ R\bar{3}m\ i$	$R6x\bar{x}z2y$
166	**$R\bar{3}m$**	(Rhombohedral axes)		
1	*a*	$\bar{3}m$	$^*\ R\bar{3}m\ a$	P
1	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P$
2	*c*	$3m$	$^*\ R\bar{3}m\ c$	$P2xxx$
3	*e*	$.2/m$	$^*\ R\bar{3}m\ e$	J
3	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ J$
6	*f*	$.2$	$^*\ R\bar{3}m\ f$	$P6x\bar{x}$
6	*g*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P6x\bar{x}$
6	*h*	$.m$	$^*\ R\bar{3}m\ h$	$P6xxz$
12	*i*	1	$^*\ R\bar{3}m\ i$	$P6xxz2y$
167	**$R\bar{3}c$**	(Hexagonal axes)		
6	*a*	32	$R\bar{3}m\ a$	$00\frac{1}{4}\ {}'R_c$
6	*b*	$\bar{3}.$	$R\bar{3}m\ a$	${}'R_c$
12	*c*	$3.$	$R\bar{3}m\ c$	${}'R_c2z$
18	*d*	$\bar{1}$	$R\bar{3}m\ e$	${}'M_c$
18	*e*	$.2$	$^*\ R\bar{3}c\ e$	$00\frac{1}{4}\ .c\ {}'R_c3x$
36	*f*	1	$^*\ R\bar{3}c\ f$	$.c\ {}'R_c6xyz$
167	**$R\bar{3}c$**	(Rhombohedral axes)		
2	*a*	32	$R\bar{3}m\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ I$
2	*b*	$\bar{3}.$	$R\bar{3}m\ a$	I
4	*c*	$3.$	$R\bar{3}m\ c$	$I2xxx$
6	*d*	$\bar{1}$	$R\bar{3}m\ e$	J^*
6	*e*	$.2$	$^*\ R\bar{3}c\ e$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ .n\ I3x\bar{x}$
12	*f*	1	$^*\ R\bar{3}c\ f$	$.n\ I6xyz$
168	**$P6$**			
1	*a*	$6..$	$P6/mmm\ a$	$P[z]$
2	*b*	$3..$	$P6/mmm\ c$	$G[z]$
3	*c*	$2..$	$P6/mmm\ f$	$N[z]$
6	*d*	1	$P6/m\ j$	$P6xy[z]$
169	**$P6_1$**			
6	*a*	1	$^*\ P6_1\ a$	$3_12_1..\ P_{Cc}E_C{}^+Q_c1xy[z]$
170	**$P6_5$**			
6	*a*	1	$^*\ P6_1a$	$3_22_1..\ P_{Cc}E_C{}^-Q_c1xy[z]$
171	**$P6_2$**			
3	*a*	$2..$	$P6/mmm\ a$	$P_C[z]$
3	*b*	$2..$	$P6_222\ c$	${}^+Q[z]$
6	*c*	1	$^*\ P6_2\ c$	$3_2..\ P_C2xy[z]$
172	**$P6_4$**			
3	*a*	$2..$	$P6/mmm\ a$	$P_C[z]$
3	*b*	$2..$	$P6_222\ c$	${}^-Q[z]$
6	*c*	1	$^*\ P6_2\ c$	$3_1..\ P_C2xy[z]$
173	**$P6_3$**			
2	*a*	$3..$	$P6/mmm\ a$	$P_c[z]$
2	*b*	$3..$	$P6_3/mmc\ c$	$E[z]$
6	*c*	1	$P6_3/m\ h$	$2_1..\ P_c3xy[z]$
174	**$P\bar{6}$**			
1	*a*	$\bar{6}..$	$P6/mmm\ a$	P
1	*b*			$00\frac{1}{2}\ P$
1	*c*			$\frac{1}{3}\frac{2}{3}0\ P$
1	*d*			$\frac{1}{3}\frac{2}{3}\frac{1}{2}\ P$
1	*e*			$\frac{2}{3}\frac{1}{3}0\ P$
1	*f*			$\frac{2}{3}\frac{1}{3}\frac{1}{2}\ P$
2	*g*	$3..$	$P6/mmm\ e$	$P2z$
2	*h*			$\frac{1}{3}\frac{2}{3}0\ P2z$

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

2	*i*			$\frac{2}{3}\frac{1}{3}0\ P2z$
3	*j*	*m..*	$^*\ P\bar{6}\ j$	$P3xy$
3	*k*			$00\frac{1}{2}\ P3xy$
6	*l*	1	$^*\ P\bar{6}\ l$	$P3xy2z$
175	***P6/m***			
1	*a*	$6/m..$	$P6/mmm\ a$	P
1	*b*			$00\frac{1}{2}\ P$
2	*c*	$\bar{6}..$	$P6/mmm\ c$	G
2	*d*			$00\frac{1}{2}\ G$
2	*e*	$6..$	$P6/mmm\ e$	$P2z$
3	*f*	$2/m..$	$P6/mmm\ f$	N
3	*g*			$00\frac{1}{2}\ N$
4	*h*	$3..$	$P6/mmm\ h$	$G2z$
6	*i*	$2..$	$P6/mmm\ i$	$N2z$
6	*j*	$m..$	$^*\ P6/m\ j$	$P6xy$
6	*k*			$00\frac{1}{2}\ P6xy$
12	*l*	1	$^*\ P6/m\ l$	$P6xy2z$
176	***P6₃/m***			
2	*a*	$\bar{6}..$	$P6/mmm\ a$	$00\frac{1}{4}\ P_c$
2	*b*	$\bar{3}..$	$P6/mmm\ a$	P_c
2	*c*	$\bar{6}..$	$P6_3/mmc\ c$	E
2	*d*			$00\frac{1}{2}\ E$
4	*e*	$3..$	$P6/mmm\ e$	P_c2z
4	*f*	$3..$	$P6_3/mmc\ f$	$E2z$
6	*g*	$\bar{1}$	$P6/mmm\ f$	N_c
6	*h*	$m..$	$^*\ P6_3/m\ h$	$00\frac{1}{4}\ 2_1..\ P_c3xy$
12	*i*	1	$^*\ P6_3/m\ i$	$m..\ P_c6xyz$
177	***P622***			
1	*a*	622	$P6/mmm\ a$	P
1	*b*			$00\frac{1}{2}\ P$
2	*c*	3.2	$P6/mmm\ c$	G
2	*d*			$00\frac{1}{2}\ G$
2	*e*	$6..$	$P6/mmm\ e$	$P2z$
3	*f*	222	$P6/mmm\ f$	N
3	*g*			$00\frac{1}{2}\ N$
4	*h*	$3..$	$P6/mmm\ h$	$G2z$
6	*i*	$2..$	$P6/mmm\ i$	$N2z$
6	*j*	$.2.$	$P6/mmm\ j$	$P6x$
6	*k*			$00\frac{1}{2}\ P6x$
6	*l*	$..2$	$P6/mmm\ l$	$P6x\bar{x}$
6	*m*			$00\frac{1}{2}\ P6x\bar{x}$
12	*n*	1	$^*\ P622\ n$	$P6x2yz$
178	***P6₁22***			
6	*a*	$.2.$	$^*\ P6_122\ a$	$3_1.2\ P_{Cc}{}^+Q_c1x$
6	*b*	$..2$	$^*\ P6_122\ b$	$00\frac{11}{12}\ 3_12.\ P_{Cc}E_C{}^+Q_c1x\bar{x}$
12	*c*	1	$^*\ P6_122\ c$	$3_1.2\ P_{Cc}{}^+Q_c1x2yz$
179	***P6₅22***			
6	*a*	$.2.$	$^*\ P6_122\ a$	$3_2.2\ P_{Cc}{}^-Q_c1x$
6	*b*	$..2$	$^*\ P6_122\ b$	$00\frac{1}{12}\ 3_22.\ P_{Cc}E_C{}^-Q_c1x\bar{x}$
12	*c*	1	$^*\ P6_122\ c$	$3_2.2\ P_{Cc}{}^-Q_c1x2yz$
180	***P6₂22***			
3	*a*	222	$P6/mmm\ a$	P_C
3	*b*			$00\frac{1}{2}\ P_C$
3	*c*	222	$^*\ P6_222\ c$	${}^+Q$
3	*d*			$00\frac{1}{2}\ {}^+Q$
6	*e*	$2..$	$P6/mmm\ e$	P_C2z
6	*f*	$2..$	$^*\ P6_222\ f$	${}^+Q2z$
6	*g*	$.2.$	$^*\ P6_222\ g$	$3_2..\ P_C2x$
6	*h*			$00\frac{1}{2}\ 3_2..\ P_C2x$
6	*i*	$..2$	$^*\ P6_222\ i$	$00\frac{1}{3}\ 3_2..\ P_C2x\bar{x}$
6	*j*			$00\frac{5}{6}\ 3_2..\ P_C2x\bar{x}$
12	*k*	1	$^*\ P6_222\ k$	$3_2..\ P_C2x2yz$
181	***P6₄22***			
3	*a*	222	$P6/mmm\ a$	P_C
3	*b*			$00\frac{1}{2}\ P_C$
3	*c*	222	$^*\ P6_222\ c$	${}^-Q$
3	*d*			$00\frac{1}{2}\ {}^-Q$
6	*e*	$2..$	$P6/mmm\ e$	P_C2z
6	*f*	$2..$	$^*\ P6_222\ f$	${}^-Q2z$
6	*g*	$.2.$	$^*\ P6_222\ g$	$3_1..\ P_C2x$
6	*h*			$00\frac{1}{2}\ 3_1..\ P_C2x$
6	*i*	$..2$	$^*\ P6_222\ i$	$00\frac{2}{3}\ 3_1..\ P_C2x\bar{x}$
6	*j*			$00\frac{1}{6}\ 3_1..\ P_C2x\bar{x}$
12	*k*	1	$^*\ P6_222\ k$	$3_1..\ P_C2x2yz$
182	***P6₃22***			
2	*a*	$32.$	$P6/mmm\ a$	P_c
2	*b*	3.2	$P6/mmm\ a$	$00\frac{1}{4}\ P_c$
2	*c*	3.2	$P6_3/mmc\ c$	E
2	*d*			$00\frac{1}{2}\ E$
4	*e*	$3..$	$P6/mmm\ e$	P_c2z
4	*f*	$3..$	$P6_3/mmc\ f$	$E2z$
6	*g*	$.2.$	$P6_3/mcm\ g$	$..2\ P_c3x$
6	*h*	$..2$	$P6_3/mmc\ h$	$00\frac{1}{4}\ .2.\ P_c3x\bar{x}$
12	*i*	1	$^*\ P6_322\ i$	$..2\ P_c3x2yz$
183	***P6mm***			
1	*a*	$6mm$	$P6/mmm\ a$	$P[z]$
2	*b*	$3m.$	$P6/mmm\ c$	$G[z]$
3	*c*	$2mm$	$P6/mmm\ f$	$N[z]$
6	*d*	$..m$	$P6/mmm\ j$	$P6x[z]$
6	*e*	$.m.$	$P6/mmm\ l$	$P6x\bar{x}[z]$
12	*f*	1	$P6/mmm\ p$	$P6x2y[z]$
184	***P6cc***			
2	*a*	$6..$	$P6/mmm\ a$	$P_c[z]$
4	*b*	$3..$	$P6/mmm\ c$	$G_c[z]$
6	*c*	$2..$	$P6/mmm\ f$	$N_c[z]$
12	*d*	1	$P6/mcc\ l$	$.c.\ P_c6xy[z]$
185	***P6₃cm***			
2	*a*	$3.m$	$P6/mmm\ a$	$P_c[z]$
4	*b*	$3..$	$P6/mmm\ c$	$G_c[z]$
6	*c*	$..m$	$P6_3/mcm\ g$	$..2\ P_c3x[z]$
12	*d*	1	$P6_3/mcm\ j$	$..2\ P_c3x2y[z]$
186	***P6₃mc***			
2	*a*	$3m.$	$P6/mmm\ a$	$P_c[z]$
2	*b*	$3m.$	$P6_3/mmc\ c$	$E[z]$

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

6	*c*	.*m*.		$P6_3/mmc$ *h*	$.2.\ P_c3x\bar{x}[z]$
12	*d*	1		$P6_3/mmc$ *j*	$.2.\ P_c3x\bar{x}2y[z]$

187 $P\bar{6}m2$

1	*a*	$\bar{6}m2$		$P6/mmm$ *a*	P
1	*b*				$00\frac{1}{2}\ P$
1	*c*				$\frac{1}{3}\frac{2}{3}0\ P$
1	*d*				$\frac{1}{3}\frac{2}{3}\frac{1}{2}\ P$
1	*e*				$\frac{2}{3}\frac{1}{3}0\ P$
1	*f*				$\frac{2}{3}\frac{1}{3}\frac{1}{2}\ P$
2	*g*	$3m.$		$P6/mmm$ *e*	$P2z$
2	*h*				$\frac{1}{3}\frac{2}{3}0\ P2z$
2	*i*				$\frac{2}{3}\frac{1}{3}0\ P2z$
3	*j*	$mm2$	*	$P\bar{6}m2$ *j*	$P3x\bar{x}$
3	*k*				$00\frac{1}{2}\ P3x\bar{x}$
6	*l*	$m..$	*	$P\bar{6}m2$ *l*	$P3x\bar{x}2y$
6	*m*				$00\frac{1}{2}\ P3x\bar{x}2y$
6	*n*	$.m.$	*	$P\bar{6}m2$ *n*	$P3x\bar{x}2z$
12	*o*	1	*	$P\bar{6}m2$ *o*	$P3x\bar{x}2y2z$

188 $P\bar{6}c2$

2	*a*	3.2		$P6/mmm$ *a*	P_c
2	*c*				$\frac{1}{3}\frac{2}{3}0\ P_c$
2	*e*				$\frac{2}{3}\frac{1}{3}0\ P_c$
2	*b*	$\bar{6}..$		$P6/mmm$ *a*	$00\frac{1}{4}\ P_c$
2	*d*				$\frac{1}{3}\frac{2}{3}\frac{1}{4}\ P_c$
2	*f*				$\frac{2}{3}\frac{1}{3}\frac{1}{4}\ P_c$
4	*g*	$3..$		$P6/mmm$ *e*	P_c2z
4	*h*				$\frac{1}{3}\frac{2}{3}0\ P_c2z$
4	*i*				$\frac{2}{3}\frac{1}{3}0\ P_c2z$
6	*j*	$..2$		$P\bar{6}m2$ *j*	$P_c3x\bar{x}$
6	*k*	$m..$	*	$P\bar{6}c2$ *k*	$00\frac{1}{4}\ ..2\ P_c3xy$
12	*l*	1	*	$P\bar{6}c2$ *l*	$m..\ P_c3x\bar{x}2yz$

189 $P\bar{6}2m$

1	*a*	$\bar{6}2m$		$P6/mmm$ *a*	P
1	*b*				$00\frac{1}{2}\ P$
2	*c*	$\bar{6}..$		$P6/mmm$ *c*	G
2	*d*				$00\frac{1}{2}\ G$
2	*e*	$3.m$		$P6/mmm$ *e*	$P2z$
3	*f*	$m2m$	*	$P\bar{6}2m$ *f*	$P3x$
3	*g*				$00\frac{1}{2}\ P3x$
4	*h*	$3..$		$P6/mmm$ *h*	$G2z$
6	*i*	$..m$	*	$P\bar{6}2m$ *i*	$P3x2z$
6	*j*	$m..$	*	$P\bar{6}2m$ *j*	$P3x2y$
6	*k*				$00\frac{1}{2}\ P3x2y$
12	*l*	1	*	$P\bar{6}2m$ *l*	$P3x2y2z$

190 $P\bar{6}2c$

2	*a*	$32.$		$P6/mmm$ *a*	P_c
2	*b*	$\bar{6}..$		$P6/mmm$ *a*	$00\frac{1}{4}\ P_c$
2	*c*	$\bar{6}..$		$P6_3/mmc$ *c*	E
2	*d*				$00\frac{1}{2}\ E$
4	*e*	$3..$		$P6/mmm$ *e*	P_c2z
4	*f*	$3..$		$P6_3/mmc$ *f*	$E2z$
6	*g*	$.2.$		$P\bar{6}2m$ *f*	P_c3x
6	*h*	$m..$	*	$P\bar{6}2c$ *h*	$00\frac{1}{4}\ .2.\ P_c3xy$
12	*i*	1	*	$P\bar{6}2c$ *i*	$m..\ P_c3x2yz$

191 $P6/mmm$

1	*a*	$6/mmm$	*	$P6/mmm$ *a*	P
1	*b*				$00\frac{1}{2}\ P$
2	*c*	$\bar{6}m2$	*	$P6/mmm$ *c*	G
2	*d*				$00\frac{1}{2}\ G$
2	*e*	$6mm$	*	$P6/mmm$ *e*	$P2z$
3	*f*	mmm	*	$P6/mmm$ *f*	N
3	*g*				$00\frac{1}{2}\ N$
4	*h*	$3m.$	*	$P6/mmm$ *h*	$G2z$
6	*i*	$2mm$	*	$P6/mmm$ *i*	$N2z$
6	*j*	$m2m$	*	$P6/mmm$ *j*	$P6x$
6	*k*				$00\frac{1}{2}\ P6x$
6	*l*	$mm2$	*	$P6/mmm$ *l*	$P6x\bar{x}$
6	*m*				$00\frac{1}{2}\ P6x\bar{x}$
12	*n*	$..m$	*	$P6/mmm$ *n*	$P6x2z$
12	*o*	$.m.$	*	$P6/mmm$ *o*	$P6x\bar{x}2z$
12	*p*	$m..$	*	$P6/mmm$ *p*	$P6x2y$
12	*q*				$00\frac{1}{2}\ P6x2y$
24	*r*	1	*	$P6/mmm$ *r*	$P6x2y2z$

192 $P6/mcc$

2	*a*	622		$P6/mmm$ *a*	$00\frac{1}{4}\ P_c$
2	*b*	$6/m..$		$P6/mmm$ *a*	P_c
4	*c*	3.2		$P6/mmm$ *c*	$00\frac{1}{4}\ G_c$
4	*d*	$\bar{6}..$		$P6/mmm$ *c*	G_c
4	*e*	$6..$		$P6/mmm$ *e*	P_c2z
6	*f*	222		$P6/mmm$ *f*	$00\frac{1}{4}\ N_c$
6	*g*	$2/m..$		$P6/mmm$ *f*	N_c
8	*h*	$3..$		$P6/mmm$ *h*	G_c2z
12	*i*	$2..$		$P6/mmm$ *i*	N_c2z
12	*j*	$.2.$		$P6/mmm$ *j*	$00\frac{1}{4}\ P_c6x$
12	*k*	$..2$		$P6/mmm$ *l*	$00\frac{1}{4}\ P_c6x\bar{x}$
12	*l*	$m..$	*	$P6/mcc$ *l*	$.c.\ P_c6xy$
24	*m*	1	*	$P6/mcc$ *m*	$.c.\ P_c6xy2z$

193 $P6_3/mcm$

2	*a*	$\bar{6}2m$		$P6/mmm$ *a*	$00\frac{1}{4}\ P_c$
2	*b*	$\bar{3}.m$		$P6/mmm$ *a*	P_c
4	*c*	$\bar{6}..$		$P6/mmm$ *c*	$00\frac{1}{4}\ G_c$
4	*d*	3.2		$P6/mmm$ *c*	G_c
4	*e*	$3.m$		$P6/mmm$ *e*	P_c2z
6	*f*	$..2/m$		$P6/mmm$ *f*	N_c
6	*g*	$m2m$	*	$P6_3/mcm$ *g*	$00\frac{1}{4}\ ..2\ P_c3x$
8	*h*	$3..$		$P6/mmm$ *h*	G_c2z
12	*i*	$..2$		$P6/mmm$ *l*	$P_c6x\bar{x}$
12	*j*	$m..$	*	$P6_3/mcm$ *j*	$00\frac{1}{4}\ ..2\ P_c3x2y$
12	*k*	$..m$	*	$P6_3/mcm$ *k*	$m..\ P_c6xz$
24	*l*	1	*	$P6_3/mcm$ *l*	$m..\ P_c6xz2y$

194 $P6_3/mmc$

2	*a*	$\bar{3}m.$		$P6/mmm$ *a*	P_c
2	*b*	$\bar{6}m2$		$P6/mmm$ *a*	$00\frac{1}{4}\ P_c$
2	*c*	$\bar{6}m2$	*	$P6_3/mmc$ *c*	E
2	*d*				$00\frac{1}{2}\ E$
4	*e*	$3m.$		$P6/mmm$ *e*	P_c2z
4	*f*	$3m.$	*	$P6_3/mmc$ *f*	$E2z$
6	*g*	$.2/m.$		$P6/mmm$ *f*	N_c
6	*h*	$mm2$	*	$P6_3/mmc$ *h*	$00\frac{1}{4}\ .2.\ P_c3x\bar{x}$

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

12	*i*	.2.		$P6/mmm$ *j*	P_c6x
12	*j*	*m*..	*	$P6_3/mmc$ *j*	$00\frac{1}{4}$ .2. $P_c3x\bar{x}2y$
12	*k*	.*m*.	*	$P6_3/mmc$ *k*	*m*.. $P_c6x\bar{x}z$
24	*l*	1	*	$P6_3/mmc$ *l*	*m*.. $P_c6x\bar{x}z2y$

195 *P*23

1	*a*	23.		$Pm\bar{3}m$ *a*	*P*
1	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
3	*c*	222..		$Pm\bar{3}m$ *c*	*J*
3	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *J*
4	*e*	.3.		$P\bar{4}3m$ *e*	*P*4*xxx*
6	*f*	2..		$Pm\bar{3}m$ *e*	*P*6*z*
6	*i*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*6*z*
6	*g*	2..		$Pm\bar{3}$ *f*	.3. *J*2*x*
6	*h*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .3. *J*2*x*
12	*j*	1	*	*P*23 *j*	*P*6*z*2*xy*

196 *F*23

4	*a*	23.		$Fm\bar{3}m$ *a*	*F*
4	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F*
4	*c*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*d*				$\frac{3}{4}\frac{3}{4}\frac{3}{4}$ *F*
16	*e*	.3.		$F\bar{4}3m$ *e*	*F*4*xxx*
24	*f*	2..		$Fm\bar{3}m$ *e*	*F*6*z*
24	*g*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*6*z*
48	*h*	1	*	*F*23 *h*	*F*6*z*2*xy*

197 *I*23

2	*a*	23.		$Im\bar{3}m$ *a*	*I*
6	*b*	222..		$Im\bar{3}m$ *b*	J^*
8	*c*	.3.		$I\bar{4}3m$ *c*	*I*4*xxx*
12	*d*	2..		$Im\bar{3}m$ *e*	*I*6*z*
12	*e*	2..		$Im\bar{3}$ *e*	.3. J^*2x
24	*f*	1	*	*I*23 *f*	*I*6*z*2*xy*

198 $P2_13$

4	*a*	.3.	*	$P2_13$ *a*	2_12_1.. *FY*1*xxx*
12	*b*	1	*	$P2_13$ *b*	2_12_1.. *FY*1*xxx*3*yz*

199 $I2_13$

8	*a*	.3.	*	$I2_13$ *a*	2_12_1.. P_2Y^*1xxx
12	*b*	2..	*	$I2_13$ *b*	2_13. *SV*1*z*
24	*c*	1	*	$I2_13$ *c*	2_12_1.. $P_2Y^*1xxx3yz$

200 $Pm\bar{3}$

1	*a*	$m\bar{3}$.		$Pm\bar{3}m$ *a*	*P*
1	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
3	*c*	*mmm*..		$Pm\bar{3}m$ *c*	*J*
3	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *J*
6	*e*	*mm*2..		$Pm\bar{3}m$ *e*	*P*6*z*
6	*h*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*6*z*
6	*f*	*mm*2..	*	$Pm\bar{3}$ *f*	.3. *J*2*x*
6	*g*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .3. *J*2*x*
8	*i*	.3.		$Pm\bar{3}m$ *g*	*P*8*xxx*
12	*j*	*m*..	*	$Pm\bar{3}$ *j*	*P*6*z*2*x*
12	*k*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*6*z*2*x*
24	*l*	1	*	$Pm\bar{3}$ *l*	*P*6*z*2*x*2*y*

201 $Pn\bar{3}$

2	*a*	23.		$Im\bar{3}m$ *a*	*I*
4	*b*	.$\bar{3}$.		$Fm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*c*				$\frac{3}{4}\frac{3}{4}\frac{3}{4}$ *F*
6	*d*	222..		$Im\bar{3}m$ *b*	J^*
8	*e*	.3.		$Pn\bar{3}m$ *e*	..2 *I*4*xxx*
12	*f*	2..		$Im\bar{3}m$ *e*	*I*6*z*
12	*g*	2..		$Im\bar{3}$ *e*	.3. J^*2x
24	*h*	1	*	$Pn\bar{3}$ *h*	*n*.. *I*6*z*2*xy*

202 $Fm\bar{3}$

4	*a*	$m\bar{3}$.		$Fm\bar{3}m$ *a*	*F*
4	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F*
8	*c*	23.		$Pm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
24	*d*	2/*m*..		$Pm\bar{3}m$ *c*	J_2
24	*e*	*mm*2..		$Fm\bar{3}m$ *e*	*F*6*z*
32	*f*	.3.		$Fm\bar{3}m$ *f*	*F*8*xxx*
48	*g*	2..		$Pm\bar{3}m$ *e*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_26z
48	*h*	*m*..	*	$Fm\bar{3}$ *h*	*F*6*z*2*x*
96	*i*	1	*	$Fm\bar{3}$ *i*	*F*6*z*2*x*2*y*

203 $Fd\bar{3}$

8	*a*	23.		$Fd\bar{3}m$ *a*	*D*
8	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *D*
16	*c*	.$\bar{3}$.		$Fd\bar{3}m$ *c*	*T*
16	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *T*
32	*e*	.3.		$Fd\bar{3}m$ *e*	..2 *D*4*xxx*
48	*f*	2..		$Fd\bar{3}m$ *f*	*D*6*z*
96	*g*	1	*	$Fd\bar{3}$ *g*	*d*.. *D*6*z*2*xy*

204 $Im\bar{3}$

2	*a*	$m\bar{3}$.		$Im\bar{3}m$ *a*	*I*
6	*b*	*mmm*..		$Im\bar{3}m$ *b*	J^*
8	*c*	.$\bar{3}$.		$Pm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
12	*d*	*mm*2..		$Im\bar{3}m$ *e*	*I*6*z*
12	*e*	*mm*2..	*	$Im\bar{3}$ *e*	.3. J^*2x
16	*f*	.3.		$Im\bar{3}m$ *f*	*I*8*xxx*
24	*g*	*m*..	*	$Im\bar{3}$ *g*	*I*6*z*2*x*
48	*h*	1	*	$Im\bar{3}$ *h*	*I*6*z*2*x*2*y*

205 $Pa\bar{3}$

4	*a*	.$\bar{3}$.		$Fm\bar{3}m$ *a*	*F*
4	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F*
8	*c*	.3.	*	$Pa\bar{3}$ *c*	*bc*.. *F*2*xxx*
24	*d*	1	*	$Pa\bar{3}$ *d*	*bc*.. *F*6*xyz*

206 $Ia\bar{3}$

8	*a*	.$\bar{3}$.		$Pm\bar{3}m$ *a*	P_2
8	*b*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
16	*c*	.3.	*	$Ia\bar{3}$ *c*	22.. P_22xxx
24	*d*	2..	*	$Ia\bar{3}$ *d*	.$\bar{3}$. $J_2S^*V^*1x$
48	*e*	1	*	$Ia\bar{3}$ *e*	22.. P_26xyz

207 *P*432

1	*a*	432		$Pm\bar{3}m$ *a*	*P*
1	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
3	*c*	42.2		$Pm\bar{3}m$ *c*	*J*
3	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *J*

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

6	*e*	4..	$Pm\bar{3}m\ e$	$P6z$
6	*f*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P6z$
8	*g*	.3.	$Pm\bar{3}m\ g$	$P8xxx$
12	*h*	2..	$Pm\bar{3}m\ h$	$.3.\ J4x$
12	*i*	..2	$Pm\bar{3}m\ i$	$P12xx$
12	*j*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P12xx$
24	*k*	1	$^{*}\ P432\ k$	$P6z4xy$

208 $P4_232$

2	*a*	23.	$Im\bar{3}m\ a$	I
4	*b*	.32	$Fm\bar{3}m\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F$
4	*c*			$\frac{3}{4}\frac{3}{4}\frac{3}{4}\ F$
6	*d*	222..	$Im\bar{3}m\ b$	J^{*}
6	*e*	2.22	$Pm\bar{3}n\ c$	W
6	*f*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ W$
8	*g*	.3.	$Pn\bar{3}m\ e$	$..2\ I4xxx$
12	*h*	2..	$Im\bar{3}m\ e$	$I6z$
12	*i*	2..	$Pm\bar{3}n\ g$	$.3.\ W2z$
12	*j*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ .3.\ W2z$
12	*k*	..2	$^{*}\ P4_232\ k$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ 4_2..\ F3x\bar{x}$
12	*l*			$\frac{3}{4}\frac{3}{4}\frac{3}{4}\ 4_2..\ F3x\bar{x}$
24	*m*	1	$^{*}\ P4_232\ m$	$..2\ I6z2xy$

209 $F432$

4	*a*	432	$Fm\bar{3}m\ a$	F
4	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ F$
8	*c*	23.	$Pm\bar{3}m\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
24	*d*	2.22	$Pm\bar{3}m\ c$	J_2
24	*e*	4..	$Fm\bar{3}m\ e$	$F6z$
32	*f*	.3.	$Fm\bar{3}m\ f$	$F8xxx$
48	*g*	..2	$Fm\bar{3}m\ h$	$F12xx$
48	*h*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ F12xx$
48	*i*	2..	$Pm\bar{3}m\ e$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_26z$
96	*j*	1	$^{*}\ F432\ j$	$F6z4xy$

210 $F4_132$

8	*a*	23.	$Fd\bar{3}m\ a$	D
8	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ D$
16	*c*	.32	$Fd\bar{3}m\ c$	T
16	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ T$
32	*e*	.3.	$Fd\bar{3}m\ e$	$..2\ D4xxx$
48	*f*	2..	$Fd\bar{3}m\ f$	$D6z$
48	*g*	..2	$^{*}\ F4_132\ g$	$22..\ T3x\bar{x}$
96	*h*	1	$^{*}\ F4_132\ h$	$..2\ D6z2xy$

211 $I432$

2	*a*	432	$Im\bar{3}m\ a$	I
6	*b*	42.2	$Im\bar{3}m\ b$	J^{*}
8	*c*	.32	$Pm\bar{3}m\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
12	*d*	2.22	$Im\bar{3}m\ d$	W^{*}
12	*e*	4..	$Im\bar{3}m\ e$	$I6z$
16	*f*	.3.	$Im\bar{3}m\ f$	$I8xxx$
24	*g*	2..	$Im\bar{3}m\ g$	$.3.\ J^{*}4x$
24	*h*	..2	$Im\bar{3}m\ h$	$I12xx$
24	*i*	..2	$^{*}\ I432\ i$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ 4..\ P_23x\bar{x}$
48	*j*	1	$^{*}\ I432\ j$	$I6z4xy$

212 $P4_332$

4	*a*	.32	$^{*}\ P4_332\ a$	^{+}Y
4	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ {}^{+}Y$
8	*c*	.3.	$^{*}\ P4_332\ c$	$4_3..\ {}^{+}Y2xxx$
12	*d*	..2	$^{*}\ P4_332\ d$	$4_3..\ {}^{+}Y3x\bar{x}$
24	*e*	1	$^{*}\ P4_332\ e$	$4_3..\ {}^{+}Y3x\bar{x}2yz$

213 $P4_132$

4	*a*	.32	$^{*}\ P4_332\ a$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ {}^{-}Y$
4	*b*			^{-}Y
8	*c*	.3.	$^{*}\ P4_332\ c$	$4_1..\ {}^{-}Y2xxx$
12	*d*	..2	$^{*}\ P4_332\ d$	$4_1..\ {}^{-}Y3x\bar{x}$
24	*e*	1	$^{*}\ P4_332\ e$	$4_1..\ {}^{-}Y3x\bar{x}2yz$

214 $I4_132$

8	*a*	.32	$^{*}\ I4_132\ a$	$^{+}Y^{*}$
8	*b*			$^{-}Y^{*}$
12	*c*	2.22	$^{*}\ I4_132\ c$	^{+}V
12	*d*			^{-}V
16	*e*	.3.	$^{*}\ I4_132\ e$	$22..\ Y^{*}2xxx$
24	*f*	2..	$^{*}\ I4_132\ f$	$.3.\ V2z$
24	*h*	..2	$^{*}\ I4_132\ h$	$4_3..\ {}^{+}Y^{*}3x\bar{x}$
24	*g*			$4_1..\ {}^{-}Y^{*}3x\bar{x}$
48	*i*	1	$^{*}\ I4_132\ i$	$22..\ Y^{*}3x\bar{x}2yz$

215 $P\bar{4}3m$

1	*a*	$\bar{4}3m$	$Pm\bar{3}m\ a$	P
1	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P$
3	*c*	$\bar{4}2.m$	$Pm\bar{3}m\ c$	J
3	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ J$
4	*e*	.3*m*	$^{*}\ P\bar{4}3m\ e$	$P4xxx$
6	*f*	2.*mm*	$Pm\bar{3}m\ e$	$P6z$
6	*g*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P6z$
12	*h*	2..	$Pm\bar{3}m\ h$	$.3.\ J4x$
12	*i*	..*m*	$^{*}\ P\bar{4}3m\ i$	$P6z2xx$
24	*j*	1	$^{*}\ P\bar{4}3m\ j$	$P6z2xx2y$

216 $F\bar{4}3m$

4	*a*	$\bar{4}3m$	$Fm\bar{3}m\ a$	F
4	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ F$
4	*c*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F$
4	*d*			$\frac{3}{4}\frac{3}{4}\frac{3}{4}\ F$
16	*e*	.3*m*	$^{*}\ F\bar{4}3m\ e$	$F4xxx$
24	*f*	2.*mm*	$Fm\bar{3}m\ e$	$F6z$
24	*g*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F6z$
48	*h*	..*m*	$^{*}\ F\bar{4}3m\ h$	$F6z2xx$
96	*i*	1	$^{*}\ F\bar{4}3m\ i$	$F6z2xx2y$

217 $I\bar{4}3m$

2	*a*	$\bar{4}3m$	$Im\bar{3}m\ a$	I
6	*b*	$\bar{4}2.m$	$Im\bar{3}m\ b$	J^{*}
8	*c*	.3*m*	$^{*}\ I\bar{4}3m\ c$	$I4xxx$
12	*d*	$\bar{4}..$	$Im\bar{3}m\ d$	W^{*}
12	*e*	2.*mm*	$Im\bar{3}m\ e$	$I6z$
24	*f*	2..	$Im\bar{3}m\ g$	$.3.\ J^{*}4x$
24	*g*	..*m*	$^{*}\ I\bar{4}3m\ g$	$I6z2xx$
48	*h*	1	$^{*}\ I\bar{4}3m\ h$	$I6z2xx2y$

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

218 $P\bar{4}3n$

2	*a*	23.	$Im\bar{3}m\ a$	I
6	*b*	222..	$Im\bar{3}m\ b$	J^*
6	*c*	$\bar{4}$..	$Pm\bar{3}n\ c$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ W$
6	*d*			W
8	*e*	.3.	$I\bar{4}3m\ c$	$I4xxx$
12	*f*	2..	$Im\bar{3}m\ e$	$I6z$
12	*g*	2..	$Pm\bar{3}n\ g$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .3. $W2z$
12	*h*			.3. $W2z$
24	*i*	1	* $P\bar{4}3n\ i$	..c $I6z2xy$

219 $F\bar{4}3c$

8	*a*	23.	$Pm\bar{3}m\ a$	P_2
8	*b*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
24	*c*	$\bar{4}$..	$Pm\bar{3}m\ c$	J_2
24	*d*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ J_2$
32	*e*	.3.	$P\bar{4}3m\ e$	P_24xxx
48	*f*	2..	$Pm\bar{3}m\ e$	P_26z
48	*g*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_26z$
96	*h*	1	* $F\bar{4}3c\ h$	..n P_26z2xy

220 $I\bar{4}3d$

12	*a*	$\bar{4}$..	* $I\bar{4}3d\ a$	S
12	*b*			$'S$
16	*c*	.3.	* $I\bar{4}3d\ c$	$\bar{4}$.. $I_2Y^{**}1xxx$
24	*d*	2..	* $I\bar{4}3d\ d$	.3. $S2z$
48	*e*	1	* $I\bar{4}3d\ e$	.3d $S4xyz$

221 $Pm\bar{3}m$

1	*a*	$m\bar{3}m$	* $Pm\bar{3}m\ a$	P
1	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P$
3	*c*	$4/mm.m$	* $Pm\bar{3}m\ c$	J
3	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ J$
6	*e*	$4m.m$	* $Pm\bar{3}m\ e$	$P6z$
6	*f*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P6z$
8	*g*	.3m	* $Pm\bar{3}m\ g$	$P8xxx$
12	*h*	$mm2$..	* $Pm\bar{3}m\ h$	.3. $J4x$
12	*i*	$m.m2$	* $Pm\bar{3}m\ i$	$P12xx$
12	*j*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P12xx$
24	*k*	m..	* $Pm\bar{3}m\ k$	$P6z4x$
24	*l*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P6z4x$
24	*m*	..m	* $Pm\bar{3}m\ m$	$P6z4xx$
48	*n*	1	* $Pm\bar{3}m\ n$	$P6z4x2y$

222 $Pn\bar{3}n$

2	*a*	432	$Im\bar{3}m\ a$	I
6	*b*	42.2	$Im\bar{3}m\ b$	J^*
8	*c*	.$\bar{3}$.	$Pm\bar{3}m\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
12	*d*	$\bar{4}$..	$Im\bar{3}m\ d$	W^*
12	*e*	4..	$Im\bar{3}m\ e$	$I6z$
16	*f*	.3.	$Im\bar{3}m\ f$	$I8xxx$
24	*g*	2..	$Im\bar{3}m\ g$	.3. J^*4x
24	*h*	..2	$Im\bar{3}m\ h$	$I12xx$
48	*i*	1	* $Pn\bar{3}n\ i$	n.. $I6z4xy$

223 $Pm\bar{3}n$

2	*a*	$m\bar{3}$.	$Im\bar{3}m\ a$	I
6	*b*	mmm..	$Im\bar{3}m\ b$	J^*
6	*c*	$\bar{4}m$.2	* $Pm\bar{3}n\ c$	W
6	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ W$
8	*e*	.32	$Pm\bar{3}m\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
12	*f*	$mm2$..	$Im\bar{3}m\ e$	$I6z$
12	*g*	$mm2$..	* $Pm\bar{3}n\ g$	.3. $W2z$
12	*h*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .3. $W2z$
16	*i*	.3.	$Im\bar{3}m\ f$	$I8xxx$
24	*j*	..2	* $Pm\bar{3}n\ j$	.3. $W4xx$
24	*k*	m..	* $Pm\bar{3}n\ k$	..2 $I6z2x$
48	*l*	1	* $Pm\bar{3}n\ l$	..2 $I6z2x2y$

224 $Pn\bar{3}m$

2	*a*	$\bar{4}3m$	$Im\bar{3}m\ a$	I
4	*b*	.$\bar{3}m$	$Fm\bar{3}m\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F$
4	*c*			$\frac{3}{4}\frac{3}{4}\frac{3}{4}\ F$
6	*d*	$\bar{4}2.m$	$Im\bar{3}m\ b$	J^*
8	*e*	.3m	* $Pn\bar{3}m\ e$	..2 $I4xxx$
12	*f*	2.22	$Im\bar{3}m\ d$	W^*
12	*g*	$2.mm$	$Im\bar{3}m\ e$	$I6z$
24	*h*	2..	$Im\bar{3}m\ g$	.3. J^*4x
24	*i*	..2	* $Pn\bar{3}m\ i$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $\bar{4}$.. $F6x\bar{x}$
24	*j*			$\frac{3}{4}\frac{3}{4}\frac{3}{4}$ $\bar{4}$.. $F6x\bar{x}$
24	*k*	..m	* $Pn\bar{3}m\ k$	..2 $I6z2xx$
48	*l*	1	* $Pn\bar{3}m\ l$	..2 $I6z2xx2y$

225 $Fm\bar{3}m$

4	*a*	$m\bar{3}m$	* $Fm\bar{3}m\ a$	F
4	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ F$
8	*c*	$\bar{4}3m$	$Pm\bar{3}m\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
24	*d*	$m.mm$	$Pm\bar{3}m\ c$	J_2
24	*e*	$4m.m$	* $Fm\bar{3}m\ e$	$F6z$
32	*f*	.3m	* $Fm\bar{3}m\ f$	$F8xxx$
48	*g*	$2.mm$	$Pm\bar{3}m\ e$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_26z$
48	*h*	$m.m2$	* $Fm\bar{3}m\ h$	$F12xx$
48	*i*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ F12xx$
96	*j*	m..	* $Fm\bar{3}m\ j$	$F6z4x$
96	*k*	..m	* $Fm\bar{3}m\ k$	$F6z4xx$
192	*l*	1	* $Fm\bar{3}m\ l$	$F6z4x2y$

226 $Fm\bar{3}c$

8	*a*	432	$Pm\bar{3}m\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*b*	$m\bar{3}$.	$Pm\bar{3}m\ a$	P_2
24	*c*	$\bar{4}m$.2	$Pm\bar{3}m\ c$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ J_2$
24	*d*	$4/m$..	$Pm\bar{3}m\ c$	J_2
48	*e*	$mm2$..	$Pm\bar{3}m\ e$	P_26z
48	*f*	4..	$Pm\bar{3}m\ e$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_26z$
64	*g*	.3.	$Pm\bar{3}m\ g$	P_28xxx
96	*h*	..2	$Pm\bar{3}m\ i$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_212xx$
96	*i*	m..	* $Fm\bar{3}c\ i$	..2 P_26z2x
192	*j*	1	* $Fm\bar{3}c\ j$	..2 $P_26z2x2y$

227 $Fd\bar{3}m$

8	*a*	$\bar{4}3m$	* $Fd\bar{3}m\ a$	D
8	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ D$
16	*c*	.$\bar{3}m$	* $Fd\bar{3}m\ c$	T
16	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ T$
32	*e*	.3m	* $Fd\bar{3}m\ e$	..2 $D4xxx$
48	*f*	$2.mm$	* $Fd\bar{3}m\ f$	$D6z$

Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

96	*g*	..*m*	* $Fd\bar{3}m\ g$	..2 $D6z2xx$
96	*h*	..2	* $Fd\bar{3}m\ h$	$\bar{4}$.. $T6x\bar{x}$
192	*i*	1	* $Fd\bar{3}m\ i$	..2 $D6z2xx2y$
228	**$Fd\bar{3}c$**			
16	*a*	23.	$Im\bar{3}m\ a$	I_2
32	*b*	.32	$Fm\bar{3}m\ a$	$\frac{1}{8}\frac{1}{8}\frac{1}{8}\ F_2$
32	*c*	.$\bar{3}$.	$Fm\bar{3}m\ a$	$\frac{3}{8}\frac{3}{8}\frac{3}{8}\ F_2$
48	*d*	$\bar{4}$..	$Im\bar{3}m\ b$	$J^*{}_2$
64	*e*	.3.	$Pn\bar{3}m\ e$	$(..2\ I4xxx)_2$
96	*f*	2..	$Im\bar{3}m\ e$	I_26z
96	*g*	..2	* $Fd\bar{3}c\ g$	$\frac{1}{8}\frac{1}{8}\frac{1}{8}\ \bar{4}2..\ F_23x\bar{x}$
192	*h*	1	* $Fd\bar{3}c\ h$	$d.2\ I_26z2xy$
229	**$Im\bar{3}m$**			
2	*a*	$m\bar{3}m$	* $Im\bar{3}m\ a$	I
6	*b*	$4/mm.m$	* $Im\bar{3}m\ b$	J^*
8	*c*	.$\bar{3}m$	$Pm\bar{3}m\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
12	*d*	$\bar{4}m.2$	* $Im\bar{3}m\ d$	W^*
12	*e*	$4m.m$	* $Im\bar{3}m\ e$	$I6z$
16	*f*	.3*m*	* $Im\bar{3}m\ f$	$I8xxx$
24	*g*	*mm*2..	* $Im\bar{3}m\ g$	.3. J^*4x
24	*h*	*m.m*2	* $Im\bar{3}m\ h$	$I12xx$
48	*i*	..2	* $Im\bar{3}m\ i$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ 4..\ P_26x\bar{x}$
48	*j*	*m*..	* $Im\bar{3}m\ j$	$I6z4x$
48	*k*	..*m*	* $Im\bar{3}m\ k$	$I6z4xx$
96	*l*	1	* $Im\bar{3}m\ l$	$I6z4x2y$
230	**$Ia\bar{3}d$**			
16	*a*	.$\bar{3}$.	$Im\bar{3}m\ a$	I_2
16	*b*	.32	* $Ia\bar{3}d\ b$	Y^{**}
24	*c*	2.22	* $Ia\bar{3}d\ c$	V^*
24	*d*	$\bar{4}$..	* $Ia\bar{3}d\ d$	S^*
32	*e*	.3.	* $Ia\bar{3}d\ e$	$\bar{4}$.. $Y^{**}2xxx$
48	*f*	2..	* $Ia\bar{3}d\ f$	.3. S^*2z
48	*g*	..2	* $Ia\bar{3}d\ g$	$\bar{4}a..\ Y^{**}3x\bar{x}$
96	*h*	1	* $Ia\bar{3}d\ h$	$\bar{4}a..\ I_26xyz$

symbols. The symbols are further affected by the settings of the space group. The present section is restricted to the fundamental features of the descriptive symbols. Details have been described by Fischer *et al.* (1973). Tables 14.2.3.1 and 14.2.3.2 give for each Wyckoff position of a plane group or a space group, respectively, the multiplicity, the Wyckoff letter, the oriented site symmetry, the reference symbol of the corresponding lattice complex and the descriptive symbol.* The comparatively short descriptive symbols condense complicated verbal descriptions of the point configurations of lattice complexes.

14.2.3.2. *Invariant lattice complexes*

Invariant lattice complexes in their characteristic Wyckoff position are represented by a capital letter eventually in combination with some superscript. The first column of Table 14.2.3.3 gives a complete list of these symbols in alphabetical order. The characteristic Wyckoff positions are shown in column 3. Lattice complexes from different crystal families but with the same coordinate description for their characteristic Wyckoff positions receive the same descriptive symbol. If necessary, the crystal family may be stated explicitly by a small letter (column 2) preceding the lattice-complex symbol: *c* cubic, *t* tetragonal, *h* hexagonal, *o* orthorhombic, *m* monoclinic, *a* anorthic (triclinic).

Table 14.2.3.3. *Descriptive symbols of invariant lattice complexes in their characteristic Wyckoff position*

Descriptive symbol	Crystal family	Characteristic Wyckoff position
C	*o* *m*	$Cmmm\ a$ $C2/m\ a$
D	*c* *o*	$Fd\bar{3}m\ a$ $Fddd\ a$
${}^vD$	*t*	$I4_1/amd\ a$
E	*h*	$P6_3/mmc\ c$
F	*c* *o*	$Fm\bar{3}m\ a$ $Fmmm\ a$
G	*h*	$P6/mmm\ c$
I	*c* *t* *o*	$Im\bar{3}m\ a$ $I4/mmm\ a$ $Immm\ a$
J	*c*	$Pm\bar{3}m\ c$
J^*	*c*	$Im\bar{3}m\ b$
M	*h*	$R\bar{3}m\ e$
N	*h*	$P6/mmm\ f$
P	*c* *h* *t* *o* *m* *a*	$Pm\bar{3}m\ a$ $P6/mmm\ a$ $P4/mmm\ a$ $Pmmm\ a$ $P2/m\ a$ $P\bar{1}\ a$
${}^+Q$	*h*	$P6_222\ c$
R	*h*	$R\bar{3}m\ a$
S	*c*	$I\bar{4}3d\ a$
S^*	*c*	$Ia\bar{3}d\ d$
T	*c* *o*	$Fd\bar{3}m\ c$ $Fddd\ c$
${}^vT$	*t*	$I4_1/amd\ c$
${}^+V$	*c*	$I4_132\ c$
V^*	*c*	$Ia\bar{3}d\ c$
W	*c*	$Pm\bar{3}n\ c$
W^*	*c*	$Im\bar{3}m\ d$
${}^+Y$	*c*	$P4_332\ a$
${}^+Y^*$	*c*	$I4_132\ a$
Y^{**}	*c*	$Ia\bar{3}d\ b$

* Some of the descriptive symbols listed in Table 14.2.3.2 differ slightly from those derived by Fischer *et al.* (1973) and used in previous editions of *International Tables for Crystallography* Vol. A.

Example

D is the descriptive symbol of the invariant cubic lattice complex $Fd\bar{3}m\ a$ as well as of the orthorhombic lattice complex $Fddd\ a$. The cubic lattice complex cD contains – among others – the point configurations corresponding to the arrangement of carbon atoms in diamond and of silicon atoms in β-cristobalite. The orthorhombic complex oD is a comprehensive complex of cD. It consists of all those point configurations that may be produced by orthorhombic deformations of the point configurations of cD.

The descriptive symbol of a noncharacteristic Wyckoff position depends on the difference between the coordinate descriptions of the respective characteristic Wyckoff position and the position under consideration. Three cases may be distinguished, which may also occur in combinations.

(i) The two coordinate descriptions differ by an origin shift. Then, the respective shift vector is added as a prefix to the descriptive symbol of the characteristic Wyckoff position.

Example

The orthorhombic invariant lattice complex C is represented in its characteristic Wyckoff position $Cmmm\ a$ by the coordinate triplets 000 and $\frac{1}{2}\frac{1}{2}0$. In $Ibam\ a$, it is described by $00\frac{1}{4}$, $\frac{1}{2}\frac{1}{2}\frac{1}{4}$ and, therefore, receives the descriptive symbol $00\frac{1}{4}\ C$.

(ii) The multiplicity of the Wyckoff position considered is higher than that of the corresponding characteristic position. Then, the coordinate description of this Wyckoff position can be transformed into that of the characteristic position by taking shorter basis vectors. Reduction of all three basis vectors by a factor of 2 is denoted by the subscript 2 on the descriptive symbol. Reduction of one or two basis vectors by a factor of 2 is denoted by one of the subscripts a, b or c or a combination of these. The subscript C means a factor of 3, cc a factor of 4 and Cc a factor of 6.

Examples

The characteristic Wyckoff position of the orthorhombic lattice complex P is $Pmmm\ a$ with coordinate description 000. It occurs also in $Pmma\ a$ with coordinate triplets 000, $\frac{1}{2}00$, and in $Pcca\ a$ with 000, $00\frac{1}{2}$, $\frac{1}{2}00$, $\frac{1}{2}0\frac{1}{2}$. The corresponding descriptive symbols are P_a and P_{ac}, respectively.

(iii) The coordinate description of a given Wyckoff position is related to that of the characteristic position by inversion or rotation of the coordinate system. Changing the superscript + into − in the descriptive symbol means that the considered Wyckoff position is mapped onto the characteristic position by an inversion through the origin, *i.e.* both Wyckoff positions are enantiomorphic. A prime preceding the capital letter denotes that a 180° rotation is required.

Examples

(1) ${}^{+}Y^{*}$ is the descriptive symbol of the invariant lattice complex $I4_132\ a$ in its characteristic position. Wyckoff position $I4_132\ b$ with the descriptive symbol ${}^{-}Y^{*}$ belongs to the same lattice complex. The point configurations of $I4_132\ a$ and $I4_132\ b$ are enantiomorphic.

(2) R is the descriptive symbol of the invariant lattice complex formed by all rhombohedral point lattices. Its characteristic position $R\bar{3}m\ a$ corresponds to the coordinate triplets 000, $\frac{2}{3}\frac{1}{3}\frac{1}{3}$, $\frac{1}{3}\frac{2}{3}\frac{2}{3}$. The same lattice complex is symbolized by $'R_c$ in the noncharacteristic position $R\bar{3}c\ b$ with coordinate description 000, $00\frac{1}{2}$, $\frac{2}{3}\frac{1}{3}\frac{1}{3}$, $\frac{2}{3}\frac{1}{3}\frac{5}{6}$, $\frac{1}{3}\frac{2}{3}\frac{2}{3}$, $\frac{1}{3}\frac{2}{3}\frac{1}{6}$.

In noncharacteristic Wyckoff positions, the descriptive symbol P may be replaced by C, I by F (tetragonal system), C by A or B (orthorhombic system), and C by A, B, I or F (monoclinic system). If the lattice complexes of rhombohedral space groups are described in rhombohedral coordinate systems, the symbols R, $'R_c$, M and $'M_c$ of the hexagonal description are replaced by P, I, J and J^{*}, respectively (preceded by the letter r, if necessary, to distinguish them from the analogous cubic invariant lattice complexes).

14.2.3.3. *Lattice complexes with degrees of freedom*

The descriptive symbols of lattice complexes with degrees of freedom consist, in general, of four parts: shift vector, distribution symmetry, central part and site-set symbol. Either of the first two parts may be absent.

Example

$0\frac{1}{2}0\ ..2\ C4xxz$ is the descriptive symbol of the lattice complex $P\bar{4}/nbm\ m$ in its characteristic position: $0\frac{1}{2}0$ is the shift vector, ..2 the distribution symmetry, C the central part and $4xxz$ the site-set symbol.

Normally, the central part is the symbol of an invariant lattice complex. Shift vector and central part together should be interpreted as described in Section 14.2.3.2. The point configurations of the regarded Wyckoff position can be derived from that described by the central part by replacing each point by a finite set of points, the site set. All points of a site set are symmetrically equivalent under the site-symmetry group of the point that they replace. A site set is symbolized by a string of numbers and letters. The product of the numbers gives the number of points in the site set, whereas the letters supply information on the pattern formed by these points. Site sets replacing different points may be differently oriented. In this case, the distribution-symmetry part of the reference symbol shows symmetry operations that relate such site sets to one another. The orientation of the corresponding symmetry elements is indicated as in the oriented site-symmetry symbols (*cf.* Section 2.2.12). If all site sets have the same orientation, no distribution symmetry is given.

Examples

(1) $I4xxx$ ($I\bar{4}3m\ 8c\ xxx$) designates a lattice complex, the point configurations of which are composed of tetrahedra $4xxx$ in parallel orientations replacing the points of a cubic body-centred lattice I. The vertices of these tetrahedra are located on body diagonals.

(2) $..2\ I4xxx$ ($Pn\bar{3}m\ 8e\ xxx$) represents the lattice complex for which, in contrast to the first example, the tetrahedra $4xxx$ around 000 and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ differ in their orientation. They are related by a twofold rotation ..2 .

(3) $00\frac{1}{4}\ P_c4x$ is the descriptive symbol of Wyckoff position $P4_2/mcm\ 8l\ x0\frac{1}{4}$. Each corresponding point configuration consists of squares of points $4x$ replacing the points of a tetragonal primitive lattice P. In comparison with $P4x$, $00\frac{1}{4}\ P_c4x$ shows a unit-cell enlargement by $\mathbf{c}' = 2\mathbf{c}$ and a subsequent shift by the vector $(00\frac{1}{4})$.

In the case of a Weissenberg complex, the central part of the descriptive symbol always consists of two (or more) symbols of invariant lattice complexes belonging to the same crystal family and forming limiting complexes of the regarded Weissenberg complex. The shift vector then refers to the first limiting complex. The corresponding site-set symbols are distinguished by containing the number 1 as the only number, *i.e.* each site set consists of only one point.

Example

In $\frac{1}{4}00\ .2.\ P_aB1z$ ($Pmma\ 2e\ \frac{1}{4}0z$), each of the two points $\frac{1}{4}00$ and $\frac{3}{4}00$, represented by $\frac{1}{4}00\ P_a$, is replaced by a site set containing only one point $1z$, *i.e.* the points are shifted along the z axis. The shifts of the two points are related by a twofold rotation .2., *i.e.* are running in opposite directions. The point configurations of the two limiting complexes P_a and B refer to the special parameter values $z = 0$ and $z = \frac{1}{4}$, respectively.

The central parts of some lattice complexes with two or three degrees of freedom are formed by the descriptive symbol of a univariant Weissenberg complex instead of that of an invariant lattice complex. This is the case only if the corresponding characteristic space-group type does not refer to a suitable invariant lattice complex.

Example

In $\frac{1}{4}00$ .2. P_aB1z2y ($Pmma$ $4k$ $\frac{1}{4}yz$), each of the two points $\frac{1}{4}0z$ and $\frac{3}{4}0\bar{z}$, represented by $\frac{1}{4}00$ .2. P_aB1z, is replaced by a site set $2y$ of two points forming a dumb-bell. These dumb-bells are oriented parallel to the y axis.

The symbol of a noncharacteristic Wyckoff position is deduced from that of the characteristic position. The four parts of the descriptive symbol are subjected to the transformation necessary to map the characteristic Wyckoff position onto the Wyckoff position under consideration.

Example

The lattice complex with characteristic Wyckoff position $Imma$ $8h$ $0yz$ has the descriptive symbol .2. B_b2yz for this position. Another Wyckoff position of this lattice complex is $Imma$ $8i$ $x\frac{1}{4}z$. The corresponding point configurations are mapped onto each other by interchanging positive x and negative y directions and shifting by $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$. Therefore, the descriptive symbol for Wyckoff position $Imma$ i is $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ 2.. A_a2xz.

In some cases, the Wyckoff position described by a lattice-complex symbol has more degrees of freedom than the lattice complex (see Section 14.2.2.1). In such a case, a letter (or a string of letters) in brackets is added to the symbol.

Examples

$tP[z]$ for $P4$ a, $aP[xyz]$ for $P1$ a.

14.2.3.4. *Properties of the descriptive symbols*

Different kinds of relations between lattice complexes are brought out.

Examples

$P \leftrightarrow P4x \leftrightarrow P4x2z$, $\quad I4xxx \leftrightarrow ..2\ I4xxx$, $\quad P4x \leftrightarrow I4x$.

In many cases, limiting-complex relations can be deduced from the symbols. This applies to limiting complexes due either to special metrical parameters (*e.g.* $cP \leftrightarrow rP$ *etc.*) or to special values of coordinates (*e.g.* both $P4x$ and $P4xx$ are limiting complexes of $P4xy$). If the site set consists of only one point, the central part of the symbol specifies all corresponding limiting complexes without degrees of freedom that are due to special values of the coordinates (*e.g.* 2_12_1. $FA_aB_bC_cI_aI_bI_c1xyz$ for the general position of $P2_12_12_1$).

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14.3. Applications of the lattice-complex concept

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14.3.1. Geometrical properties of point configurations

To study the geometrical properties of all point configurations in three-dimensional space, it is not necessary to consider all Wyckoff positions of the space groups or all 1128 types of Wyckoff set. Instead, one may restrict the investigations to the characteristic Wyckoff positions of the 402 lattice complexes. The results can then be transferred to all noncharacteristic Wyckoff positions of the lattice complexes, as listed in Tables 14.2.3.1 and 14.2.3.2.

The determination of all types of sphere packings with cubic or tetragonal symmetry forms an example for this kind of procedure (Fischer, 1973, 1974, 1991*a*,*b*, 1993). The cubic lattice complex *I*4*xxx*, for example, allows two types of sphere packings within its characteristic Wyckoff position $I\bar{4}3m$ 8*c* *xxx* .3*m*, namely 9/3/*c*2 for $x = 3/16$ and 6/4/*c*1 for $3/16 < x < \frac{1}{4}$ (*cf.* Fischer, 1973). Ag_3PO_4 crystallizes with symmetry $P\bar{4}3n$ (Deschizeaux-Cheruy *et al.*, 1982) and the oxygen atoms occupy Wyckoff position 8*e* *xxx* .3., which also belongs to *I*4*xxx*. Comparison of the coordinate parameter $x = 0.1491$ for the oxygen atoms with the sphere-packing parameters listed for $I\bar{4}3m$ *c* shows directly that the oxygen arrangement in this crystal structure does not form a sphere packing.

Other examples for this approach are the derivation of crystal potentials (Naor, 1958), of coordinate restrictions in crystal structures (Smirnova, 1962), of Patterson diagrams (Koch & Hellner, 1971), of Dirichlet domains (Koch, 1973, 1984) and of sphere packings for subperiodic groups (Koch & Fischer, 1978).

The 30 lattice complexes in two-dimensional space correspond uniquely to the 'henomeric types of dot pattern' introduced by Grünbaum and Shephard (*cf. e.g.* Grünbaum & Shephard, 1981; Grünbaum, 1983).

14.3.2. Relations between crystal structures

Frequently, different crystal structures show the same geometrical arrangement for some of their atoms, even though their space groups do not belong to the same type. In these cases, the corresponding Wyckoff positions either belong to the same lattice complex or there exist close relationships between them, *e.g.* limiting-complex relations.

Examples

(1) The Fe atoms in pyrite FeS_2 occupy Wyckoff position 4*a* 000 $.\bar{3}.$ of $Pa\bar{3}$ (descriptive symbol *F*) that belongs to the invariant lattice complex $Fm\bar{3}m$ *a*. Accordingly, the Fe atoms in pyrite form a face-centred cubic lattice as do the Cu atoms in the element structure of copper.

(2) Cuprite Cu_2O crystallizes with symmetry $Pn\bar{3}m$. The oxygen atoms occupy Wyckoff position 2*a* 000 $\bar{4}3m$ (descriptive symbol *I*) and the copper atoms position 4*b* $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $.\bar{3}m$ (descriptive symbol $\frac{1}{4}\frac{1}{4}\frac{1}{4}F$). Position 2*a* belongs to lattice complex $Im\bar{3}m$ *a* and position 4*b* to $Fm\bar{3}m$ *a*. Therefore, the O atoms form a body-centred cubic lattice like the W atoms in the structure of tungsten, and the copper atoms form a face-centred cubic lattice. The tungsten configuration is shifted by $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ with respect to the copper configuration.

(3) K_2NaAlF_6 (elpasolite, *cf.* Morss, 1974) and $K_2PbNi(NO_2)_6$ (*cf.* Takagi *et al.*, 1975) crystallize with symmetry $Fm\bar{3}m$ and $Fm\bar{3}$, respectively.

K_2NaAlF_6

Al	4*a*	$m\bar{3}m$	000	*F*
Na	4*b*	$m\bar{3}m$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}F$
K	8*c*	$\bar{4}3m$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}P_2$
F	24*e*	4*m*.*m*	*x*00	*F*6*z*
			$x = 0.219$	

$K_2PbNi(NO_2)_6$

Ni	4*a*	$m\bar{3}.$	000	*F*
Pb	4*b*	$m\bar{3}.$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}F$
K	8*c*	23.	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}P_2$
N	24*e*	*mm*2..	*x*00	*F*6*z*
			$x = 0.1966$	
O	48*h*	*m*..	0*yz*	*F*6*z*2*x*

As the descriptive lattice-complex symbols for the various atomic positions show immediately, the two crystal structures are very similar. The only difference originates from the replacement of the fluorine atoms in elpasolite by NO_2 groups in $K_2PbNi(NO_2)_6$, which causes the symmetry reduction from $Fm\bar{3}m$ to $Fm\bar{3}$.

(4) The crystal structure of CoU (Baenziger *et al.*, 1950) may be interpreted as a slightly distorted CsCl (or β-brass, CuZn)-type structure. CsCl corresponds to Wyckoff positions 1*a* and 1*b* of $Pm\bar{3}m$ with descriptive symbol *P* and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*, respectively; Co and U both occupy Wyckoff position 8*a* .3. *xxx* of $I2_13$ with $x = 0.0347$ for U and $x = 0.294$ for Co. As the descriptive symbol $2_12_1..\ P_2Y^*1xxx$ shows, this Wyckoff position belongs to a Weissenberg complex with two invariant limiting complexes, namely *P* ($Pm\bar{3}m$ *a*) and Y^* ($I4_132$ *a*). $x = 0$ corresponds to P_2, $x = \frac{1}{4}$ to $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2, $x = \frac{1}{8}$ to $^{+}Y^*$ and $x = \frac{7}{8}$ to $^{-}Y^*$. Consequently, the uranium and cobalt atoms form approximately a P_2 and a $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2 configuration, respectively.

Publications by Hellner (1965, 1976*a*,*b*,*c*, 1977, 1979), Loeb (1970), Smirnova & Vasserman (1971), Sakamoto & Takahasi (1971), Niggli (1971), Fischer & Koch (1974), Hellner *et al.* (1981) and Hellner & Sowa (1985) refer to this aspect.

14.3.3. Reflection conditions

Wyckoff positions belonging to the same lattice complex show analogous reflection conditions. Therefore, lattice complexes have also been used to check the reflection conditions for all Wyckoff positions in the space-group tables of this volume.

The descriptive symbols may supply information on the reflection conditions. If the symbol does not contain any distribution-symmetry part, the reflection conditions of the Wyckoff position are indicated by the symbol of the invariant lattice complex in the central part (*e.g.* $P4/nmm$ *g*: *C*4*xx* shows that the reflection condition is that of a *C* lattice, $hkl: h + k = 2n$). In the case that the site set consists of only one point, *i.e.* the Wyckoff position belongs to a Weissenberg complex, all conditions for general reflections *hkl* that may arise from special choices of the coordinates can be read from the central part of the symbol (*e.g.* $P4/nmm$ *c*: $0\frac{1}{2}0$ ..2 $CI1z$ indicates that, by special choice of z, either *hkl*: $h+k=2n$ or *hkl*: $h+k+l=2n$ may be produced).

14.3.4. Phase transitions

If a crystal undergoes a phase transition from a high- to a low-symmetry modification, the transition may be connected with a group–subgroup degradation. In such a case, the comparison of the lattice complexes corresponding to the Wyckoff positions of the original space group on the one hand and of its various subgroups on the other hand very often shows which of these subgroups are suitable for the low-symmetry modification.

This kind of procedure will be demonstrated with the aid of a space group $R\bar{3}m$ and its three translation-equivalent subgroups with index 2, namely $R32$, $R\bar{3}$ and $R3m$. In the course of the subgroup degradation, the Wyckoff positions of $R\bar{3}m$ behave differently:

The descriptive symbols R and $00\frac{1}{2}$ R refer to Wyckoff positions $R\bar{3}m$ 3*a* and 3*b* as well as to Wyckoff positions $R32$ 3*a* and 3*b* and $R\bar{3}$ 3*a* and 3*b*. Therefore, all corresponding point configurations and atomic arrangements remain unchanged in these subgroups. In subgroup $R3m$, however, the respective Wyckoff position is 3*a* with descriptive symbol $R[z]$, *i.e.* a shift parallel to [001] of the entire point configuration is allowed.

The descriptive symbol $R2z$ for $R\bar{3}m$ 6*c* occurs also for $R32$ 6*c* and $R\bar{3}$ 6*c*. Again both subgroups do not allow any deformations of the corresponding point configurations or atomic arrangements. Symmetry reduction to $R3m$, however, yields a splitting of each $R2z$ configuration into two $R[z]$ configurations. The two z parameters may be chosen independently.

As M and $00\frac{1}{2}$ M are the descriptive symbols not only of $R\bar{3}m$ 9*e* and 9*d* but also of $R\bar{3}$ 9*e* and 9*d*, $R\bar{3}$ does not enable any deformation of the corresponding atomic arrangements. In $R32$ and in $R3m$, however, the respective point configurations may be deformed differently, as the descriptive symbols show: $R3x$ and $00\frac{1}{2}$ $R3x$ ($R32$ 9*d* and 9*e*), $R3x\bar{x}[z]$ ($R3m$ 9*b*).

Wyckoff positions $R\bar{3}m$ 18*f* and 18*g* ($R6x$ and $00\frac{1}{2}$ $R6x$) correspond to $R32$ 9*d* and 9*e* ($R3x$ and $00\frac{1}{2}$ $R3x$), to $R\bar{3}$ 18*f* ($R6xyz$), and to $R3m$ 18*c* ($R3x\bar{x}2y[z]$). In $R32$, the hexagons $6x$ around the points of the R lattice are split into two oppositely oriented triangles $3x$, which may have different size. In $R\bar{3}$ and in $R3m$, the hexagons may be deformed differently.

Wyckoff position $R\bar{3}m$ 18*h* ($R6x\bar{x}z$) corresponds to sets of trigonal antiprisms around the points of an R lattice. These antiprisms may be distorted in $R32$ 18*f* ($R3x2yz$) or rotated in $R\bar{3}$ 18*f* ($R6xyz$). In $R3m$ 9*b* ($R3x\bar{x}[z]$), each antiprism is split into two parallel triangles that may differ in size.

In each of the three subgroups, any point configuration belonging to the general position $R\bar{3}m$ 36*i* splits into two parts. Each of these parts may be deformed differently.

14.3.5. Incorrect space-group assignment

In the literature, some crystal structures are still described within space groups that are only subgroups of the correct symmetry groups. Many such mistakes (but not all of them) could be avoided by simply looking at the lattice complexes (and their descriptive symbols) that correspond to the Wyckoff positions of the different kinds of atoms. Whenever the same (or an analogous) lattice-complex description of a crystal structure is also possible within a supergroup, then the crystal structure has at least that symmetry.

Examples

(1) The crystal structure of β-$LiRhO_2$ has been refined in space group $F4_132$ (*cf.* Hobbie & Hoppe, 1986).

Rh	16*c*	.32	$\frac{1}{8}\frac{1}{8}\frac{1}{8}$	T
Li	16*d*	.32	$\frac{5}{8}\frac{5}{8}\frac{5}{8}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ T
O	32*e*	.3.	xxx	..2 $D4xxx$

The same atomic arrangement is possible in the supergroup $Fd\bar{3}m$ of $F4_132$, as can easily be read from Table 14.2.3.2:

Rh	16*c*	$.\bar{3}m$	$\frac{1}{8}\frac{1}{8}\frac{1}{8}$	T
Li	16*d*	$.\bar{3}m$	$\frac{5}{8}\frac{5}{8}\frac{5}{8}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ T
O	32*e*	$.3m$	xxx	..2 $D4xxx$

Therefore, β-$LiRhO_2$ should be described in $Fd\bar{3}m$.

(2) $KIAs_4O_6$ (Pertlik, 1988) has been described with symmetry $P622$.

I	1*a*	622	000	P
K	1*b*	622	$00\frac{1}{2}$	$00\frac{1}{2}$ P
As	4*h*	3..	$\frac{1}{3}\frac{2}{3}z$	$G2z$
O	6*i*	2..	$\frac{1}{2}0z$	$N2z$

Space group $P6/mmm$ allows the same atomic arrangement:

I	1*a*	$6/mmm$	000	P
K	1*b*	$6/mmm$	$00\frac{1}{2}$	$00\frac{1}{2}$ P
As	4*h*	$3m.$	$\frac{1}{3}\frac{2}{3}z$	$G2z$
O	6*i*	$2mm$	$\frac{1}{2}0z$	$N2z$

Therefore, $KIAs_4O_6$ should be described in $P6/mmm$.

14.3.6. Application of descriptive lattice-complex symbols

Descriptive symbols of lattice complexes – at least those of the invariant lattice complexes – have been used for the description of crystal structures (*cf.* Section 14.3.2 and the literature cited there), for the nomenclature of three-periodic surfaces (von Schnering & Nesper, 1987) and in connection with orbifolds of space groups (Johnson *et al.*, 2001).

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15.1. Introduction and definitions

BY E. KOCH, W. FISCHER AND U. MÜLLER

15.1.1. Introduction

The mathematical concept of normalizers forms the common basis for the solution of several crystallographic problems:

It is generally known, for instance, that the coordinate description of a crystal structure trivially depends on the coordinate system used for the description, *i.e.* on the setting of the space group and the site symmetry of the origin. It is less well known, however, that for most crystal structures there exist several different but equivalent coordinate descriptions, even if the space-group setting and the site symmetry of the origin are unchanged. The number of such descriptions varies between 1 and 24 and depends only on the type of the Euclidean normalizer of the corresponding space group. In principle, none of these descriptions stands out against the others.

In crystal-structure determination with direct methods, the phases of some suitably chosen structure factors have to be restricted to certain values or to certain ranges in order to specify the origin and the enantiomorph. The information necessary for a correct selection of such phases and for their appropriate restrictions follows directly from the Euclidean normalizer of the space group. Similar examples are the positioning of the first atom(s) within an asymmetric unit when using trial-and-error or Patterson methods, the choice of a basis system for indexing the reflections of a diffraction pattern or the indexing of the first morphological face(s) of a crystal.

For the following problems, normalizers also play an important role: They supply information on the interchangeability of Wyckoff positions and their assignment to Wyckoff sets (*cf.* Section 8.3.2 and Chapter 14.1), needed *e.g.* for the definition of lattice complexes. They are important for the comparison of crystal structures, for their assignment to structure types and for the choice of a standard description for each crystal structure (Parthé & Gelato, 1984, 1985). They allow the derivation of 'privileged origins' for each space group (Burzlaff & Zimmermann, 1980) and facilitate the complete deduction of subgroups and supergroups of a crystallographic group. They enable an easy classification of magnetic (black–white or Shubnikov) space groups and of colour space groups. They may also be used to reduce the parameter range in the study of geometrical properties of point configurations, *e.g.* their inherent symmetry or their sphere packings and Dirichlet partitions (*cf. e.g.* Koch, 1984).

In the past, most of these problems have been treated by crystallographers without the aid of normalizers, but the use of normalizers simplifies the solution of all these problems and clarifies the common background (for references, see Fischer & Koch, 1983).

15.1.2. Definitions

Any pair, consisting of a group $\mathcal{G}$ and one of its supergroups $\mathcal{S}$, is uniquely related to a third intermediate group $\mathcal{N}_{\mathcal{S}}(\mathcal{G})$, called the *normalizer of* $\mathcal{G}$ *with respect to* $\mathcal{S}$. $\mathcal{N}_{\mathcal{S}}(\mathcal{G})$ is defined as the set of all elements $\mathbf{S} \in \mathcal{S}$ that map $\mathcal{G}$ onto itself by conjugation (*cf.* Section 8.3.6).

$$\mathcal{N}_{\mathcal{S}}(\mathcal{G}) := \{\mathbf{S} \in \mathcal{S} |\ \mathbf{S}^{-1} \mathcal{G}\, \mathbf{S} = \mathcal{G}\}.$$

The normalizer $\mathcal{N}_{\mathcal{S}}(\mathcal{G})$ may coincide either with $\mathcal{G}$ or with $\mathcal{S}$ or it may be a proper intermediate group. In any case, $\mathcal{G}$ is a normal subgroup of its normalizer.

For most crystallographic problems, two kinds of normalizers are of special interest: (i) the normalizer of a space group (plane group) $\mathcal{G}$ with respect to the group $\mathcal{E}$ of all Euclidean mappings (motions, isometries) in E^3 (E^2), called the *Euclidean normalizer of* $\mathcal{G}$

$$\mathcal{N}_{\mathcal{E}}(\mathcal{G}) := \{\mathbf{S} \in \mathcal{E} |\ \mathbf{S}^{-1} \mathcal{G}\, \mathbf{S} = \mathcal{G}\};$$

(ii) the normalizer of a space group (plane group) $\mathcal{G}$ with respect to the group $\mathcal{A}$ of all affine mappings in E^3 (E^2), called the *affine normalizer of* $\mathcal{G}$

$$\mathcal{N}_{\mathcal{A}}(\mathcal{G}) := \{\mathbf{S} \in \mathcal{A} |\ \mathbf{S}^{-1} \mathcal{G}\, \mathbf{S} = \mathcal{G}\}.$$

The Euclidean normalizers of the space groups were first derived by Hirshfeld (1968) under the name *Cheshire groups*. They have been tabulated in more detail by Gubler (1982*a*,*b*) and Fischer & Koch (1983). The Euclidean normalizers of triclinic and monoclinic space groups with specialized metric have been determined by Koch & Müller (1990). The affine normalizers of the space groups have been listed by Burzlaff & Zimmermann (1980), Billiet *et al.* (1982) and Gubler (1982*a*,*b*). They have also been used for the derivation of Wyckoff sets and the definition of lattice complexes by Koch & Fischer (1975), even though there the automorphism groups of the space groups were tabulated instead of their affine normalizers.

International Tables for Crystallography (2006). Vol. A, Chapter 15.2, pp. 879–899.

15.2. Euclidean and affine normalizers of plane groups and space groups

By E. Koch, W. Fischer and U. Müller

15.2.1. Euclidean normalizers of plane groups and space groups

Since each symmetry operation of the Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ maps the space group $\mathcal{G}$ onto itself, it also maps the set of all symmetry elements of $\mathcal{G}$ onto itself. Therefore, the Euclidean normalizer of a space group can be interpreted as the group of motions that maps the pattern of symmetry elements of the space group onto itself, *i.e.* as the 'symmetry of the symmetry pattern'.

For most space (plane) groups, the Euclidean normalizers are space (plane) groups again. Exceptions are those groups where origins are not fully fixed by symmetry, *i.e.* all space groups of the geometrical crystal classes 1, *m*, 2, 2*mm*, 3, 3*m*, 4, 4*mm*, 6 and 6*mm*, and all plane groups of the geometrical crystal classes 1 and *m*. The Euclidean normalizer of each such group contains continuous translations (*i.e.* translations of infinitesimal length) in one, two or three independent lattice directions and, therefore, is not a space (plane) group but a supergroup of a space (plane) group.

If one regards a certain type of space (plane) group, usually the Euclidean normalizers of all corresponding groups belong also to only one type of normalizer. This is true for all cubic, hexagonal, trigonal and tetragonal space groups (hexagonal and square plane groups) and, in addition, for 21 types of orthorhombic space group (4 types of rectangular plane group), *e.g.* for *Pnma*.

In contrast to this, the Euclidean normalizer of a space (plane) group belonging to one of the other 38 orthorhombic (3 rectangular) types may interchange two or even three lattice directions if the corresponding basis vectors have equal length (example: *Pmmm* with $a = b$). Then, the Euclidean normalizer of this group belongs to the tetragonal (square) or even to the cubic crystal system, whereas another space (plane) group of the same type but with general metric has an orthorhombic (rectangular) Euclidean normalizer.

For each space (plane)-group type belonging to the monoclinic (oblique) or triclinic system, there also exist groups with specialized metric that have Euclidean normalizers of higher symmetry than for the general case (*cf.* Koch & Müller, 1990). The description of these special cases, however, is by far more complicated than for the orthorhombic system.

The symmetry of the Euclidean normalizer of a monoclinic (oblique) space (plane) group depends only on two metrical parameters. A clear presentation of all cases with specialized metric may be achieved by choosing the cosine of the monoclinic angle and the related axial ratio as parameters. To cover all different metrical situations exactly once, not all pairs of parameter values are allowed for a given type of space (plane) group, but one has to restrict the study to a certain parameter range depending on the type, the setting and the cell choice of the space (plane) group. Parthé & Gelato (1985) have discussed in detail such parameter regions for the first setting of the monoclinic space groups. Figs. 15.2.1.1 to 15.2.1.4 are based on these studies.

Fig. 15.2.1.1 shows a suitably chosen parameter region for the five space-group types $P2$, $P2_1$, Pm, $P2/m$ and $P2_1/m$ and for the plane-group types $p1$ and $p2$. Each such space (plane) group with general metric may be uniquely assigned to an inner point of this region and any metrical specialization corresponds either to one of the three boundary lines or to one of their points of intersection and gives rise to a symmetry enhancement of the respective Euclidean normalizer.

For each of the other eight types of monoclinic space groups, *i.e.* $C2$, Pc, Cm, Cc, $C2/m$, $P2/c$, $P2_1/c$ and $C2/c$, and for each setting three possibilities of cell choice are listed in Part 7, which can be distinguished by different space-group symbols (example: $C12/m1$,

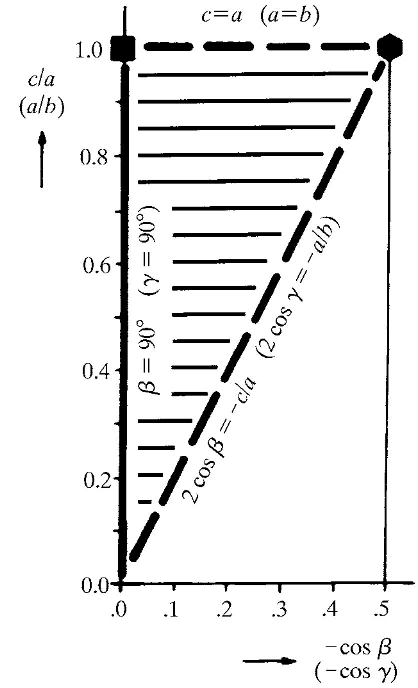

Fig. 15.2.1.1. Parameter range for space groups of types $P2, P2_1, Pm, P2/m$ and $P2_1/m$ (plane groups of types $p1$ and $p2$). The information in parentheses refers to unique axis *c*.

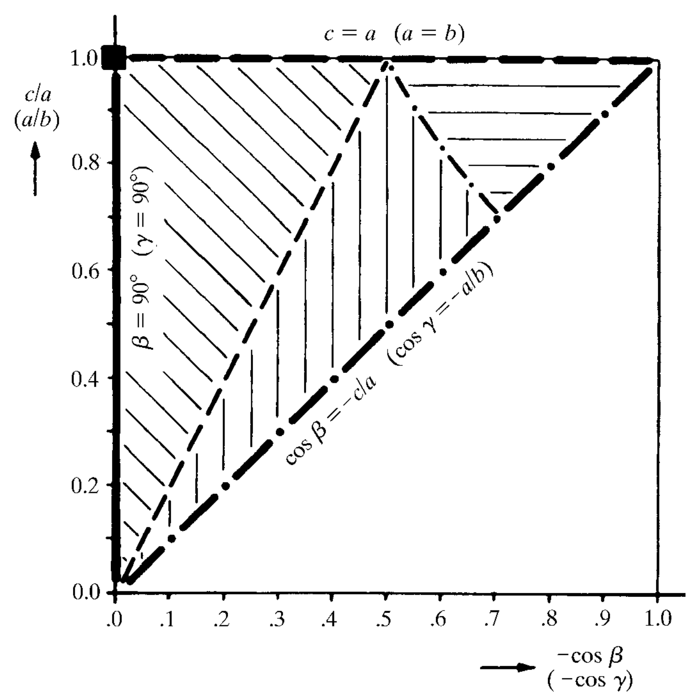

Fig. 15.2.1.2. Parameter range for space groups of types $C2$, Pc, Cm, Cc, $C2/m$, $P2/c$, $P2_1/c$ and $C2/c$:
unique axis *b*, cell choice 2: $P1n1$, $P12/n1$, $P12_1/n1$;
unique axis *b*, cell choice 3: $I121$, $I1m1$, $I1a1$, $I12/m1$, $I12/a1$;
unique axis *c*, cell choice 2: $P11n$, $P112/n$, $P112_1/n$;
unique axis *c*, cell choice 3: $I112$, $I11m$, $I11b$, $I112/m$, $I112/b$.
The information in parentheses refers to unique axis *c*.

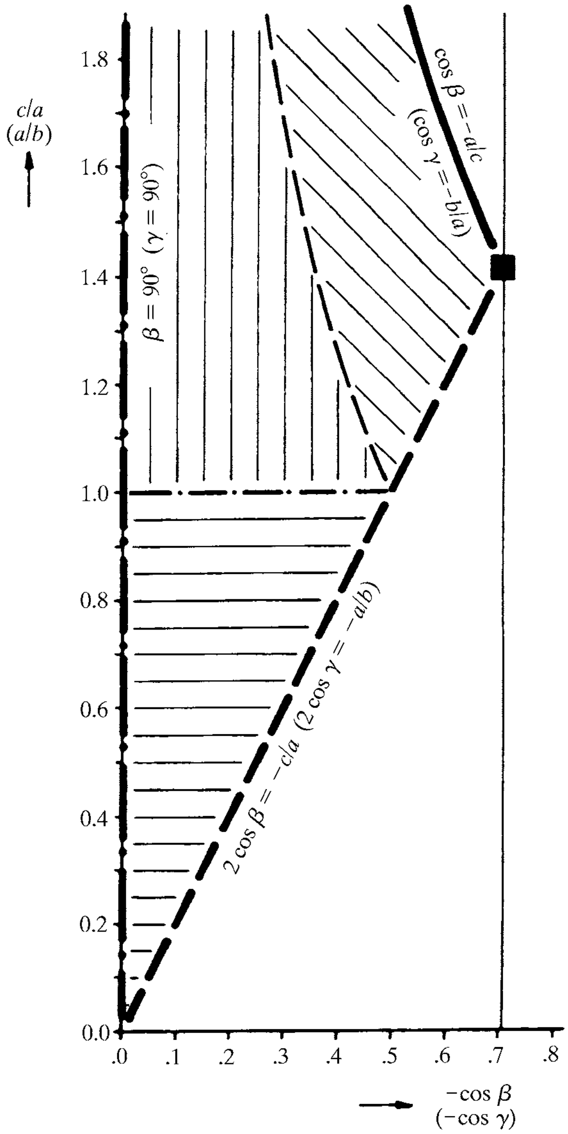

Fig. 15.2.1.3. Parameter range for space groups of types $C2$, Pc, Cm, Cc, $C2/m$, $P2/c$, $P2_1/c$ and $C2/c$:
unique axis b, cell choice 1: $P1c1$, $P12/c1$, $P12_1/c1$;
unique axis b, cell choice 2: $A121$, $A1m1$, $A1n1$, $A12/m1$, $A12/n1$;
unique axis c, cell choice 1: $P11a$, $P112/a$, $P112_1/a$;
unique axis c, cell choice 2: $B112$, $B11m$, $B11n$, $B112/m$, $B112/n$.
The information in parentheses refers to unique axis c.

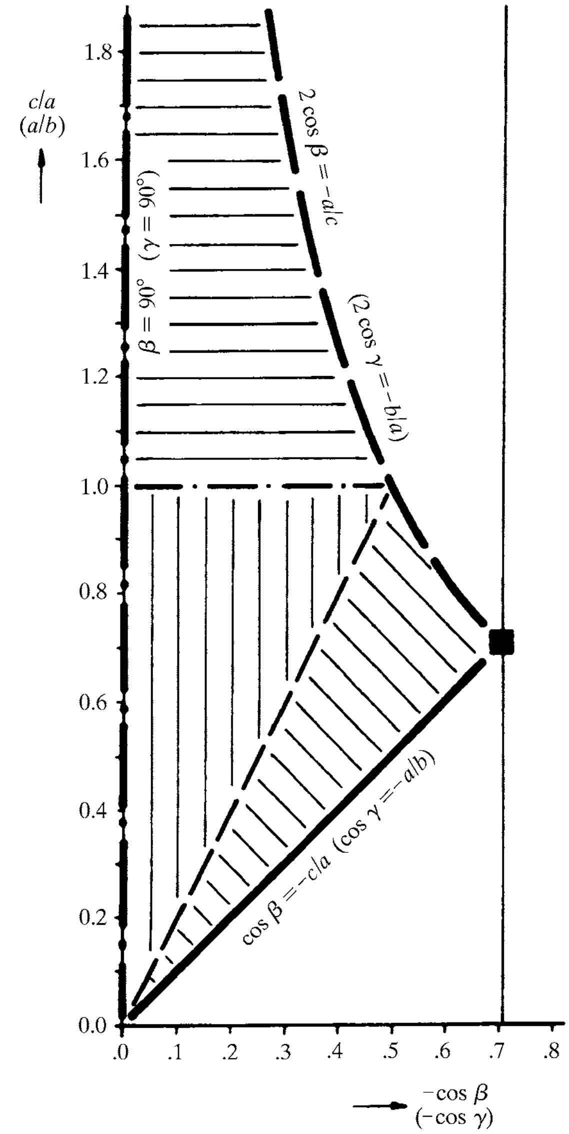

Fig. 15.2.1.4. Parameter range for space groups of types $C2$, Pc, Cm, Cc, $C2/m$, $P2/c$, $P2_1/c$ and $C2/c$:
unique axis b, cell choice 1: $C121$, $C1m1$, $C1c1$, $C12/m1$, $C12/c1$;
unique axis b, cell choice 3: $P1a1$, $P12/a1$, $P12_1/a1$, $C12/c1$;
unique axis c, cell choice 1: $A112$, $A11m$, $A11a$, $A112/m$, $A112/a$;
unique axis c, cell choice 3: $P11b$, $P112/b$, $P112_1/b$, $A112/a$.
The information in parentheses refers to unique axis c.

$A12/m1$, $I12/m1$, $A112/m$, $B112/m$, $I112/m$). For each setting, there exist two ways to choose a suitable range for the metrical parameters such that each group corresponds to exactly one point:

(i) One arbitrarily restricts oneself to cell choice 1, 2 or 3. Then, the suitable parameter range (displayed in one of the Figs. 15.2.1.2, 15.2.1.3 or 15.2.1.4) is larger than the range shown in Fig. 15.2.1.1 because, in contrast to the space-group types discussed above, some of the possible metrical specializations do not give rise to any symmetry enhancement of the Euclidean normalizers. These special metrical cases refer to the light lines subdividing the parameter regions of Figs. 15.2.1.2 to 15.2.1.4. Again, all inner points of these regions correspond to space groups with Euclidean normalizers without enhanced symmetry, and all points on the heavy-line boundaries refer to space groups, the Euclidean normalizers of which show symmetry enhancement.

(ii) For all types of monoclinic space groups, one regards only the small parameter region shown in Fig. 15.2.1.1, but in return takes into consideration all three possibilities for the cell choice. Then, however, not all boundaries of this small parameter region correspond to Euclidean normalizers with enhanced symmetry. (Similar considerations are true for oblique plane groups.)

For triclinic space groups, five metrical parameters are necessary and, therefore, it is impossible to describe the special metrical cases in an analogous way.

In general, between a space group (or plane group) $\mathcal{G}$ and its Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$, two uniquely defined intermediate groups $\mathcal{K}(\mathcal{G})$ and $\mathcal{L}(\mathcal{G})$ exist, such that

$$\mathcal{G} \leq \mathcal{K}(\mathcal{G}) \leq \mathcal{L}(\mathcal{G}) \leq \mathcal{N}_{\mathcal{E}}(\mathcal{G})$$

holds. $\mathcal{K}(\mathcal{G})$ is that class-equivalent supergroup of $\mathcal{G}$ that is at the same time a translation-equivalent subgroup of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$. It is well defined according to a theorem of Hermann (1929). The group $\mathcal{L}(\mathcal{G})$ differs from $\mathcal{K}(\mathcal{G})$ only if $\mathcal{G}$ is noncentrosymmetric but $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is centrosymmetric; then $\mathcal{L}(\mathcal{G})$ is that centrosymmetric supergroup of $\mathcal{K}(\mathcal{G})$ of index 2 that is again a subgroup of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$. It belongs to the

Table 15.2.1.1. *Euclidean normalizers of the plane groups*

For the restrictions of the cell metric of the two oblique plane groups see text and Fig. 15.2.1.3.

Plane group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Twofold rotation	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
1	$p1$	General	p^22	$\varepsilon_1\mathbf{a},\ \varepsilon_2\mathbf{b}$	$r, 0; 0, s$	$-x, -y$		$\infty^2\cdot 2\cdot 1$
		$a<b,\ \gamma=90°$	p^22mm	$\varepsilon_1\mathbf{a},\ \varepsilon_2\mathbf{b}$	$r, 0; 0, s$	$-x, -y$	$-x,\ y$	$\infty^2\cdot 2\cdot 2$
		$2\cos\gamma=-a/b,\ 90<\gamma<120°$	c^22mm	$\varepsilon_1\mathbf{a},\ \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{b})$	$r, 0; 0, s$	$-x, -y$	$x-y, -y$	$\infty^2\cdot 2\cdot 2$
		$a=b,\ 90<\gamma<120°$	c^22mm	$\varepsilon_1(\mathbf{a}-\mathbf{b}),\ \varepsilon_2(\mathbf{a}+\mathbf{b})$	$r, 0; 0, s$	$-x, -y$	y, x	$\infty^2\cdot 2\cdot 2$
		$a=b, \gamma=90°$	p^24mm	$\varepsilon\mathbf{a},\ \varepsilon\mathbf{b}$	$r, 0; 0, s$	$-x, -y$	$-x,\ y;\ y,\ x$	$\infty^2\cdot 2\cdot 4$
		$a=b, \gamma=120°$	p^26mm	$\varepsilon\mathbf{a},\ \varepsilon\mathbf{b}$	$r, 0; 0, s$	$-x, -y$	$y,\ x;\ x,\ x-y$	$\infty^2\cdot 2\cdot 6$
2	$p2$	General	$p2$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
		$a<b, \gamma=90°$	$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		$-x,\ y$	$4\cdot 1\cdot 2$
		$2\cos\gamma=-a/b,\ 90<\gamma<120°$	$c2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		$x-y,\ -y$	$4\cdot 1\cdot 2$
		$a=b,\ 90<\gamma<120°$	$c2mm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b})$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		$y,\ x$	$4\cdot 1\cdot 2$
		$a=b, \gamma=90°$	$p4mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		$-x,\ y;\ y,\ x$	$4\cdot 1\cdot 4$
		$a=b, \gamma=120°$	$p6mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		$y,\ x;\ x,\ x-y$	$4\cdot 1\cdot 6$
3	$p1m1$		p^12mm	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2}, 0; 0, s$	$-x, -y$		$(2\cdot\infty)\cdot 2\cdot 1$
4	$p1g1$		p^12mm	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2}, 0; 0, s$	$-x, -y$		$(2\cdot\infty)\cdot 2\cdot 1$
5	$c1m1$		p^12mm	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$0, s$	$-x, -y$		$\infty\cdot 2\cdot 1$
6	$p2mm$	$a\neq b$	$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
		$a=b$	$p4mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		y, x	$4\cdot 1\cdot 2$
7	$p2mg$		$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
8	$p2gg$	$a\neq b$	$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
		$a=b$	$p4mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		y, x	$4\cdot 1\cdot 2$
9	$c2mm$	$a\neq b$	$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0$			$2\cdot 1\cdot 1$
		$a=b$	$p4mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0$		y, x	$2\cdot 1\cdot 2$
10	$p4$		$p4mm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b})$	$\frac{1}{2}, \frac{1}{2}$		y, x	$2\cdot 1\cdot 2$
11	$p4mm$		$p4mm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b})$	$\frac{1}{2}, \frac{1}{2}$			$2\cdot 1\cdot 1$
12	$p4gm$		$p4mm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b})$	$\frac{1}{2}, \frac{1}{2}$			$2\cdot 1\cdot 1$
13	$p3$		$p6mm$	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}), \frac{1}{3}(-\mathbf{a}+\mathbf{b})$	$\frac{2}{3}, \frac{1}{3}$	$-x, -y$	y, x	$3\cdot 2\cdot 2$
14	$p3m1$		$p6mm$	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}), \frac{1}{3}(-\mathbf{a}+\mathbf{b})$	$\frac{2}{3}, \frac{1}{3}$	$-x, -y$		$3\cdot 2\cdot 1$
15	$p31m$		$p6mm$	$\mathbf{a}, \mathbf{b}$		$-x, -y$		$1\cdot 2\cdot 1$
16	$p6$		$p6mm$	$\mathbf{a}, \mathbf{b}$			y, x	$1\cdot 1\cdot 2$
17	$p6mm$		$p6mm$	$\mathbf{a}, \mathbf{b}$				$1\cdot 1\cdot 1$

Laue class of $\mathcal{G}$. If $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is noncentrosymmetric, an intermediate group $\mathcal{L}(\mathcal{G})$ cannot exist.

The groups $\mathcal{K}(\mathcal{G})$ and $\mathcal{L}(\mathcal{G})$ are of special interest in connection with direct methods for structure determination: they cause the parity classes of reflections; $\mathcal{K}(\mathcal{G})$ defines the permissible origin shifts and the parameter ranges for the phase restrictions in the specification of the origin; and $\mathcal{L}(\mathcal{G})$ gives information on possible phase restrictions for the selection of the enantiomorph. For any space (plane) group $\mathcal{G}$, the translation subgroups of $\mathcal{K}(\mathcal{G})$, $\mathcal{L}(\mathcal{G})$, $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and even $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ coincide.

The Euclidean normalizers of the plane groups are listed in Table 15.2.1.1, those of triclinic space groups in Table 15.2.1.2, of monoclinic and orthorhombic space groups in Table 15.2.1.3, and those of all other space groups in Table 15.2.1.4. Herein all settings and choices of cell and origin as tabulated in Parts 6 and 7 are taken into account and, in addition, all metrical specializations giving rise to Euclidean normalizers with enhanced symmetry. Each setting, cell choice, origin or metrical specialization corresponds to one line in the tables. (Exceptions are some orthorhombic space groups with tetragonal metric: if $a=b$ as well as $b=c$ and $c=a$ give rise to a symmetry enhancement of the Euclidean normalizer, only the case $a=b$ is listed in Table 15.2.1.3.)

The first column of Tables 15.2.1.1, 15.2.1.3 and 15.2.1.4 shows the number of the plane group or space group, the second column its Hermann–Mauguin symbol together with information on the setting, cell choice and origin, if necessary. Special metrical conditions affecting the Euclidean normalizer are tabulated in the third column of Tables 15.2.1.1 and 15.2.1.3. The term 'general' means that only the general metrical conditions for the respective crystal system are valid. In Table 15.2.1.4, a corresponding column is superfluous because here a metrical specialization of the space group does not influence the type of the Euclidean normalizer.

The Euclidean normalizer of the space (plane) group is identified in the fourth column of Table 15.2.1.3 (15.2.1.1) or in the third column of Table 15.2.1.4. As Euclidean normalizers are groups of motions, they can normally be designated by Hermann–Mauguin symbols. If, however, the origin of the space (plane) group is not fixed by symmetry (examples: $P4$, $P1m1$, $P1$), the Euclidean normalizer contains continuous translations in one, two or three (one or two) independent directions. In these cases, P^1, B^1, C^1, P^2 or

Table 15.2.1.2. *Euclidean normalizers of the triclinic space groups*

Basis vectors of the Euclidean normalizers ($\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$ refer to the possibly centred conventional unit cell for the respective Bravais lattice):
$P1 : \varepsilon\mathbf{a}_c, \varepsilon\mathbf{b}_c, \varepsilon\mathbf{c}_c$; $P\bar{1} : \frac{1}{2}\mathbf{a}_c, \frac{1}{2}\mathbf{b}_c, \frac{1}{2}\mathbf{c}_c$.

Bravais type	Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ of 1 $P1$	2 $P\bar{1}$
aP	$P^3\bar{1}$	$P\bar{1}$
mP	$P^3 2/m$	$P2/m$
mA	$P^3 2/m$	$A2/m$
oP	P^3mmm	$Pmmm$
oC	P^3mmm	$Cmmm$
oF	P^3mmm	$Fmmm$
oI	P^3mmm	$Immm$
tP	$P^3 4/mmm$	$P4/mmm$
tI	$P^3 4/mmm$	$I4/mmm$
hP	$P^3 6/mmm$	$P6/mmm$
hR	$P^3\bar{3}m1$	$R\bar{3}m$
cP	$P^3m\bar{3}m$	$Pm\bar{3}m$
cF	$P^3m\bar{3}m$	$Fm\bar{3}m$
cI	$P^3m\bar{3}m$	$Im\bar{3}m$

P^3 (p^1, c^1, p^2), respectively, are used instead of the Bravais letter.* Setting and origin choice for the Euclidean normalizers are indicated as for space groups. In a few cases, origin choices not tabulated in Part 7 are needed.

In the next column, the basis of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is described in terms of the basis of $\mathcal{G}$. A factor ε is used to indicate continuous translations.

The following three columns specify a set of additional symmetry operations that generate $\mathcal{K}(\mathcal{G})$, $\mathcal{L}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ successively from the space group $\mathcal{G}$: The first of them shows the vector components of the additional translations generating $\mathcal{K}(\mathcal{G})$ from $\mathcal{G}$; components referring to continuous translations are labelled r, s and t. If $\mathcal{L}(\mathcal{G})$ differs from $\mathcal{K}(\mathcal{G})$, *i.e.* if $\mathcal{G}$ is noncentrosymmetric and $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is centrosymmetric, the position of an additional centre of symmetry is given in the second of these columns. The respective inversion generates $\mathcal{L}(\mathcal{G})$ from $\mathcal{K}(\mathcal{G})$. (For plane groups, additional twofold rotations play the role of these inversions.) If, however, $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is noncentrosymmetric and, therefore, $\mathcal{L}(\mathcal{G})$ is undefined, this fact is indicated by a slash. The last of these columns contains entries only if $\mathcal{G}$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ belong to different Laue classes. The corresponding additional generators are listed as coordinate triplets.

In the last column, the subgroup index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is specified as the product $k_g l_k n_l$, where k_g means the index of $\mathcal{G}$ in $\mathcal{K}(\mathcal{G})$, l_k the index of $\mathcal{K}(\mathcal{G})$ in $\mathcal{L}(\mathcal{G})$ and n_l the index of $\mathcal{L}(\mathcal{G})$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$. [In the case of a noncentrosymmetric normalizer, the index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is given as the product $k_g n_k$, where k_g means the index of $\mathcal{G}$ in $\mathcal{K}(\mathcal{G})$ and n_k the index of $\mathcal{K}(\mathcal{G})$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$.] For continuous translations, k_g is always infinite. Nevertheless, it is useful to distinguish different cases: ∞, ∞^2 and ∞^3 refer to one, two and three independent directions with continuous translations. An additional factor of 2^n or 3^n indicates the existence of n additional independent translations which are not continuous.

For triclinic space groups, each metrical specialization gives rise to a symmetry enhancement of the Euclidean normalizer. The corresponding conditions for the metrical parameters, however, cannot be described as easily as in the monoclinic case (for further information see Part 9 and literature on 'reduced cells' cited therein). Table 15.2.1.2 shows the Euclidean normalizers for $P1$ and $P\bar{1}$. Each special metrical condition is designated by the Bravais type of the corresponding translation lattice. In the case of $P\bar{1}$, the Euclidean normalizer is always the inherent symmetry group of a suitably chosen point lattice with basis vectors $\frac{1}{2}\mathbf{a}_c$, $\frac{1}{2}\mathbf{b}_c$ and $\frac{1}{2}\mathbf{c}_c$. Here, $\mathbf{a}_c$, $\mathbf{b}_c$ and $\mathbf{c}_c$ do not refer to the primitive unit cell of $P\bar{1}$ but to the possibly centred conventional cell for the respective Bravais lattice. In the case of $P1$, the Euclidean normalizer always contains continuous translations in three independent directions, symbolized by P^3. These normalizers may be easily derived from those for $P\bar{1}$.

15.2.2. Affine normalizers of plane groups and space groups

The affine normalizer $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ of a space (plane) group $\mathcal{G}$ either is a true supergroup of its Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$, or both normalizers coincide:

$$\mathcal{N}_{\mathcal{A}}(\mathcal{G}) \geq \mathcal{N}_{\mathcal{E}}(\mathcal{G}).$$

As any translation is an isometry, each translation belonging to $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ also belongs to $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$. Therefore, the affine normalizer and the Euclidean normalizer of a space (plane) group necessarily have identical translation subgroups.

By analogy to the isometries of the Euclidean normalizer, the additional mappings of the affine normalizer also map the set of all symmetry elements of the space (plane) group onto itself.

In contrast to the Euclidean normalizers, the affine normalizers of all space (plane) groups of a certain type belong to only one type of normalizer, *i.e.* they are isomorphic groups. Therefore, the type of the affine normalizer $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ never depends on the metrical properties of the space group $\mathcal{G}$.

If for all space (plane) groups of a certain type the Euclidean normalizers also belong to one type, then for each such space (plane) group the Euclidean and the affine normalizers are identical, irrespective of any metrical specialization, *i.e.* $\mathcal{N}_{\mathcal{E}}(\mathcal{G}) = \mathcal{N}_{\mathcal{A}}(\mathcal{G})$ holds. Then, the affine normalizers are pure groups of motions and do not contain any further affine mappings. This is true for all cubic, hexagonal, trigonal and tetragonal space groups (for all hexagonal and square plane groups) and, in addition, for the space groups of 21 further orthorhombic types (plane groups of 2 further rectangular types) [examples: $\mathcal{N}_{\mathcal{A}}(Pcca) = Pmmm$, $\mathcal{N}_{\mathcal{A}}(Pnc2) = P^1mmm$].

For each of the other 38 types of orthorhombic space group (5 types of rectangular plane groups), the type of the affine normalizer corresponds to the type of the highest-symmetry Euclidean normalizers belonging to that space (plane)-group type. Therefore, it may also be symbolized by (possibly modified) Hermann–Mauguin symbols [examples: $\mathcal{N}_{\mathcal{A}}(Pbca) = Pm\bar{3}$, $\mathcal{N}_{\mathcal{A}}(Pccn) = P4/mmm$, $\mathcal{N}_{\mathcal{A}}(Pcc2) = P^1 4/mmm$].

As the affine normalizer of a monoclinic or triclinic space group (oblique plane group) is not isomorphic to any group of motions, it cannot be characterized by a modified Hermann–Mauguin symbol. It may be described, however, by one or two matrix–vector pairs together with the appropriate restrictions on the coefficients. Similar information has been given by Billiet *et al.* (1982) for the standard description of each group. The problem has been discussed in more detail by Gubler (1982*a*,*b*).

In Table 15.2.2.1, the affine normalizers of all triclinic and monoclinic space groups are given. The first two columns correspond to those of Table 15.2.1.3 or 15.2.1.4. The affine normalizers are completely described in column 3 by one or two general matrix–vector pairs. All unimodular matrices and vectors used in Table 15.2.2.1 are listed explicitly in Table 15.2.2.2. The matrix–vector representation of an affine normalizer consists of all

(*continued on page* 894)

* In the previous editions, the symbols Z^1, Z^2 and Z^3 (z^1, z^2) were used.

Table 15.2.1.3. *Euclidean normalizers of the monoclinic and orthorhombic space groups*

For the restrictions of the cell metric of monoclinic space groups see text and Figs. 15.2.1.1 to 15.2.1.4. The symbols in parentheses following a space-group symbol refer to the location of the origin ('origin choice' in Part 7).

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
3	$P121$	General	$P^{1}12/m1$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0		$(4\cdot\infty)\cdot 2\cdot 1$
		$a>c, \beta=90°$	$P^{1}mmm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$\bar{x},y,z$	$(4\cdot\infty)\cdot 2\cdot 2$
		$2\cos\beta=-c/a, 90<\beta<120°$	$B^{1}mmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c},\ \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$x,y,x-z$	$(4\cdot\infty)\cdot 2\cdot 2$
		$a=c, 90<\beta<120°$	$B^{1}mmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	z,y,x	$(4\cdot\infty)\cdot 2\cdot 2$
		$a=c,\ \beta=90°$	$P^{1}4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$\bar{x},y,z;\ z,y,x$	$(4\cdot\infty)\cdot 2\cdot 4$
		$a=c,\ \beta=120°$	$P^{1}6/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$z,y,x;\ \bar{x}+z,y,z$	$(4\cdot\infty)\cdot 2\cdot 6$
3	$P112$	General	$P^{1}112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c},$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0		$(4\cdot\infty)\cdot 2\cdot 1$
		$a<b,\ \gamma=90°$	$P^{1}mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$\bar{x},y,z$	$(4\cdot\infty)\cdot 2\cdot 2$
		$2\cos\gamma=-a/b, 90<\gamma<120°$	$C^{1}mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$\bar{x}+y,y,z$	$(4\cdot\infty)\cdot 2\cdot 2$
		$a=b, 90<\gamma<120°$	$C^{1}mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	y,x,z	$(4\cdot\infty)\cdot 2\cdot 2$
		$a=b,\ \gamma=90°$	$P^{1}4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$\bar{x},y,z;\ y,x,z$	$(4\cdot\infty)\cdot 2\cdot 4$
		$a=b,\ \gamma=120°$	$P^{1}6/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$y,x,z;\ x,x-y,z$	$(4\cdot\infty)\cdot 2\cdot 6$
4	$P12_{1}1$	General	$P^{1}12/m1$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0		$(4\cdot\infty)\cdot 2\cdot 1$
		$a>c,\ \beta=90°$	$P^{1}mmm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$\bar{x},y,z$	$(4\cdot\infty)\cdot 2\cdot 2$
		$2\cos\beta=-c/a, 90<\beta<120°$	$B^{1}mmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$x,y,x-z$	$(4\cdot\infty)\cdot 2\cdot 2$
		$a=c, 90<\beta<120°$	$B^{1}mmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	z,y,x	$(4\cdot\infty)\cdot 2\cdot 2$
		$a=c,\ \beta=90°$	$P^{1}4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$\bar{x},y,z;\ z,y,x$	$(4\cdot\infty)\cdot 2\cdot 4$
		$a=c,\ \beta=120°$	$P^{1}6/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$z,y,x;\ \bar{x}+z,y,z$	$(4\cdot\infty)\cdot 2\cdot 6$
4	$P112_{1}$	General	$P^{1}112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0		$(4\cdot\infty)\cdot 2\cdot 1$
		$a<b,\ \gamma=90°$	$P^{1}mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$\bar{x},y,z$	$(4\cdot\infty)\cdot 2\cdot 2$
		$2\cos\gamma=-a/b, 90<\gamma<120°$	$C^{1}mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$\bar{x}+y,y,z$	$(4\cdot\infty)\cdot 2\cdot 2$
		$a=b, 90<\gamma<120°$	$C^{1}mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	y,x,z	$(4\cdot\infty)\cdot 2\cdot 2$
		$a=b,\ \gamma=90°$	$P^{1}4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$\bar{x},y,z;\ y,x,z$	$(4\cdot\infty)\cdot 2\cdot 4$
		$a=b,\ \gamma=120°$	$P^{1}6/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$y,x,z;\ x,x-y,z$	$(4\cdot\infty)\cdot 2\cdot 6$
5	$C121$	General	$P^{1}12/m1$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0		$(2\cdot\infty)\cdot 2\cdot 1$
		$\beta=90°$	$P^{1}mmm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$\bar{x},y,z$	$(2\cdot\infty)\cdot 2\cdot 2$
		$\cos\beta=-c/a, 90<\beta<135°$	$P^{1}mmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$x,y,2x-z$	$(2\cdot\infty)\cdot 2\cdot 2$
		$2\cos\beta=-a/c, 90<\beta<135°$	$B^{1}mmm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{a}+\mathbf{c}$	$0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$\bar{x}+z,y,z$	$(2\cdot\infty)\cdot 2\cdot 2$
		$a=c\sqrt{2}, \beta=135°$	$P^{1}4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{c}, \varepsilon\mathbf{b}$	$0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$x,y,2x-z;\ \bar{x}+z,y,z$	$(2\cdot\infty)\cdot 2\cdot 4$
5	$A121$	General	$P^{1}12/m1$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0$	0, 0, 0		$(2\cdot\infty)\cdot 2\cdot 1$
		$\beta=90°$	$P^{1}mmm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0$	0, 0, 0	$\bar{x},y,z$	$(2\cdot\infty)\cdot 2\cdot 2$
		$\cos\beta=-a/c, 90<\beta<135°$	$P^{1}mmm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}(\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0;\ 0,s,0$	0, 0, 0	$\bar{x}+2z,y,z$	$(2\cdot\infty)\cdot 2\cdot 2$
		$2\cos\beta=-c/a, 90<\beta<135°$	$B^{1}mmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0$	0, 0, 0	$x,y,x-z$	$(2\cdot\infty)\cdot 2\cdot 2$
		$c=a\sqrt{2}, \beta=135°$	$P^{1}4/mmm$	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}$	$\frac{1}{2},0,0;\ 0,s,0$	0, 0, 0	$x,y,x-z;\ \bar{x}+2z,y,z$	$(2\cdot\infty)\cdot 2\cdot 4$
5	$I121$	General	$P^{1}12/m1$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0$	0, 0, 0		$(2\cdot\infty)\cdot 2\cdot 1$
		$a>c,\ \beta=90°$	$P^{1}mmm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0$	0, 0, 0	$\bar{x},y,z$	$(2\cdot\infty)\cdot 2\cdot 2$

Table 15.2.1.3. *Euclidean normalizers of the monoclinic and orthorhombic space groups* (*cont.*)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
		$\cos\beta = -c/a, 90 < \beta < 180°$	P^1mmm	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0$	$0,0,0$	$x,y,2x-z$	$(2\cdot\infty)\cdot 2\cdot 2$
		$a = c, 90 < \beta < 180°$	B^1mmm	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0;\ 0,s,0$	$0,0,0$	z,y,x	$(2\cdot\infty)\cdot 2\cdot 2$
		$a = c,\ \beta = 90°$	P^14/mmm	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2},0,0;\ 0,s,0$	$0,0,0$	$\bar{x},y,z;\ z,y,x$	$(2\cdot\infty)\cdot 2\cdot 4$
5	$A112$	General	P^1112/m	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	$0,0,0$		$(2\cdot\infty)\cdot 2\cdot 1$
		$\gamma = 90°$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	$0,0,0$	$\bar{x},y,z$	$(2\cdot\infty)\cdot 2\cdot 2$
		$\cos\gamma = -a/b, 90 < \gamma < 135°$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	$0,0,0$	$\bar{x}+2y,y,z$	$(2\cdot\infty)\cdot 2\cdot 2$
		$2\cos\gamma = -b/a, 90 < \gamma < 135°$	C^1mmm	$\mathbf{a}+\frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	$0,0,0$	$x,x-y,z$	$(2\cdot\infty)\cdot 2\cdot 2$
		$b = a\sqrt{2}, \gamma = 135°$	P^14/mmm	$-\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	$0,0,0$	$\bar{x}+2y,y,z;\ x,x-y,z$	$(2\cdot\infty)\cdot 2\cdot 4$
5	$B112$	General	P^1112/m	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$		$(2\cdot\infty)\cdot 2\cdot 1$
		$\gamma = 90°$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$	$\bar{x},y,z$	$(2\cdot\infty)\cdot 2\cdot 2$
		$\cos\gamma = -b/a, 90 < \gamma < 135°$	P^1mmm	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$	$x,2x-y,z$	$(2\cdot\infty)\cdot 2\cdot 2$
		$2\cos\gamma = -a/b, 90 < \gamma < 135°$	C^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \varepsilon\mathbf{c}$	$0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$	$\bar{x}+y,y,z$	$(2\cdot\infty)\cdot 2\cdot 2$
		$a = b\sqrt{2}, \gamma = 135°$	P^14/mmm	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$	$x,2x-y,z;\ \bar{x}+y,y,z$	$(2\cdot\infty)\cdot 2\cdot 4$
5	$I112$	General	P^1112/m	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	$0,0,0$		$(2\cdot\infty)\cdot 2\cdot 1$
		$a < b,\ \gamma = 90°$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	$0,0,0$	$\bar{x},y,z$	$(2\cdot\infty)\cdot 2\cdot 2$
		$\cos\gamma = -a/b, 90 < \gamma < 180°$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	$0,0,0$	$\bar{x}+2y,y,z$	$(2\cdot\infty)\cdot 2\cdot 2$
		$a = b, 90 < \gamma < 180°$	C^1mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	$0,0,0$	y,x,z	$(2\cdot\infty)\cdot 2\cdot 2$
		$a = b,\ \gamma = 90°$	P^14/mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	$0,0,0$	$\bar{x},y,z;\ y,x,z$	$(2\cdot\infty)\cdot 2\cdot 4$
6	$P1m1$	General	$P^212/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$		$(2\cdot\infty^2)\cdot 2\cdot 1$
		$a > c,\ \beta = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$	$\bar{x},y,z$	$(2\cdot\infty^2)\cdot 2\cdot 2$
		$2\cos\beta = -c/a, 90 < \beta < 120°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\frac{1}{2}\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$	$x,y,x-z$	$(2\cdot\infty^2)\cdot 2\cdot 2$
		$a = c, 90 < \beta < 120°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2(-\mathbf{a}+\mathbf{c})$	$r,0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$	z,y,x	$(2\cdot\infty^2)\cdot 2\cdot 2$
		$a = c,\ \beta = 90°$	P^24/mmm	$\varepsilon\mathbf{c}, \varepsilon\mathbf{a}, \frac{1}{2}\mathbf{b}$	$r,0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$	$\bar{x},y,z;\ z,y,x$	$(2\cdot\infty^2)\cdot 2\cdot 4$
		$a = c,\ \beta = 120°$	P^26/mmm	$\varepsilon\mathbf{c}, \varepsilon\mathbf{a}, \frac{1}{2}\mathbf{b}$	$r,0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$	$z,y,x;\ \bar{x}+z,y,z$	$(2\cdot\infty^2)\cdot 2\cdot 6$
6	$P11m$	General	P^2112/m	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	$0,0,0$		$(2\cdot\infty^2)\cdot 2\cdot 1$
		$a < b,\ \gamma = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	$0,0,0$	$\bar{x},y,z$	$(2\cdot\infty^2)\cdot 2\cdot 2$
		$2\cos\gamma = -a/b, 90 < \gamma < 120°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r,0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	$0,0,0$	$\bar{x}+y,y,z$	$(2\cdot\infty^2)\cdot 2\cdot 2$
		$a = b, 90 < \gamma < 120°$	P^2mmm	$\varepsilon_1(\mathbf{a}-\mathbf{b}), \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r,0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	$0,0,0$	y,x,z	$(2\cdot\infty^2)\cdot 2\cdot 2$
		$a = b, \gamma = 90°$	P^24/mmm	$\varepsilon\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	$0,0,0$	$\bar{x},y,z;\ y,x,z$	$(2\cdot\infty^2)\cdot 2\cdot 4$
		$a = b,\ \gamma = 120°$	P^26/mmm	$\varepsilon\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	$0,0,0$	$y,x,z;\ x,x-y,z$	$(2\cdot\infty^2)\cdot 2\cdot 6$
7	$P1c1$	General	$P^212/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$		$(2\cdot\infty^2)\cdot 2\cdot 1$
		$\beta = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$	$\bar{x},y,z$	$(2\cdot\infty^2)\cdot 2\cdot 2$
		$\cos\beta = -a/c, 90 < \beta < 135°$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2(\mathbf{a}+\mathbf{c})$	$r,0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$	$\bar{x}+2z,y,z$	$(2\cdot\infty^2)\cdot 2\cdot 2$
		$2\cos\beta = -c/a, 90 < \beta < 135°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\frac{1}{2}\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$	$x,y,x-z$	$(2\cdot\infty^2)\cdot 2\cdot 2$
		$c = a\sqrt{2}, \beta = 135°$	P^24/mmm	$\varepsilon\mathbf{a}, -\varepsilon(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}$	$r,0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$	$x,y,x-z;\ \bar{x}+2z,y,z$	$(2\cdot\infty^2)\cdot 2\cdot 4$
7	$P1n1$	General	$P^212/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$		$(2\cdot\infty^2)\cdot 2\cdot 1$
		$a > c,\ \beta = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$	$\bar{x},y,z$	$(2\cdot\infty^2)\cdot 2\cdot 2$
		$\cos\beta = -c/a, 90 < \beta < 180°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	$0,0,0$	$x,y,2x-z$	$(2\cdot\infty^2)\cdot 2\cdot 2$

Table 15.2.1.3. *Euclidean normalizers of the monoclinic and orthorhombic space groups* (*cont.*)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
		$a = c, 90 < \beta < 180°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2(-\mathbf{a}+\mathbf{c})$	$r, 0, 0; 0, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$	z, y, x	$(2 \cdot \infty^2) \cdot 2 \cdot 2$
		$a = c,\ \beta = 90°$	P^24/mmm	$\varepsilon\mathbf{c}, \varepsilon\mathbf{a}, \frac{1}{2}\mathbf{b}$	$r, 0, 0; 0, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z; z, y, x$	$(2 \cdot \infty^2) \cdot 2 \cdot 4$
7	$P1a1$	General	$P^212/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0; 0, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$		$(2 \cdot \infty^2) \cdot 2 \cdot 1$
		$\beta = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0; 0, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z$	$(2 \cdot \infty^2) \cdot 2 \cdot 2$
		$\cos\beta = -c/a, 90 < \beta < 135°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0; 0, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$	$x, y, 2x - z$	$(2 \cdot \infty^2) \cdot 2 \cdot 2$
		$2\cos\beta = -a/c, 90 < \beta < 135°$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{c})$	$r, 0, 0; 0, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$	$\bar{x} + z, y, z$	$(2 \cdot \infty^2) \cdot 2 \cdot 2$
		$a = c\sqrt{2}, \beta = 135°$	P^24/mmm	$-\varepsilon(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{c}, \frac{1}{2}\mathbf{b}$	$r, 0, 0; 0, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$	$x, y, 2x - z; \bar{x} + z, y, z$	$(2 \cdot \infty^2) \cdot 2 \cdot 4$
7	$P11a$	General	P^2112/m	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$(2 \cdot \infty^2) \cdot 2 \cdot 1$
		$\gamma = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}, y, z$	$(2 \cdot \infty^2) \cdot 2 \cdot 2$
		$\cos\gamma = -b/a, 90 < \gamma < 135°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{b}), \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	$x, 2x - y, z$	$(2 \cdot \infty^2) \cdot 2 \cdot 2$
		$2\cos\gamma = -a/b, 90 < \gamma < 135°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x} + y, y, z$	$(2 \cdot \infty^2) \cdot 2 \cdot 2$
		$a = b\sqrt{2}, \gamma = 135°$	P^24/mmm	$\varepsilon\mathbf{b}, -\varepsilon(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	$x, 2x - y, z; x - y, \bar{y}, z$	$(2 \cdot \infty^2) \cdot 2 \cdot 4$
7	$P11n$	General	P^2112/m	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$(2 \cdot \infty^2) \cdot 2 \cdot 1$
		$a < b,\ \gamma = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}, y, z$	$(2 \cdot \infty^2) \cdot 2 \cdot 2$
		$\cos\gamma = -a/b, 90 < \gamma < 180°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x} + 2y, y, z$	$(2 \cdot \infty^2) \cdot 2 \cdot 2$
		$a = b, 90 < \gamma < 180°$	P^2mmm	$\varepsilon_1(\mathbf{a}-\mathbf{b}), \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	y, x, z	$(2 \cdot \infty^2) \cdot 2 \cdot 2$
		$a = b,\ \gamma = 90°$	P^24/mmm	$\varepsilon\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}, y, z; y, x, z$	$(2 \cdot \infty^2) \cdot 2 \cdot 4$
7	$P11b$	General	P^2112/m	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$(2 \cdot \infty^2) \cdot 2 \cdot 1$
		$\gamma = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}, y, z$	$(2 \cdot \infty^2) \cdot 2 \cdot 2$
		$\cos\gamma = -a/b, 90 < \gamma < 135°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x} + 2y, y, z$	$(2 \cdot \infty^2) \cdot 2 \cdot 2$
		$2\cos\gamma = -b/a, 90 < \gamma < 135°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\frac{1}{2}\mathbf{b}), \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	$x, x - y, z$	$(2 \cdot \infty^2) \cdot 2 \cdot 2$
		$b = a\sqrt{2}, \gamma = 135°$	P^24/mmm	$-\varepsilon(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{a}, \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x} + 2y, y, z; x, x - y, z$	$(2 \cdot \infty^2) \cdot 2 \cdot 4$
8	$C1m1$	General	$P^212/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0; 0, 0, t$	$0, 0, 0$		$\infty^2 \cdot 2 \cdot 1$
		$\beta = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0; 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z$	$\infty^2 \cdot 2 \cdot 2$
		$\cos\beta = -c/a, 90 < \beta < 135°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0; 0, 0, t$	$0, 0, 0$	$x, y, 2x - z$	$\infty^2 \cdot 2 \cdot 2$
		$2\cos\beta = -a/c, 90 < \beta < 135°$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{c})$	$r, 0, 0; 0, 0, t$	$0, 0, 0$	$\bar{x} + z, y, z$	$\infty^2 \cdot 2 \cdot 2$
		$a = c\sqrt{2}, \beta = 135°$	P^24/mmm	$-\varepsilon(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{c}, \frac{1}{2}\mathbf{b}$	$r, 0, 0; 0, 0, t$	$0, 0, 0$	$x, y, 2x - z; \bar{x} + z, y, z$	$\infty^2 \cdot 2 \cdot 4$
8	$A1m1$	General	$P^212/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0; 0, 0, t$	$0, 0, 0$		$\infty^2 \cdot 2 \cdot 1$
		$\beta = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0; 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z$	$\infty^2 \cdot 2 \cdot 2$
		$\cos\beta = -a/c, 90 < \beta < 135°$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2(\mathbf{a}+\mathbf{c})$	$r, 0, 0; 0, 0, t$	$0, 0, 0$	$\bar{x} + 2z, y, z$	$\infty^2 \cdot 2 \cdot 2$
		$2\cos\beta = -c/a, 90 < \beta < 135°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\frac{1}{2}\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0; 0, 0, t$	$0, 0, 0$	$x, y, x - z$	$\infty^2 \cdot 2 \cdot 2$
		$c = a\sqrt{2}, \beta = 135°$	P^24/mmm	$\varepsilon\mathbf{a}, -\varepsilon(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}$	$r, 0, 0; 0, 0, t$	$0, 0, 0$	$x, y, x - z; \bar{x} + 2z, y, z$	$\infty^2 \cdot 2 \cdot 4$
8	$I1m1$	General	$P^212/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0; 0, 0, t$	$0, 0, 0$		$\infty^2 \cdot 2 \cdot 1$
		$a > c, \beta = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0; 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z$	$\infty^2 \cdot 2 \cdot 2$
		$\cos\beta = -c/a, 90 < \beta < 180°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0; 0, 0, t$	$0, 0, 0$	$x, y, 2x - z$	$\infty^2 \cdot 2 \cdot 2$
		$a = c, 90 < \beta < 180°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2(-\mathbf{a}+\mathbf{c})$	$r, 0, 0; 0, 0, t$	$0, 0, 0$	z, y, x	$\infty^2 \cdot 2 \cdot 2$
		$a = c, \beta = 90°$	P^24/mmm	$\varepsilon_1\mathbf{c}, \varepsilon_2\mathbf{a}, \frac{1}{2}\mathbf{b}$	$r, 0, 0; 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z; z, y, x$	$\infty^2 \cdot 2 \cdot 4$

Table 15.2.1.3. *Euclidean normalizers of the monoclinic and orthorhombic space groups* (*cont.*)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
8	$A11m$	General	$P^2 112/m$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$		$\infty^2\cdot 2\cdot 1$
		$\gamma = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$\bar{x},y,z$	$\infty^2\cdot 2\cdot 2$
		$\cos\gamma = -a/b, 90 < \gamma < 135°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$\bar{x}+2y,y,z$	$\infty^2\cdot 2\cdot 2$
		$2\cos\gamma = -b/a, 90 < \gamma < 135°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\frac{1}{2}\mathbf{b}), \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$x,x-y,z$	$\infty^2\cdot 2\cdot 2$
		$b = a\sqrt{2}, \gamma = 135°$	$P^2 4/mmm$	$-\varepsilon(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{a}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$\bar{x}+2y,y,z; x,x-y,z$	$\infty^2\cdot 2\cdot 4$
8	$B11m$	General	$P^2 112/m$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$		$\infty^2\cdot 2\cdot 1$
		$\gamma = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$\bar{x},y,z$	$\infty^2\cdot 2\cdot 2$
		$\cos\gamma = -b/a, 90 < \gamma < 135°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{b}), \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$x,2x-y,z$	$\infty^2\cdot 2\cdot 2$
		$2\cos\gamma = -a/b, 90 < \gamma < 135°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$\bar{x}+y,y,z$	$\infty^2\cdot 2\cdot 2$
		$a = b\sqrt{2}, \gamma = 135°$	$P^2 4/mmm$	$\varepsilon_2\mathbf{b}, -\varepsilon(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$x,2x-y,z; \bar{x}+y,y,z$	$\infty^2\cdot 2\cdot 4$
8	$I11m$	General	$P^2 112/m$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$		$\infty^2\cdot 2\cdot 1$
		$a < b, \gamma = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$\bar{x},y,z$	$\infty^2\cdot 2\cdot 2$
		$\cos\gamma = -a/b, 90 < \gamma < 180°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$\bar{x}+2y,y,z$	$\infty^2\cdot 2\cdot 2$
		$a = b, 90 < \gamma < 180°$	P^2mmm	$\varepsilon_1(\mathbf{a}-\mathbf{b}), \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	y,x,z	$\infty^2\cdot 2\cdot 2$
		$a = b, \gamma = 90°$	$P^2 4/mmm$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$\bar{x},y,z; y,x,z$	$\infty^2\cdot 2\cdot 4$
9	$C1c1$	General	$P^2 12/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;0,0,t$	$0,0,0$		$\infty^2\cdot 2\cdot 1$
		$\beta = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;0,0,t$	$0,0,0$	$\bar{x},y,z$	$\infty^2\cdot 2\cdot 2$
		$\cos\beta = -c/a, 90 < \beta < 135°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;0,0,t$	$0,0,0$	$x,y,2x-z$	$\infty^2\cdot 2\cdot 2$
		$2\cos\beta = -a/c, 90 < \beta < 135°$	P^2bmb	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{c})$	$r,0,0;0,0,t$	$0,0,0$	$\bar{x}+z,y+\frac{1}{4},z$	$\infty^2\cdot 2\cdot 2$
		$a = c\sqrt{2}, \beta = 135°$	$P^2 4_2/mmc$	$-\varepsilon(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{c}, \frac{1}{2}\mathbf{b}$	$r,0,0;0,0,t$	$0,0,0$	$x,y,2x-z; \bar{x}+z,y+\frac{1}{4},z$	$\infty^2\cdot 2\cdot 4$
9	$A1n1$	General	$P^2 12/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;0,0,t$	$0,0,0$		$\infty^2\cdot 2\cdot 1$
		$\beta = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;0,0,t$	$0,0,0$	$\bar{x},y,z$	$\infty^2\cdot 2\cdot 2$
		$\cos\beta = -a/c, 90 < \beta < 135°$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2(\mathbf{a}+\mathbf{c})$	$r,0,0;0,0,t$	$0,0,0$	$\bar{x}+2z,y,z$	$\infty^2\cdot 2\cdot 2$
		$2\cos\beta = -c/a, 90 < \beta < 135°$	P^2bmb	$\varepsilon_1(\mathbf{a}+\frac{1}{2}\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;0,0,t$	$0,0,0$	$x,y+\frac{1}{4},x-z$	$\infty^2\cdot 2\cdot 2$
		$c = a\sqrt{2}, \beta = 135°$	$P^2 4_2/mmc$	$\varepsilon\mathbf{a}, -\varepsilon(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}$	$r,0,0;0,0,t$	$0,0,0$	$x,y+\frac{1}{4},x-z; \bar{x}+2z,y,z$	$\infty^2\cdot 2\cdot 4$
9	$I1a1$	General	$P^2 12/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;0,0,t$	$0,0,0$		$\infty^2\cdot 2\cdot 1$
		$a > c, \beta = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;0,0,t$	$0,0,0$	$\bar{x},y,z$	$\infty^2\cdot 2\cdot 2$
		$\cos\beta = -c/a, 90 < \beta < 180°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r,0,0;0,0,t$	$0,0,0$	$x,y,2x-z$	$\infty^2\cdot 2\cdot 2$
		$a = c, 90 < \beta < 180°$	P^2bmb	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2(-\mathbf{a}+\mathbf{c})$	$r,0,0;0,0,t$	$0,0,0$	$z,y+\frac{1}{4},x$	$\infty^2\cdot 2\cdot 2$
		$a = c, \beta = 90°$	$P^2 4_2/mmc$	$\varepsilon\mathbf{c}, \varepsilon\mathbf{a}, \frac{1}{2}\mathbf{b}$	$r,0,0;0,0,t$	$0,0,0$	$\bar{x},y,z; z,y+\frac{1}{4},x$	$\infty^2\cdot 2\cdot 4$
9	$A11a$	General	$P^2 112/m$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$		$\infty^2\cdot 2\cdot 1$
		$\gamma = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$\bar{x},y,z$	$\infty^2\cdot 2\cdot 2$
		$\cos\gamma = -a/b, 90 < \gamma < 135°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$\bar{x}+2y,y,z$	$\infty^2\cdot 2\cdot 2$
		$2\cos\gamma = -b/a, 90 < \gamma < 135°$	P^2ccm	$\varepsilon_1(\mathbf{a}+\frac{1}{2}\mathbf{b}), \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$x,x-y,z+\frac{1}{4}$	$\infty^2\cdot 2\cdot 2$
		$b = a\sqrt{2}, \gamma = 135°$	$P^2 4_2/mmc$	$-\varepsilon(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{a}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$\bar{x}+2y,y,z; x,x-y,z+\frac{1}{4}$	$\infty^2\cdot 2\cdot 4$
9	$B11n$	General	$P^2 112/m$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$		$\infty^2\cdot 2\cdot 1$
		$\gamma = 90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$\bar{x},y,z$	$\infty^2\cdot 2\cdot 2$
		$\cos\gamma = -b/a, 90 < \gamma < 135°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{b}), \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0;0,s,0$	$0,0,0$	$x,2x-y,z$	$\infty^2\cdot 2\cdot 2$

Table 15.2.1.3. *Euclidean normalizers of the monoclinic and orthorhombic space groups* (*cont.*)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
		$2\cos\gamma=-a/b, 90<\gamma<135°$	P^2ccm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r,0,0; 0,s,0$	$0,0,0$	$\bar{x}+y,y,z+\frac{1}{4}$	$\infty^2\cdot 2\cdot 2$
		$a=b\sqrt{2}, \gamma=135°$	P^24_2/mmc	$\varepsilon\mathbf{b}, -\varepsilon(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r,0,0; 0,s,0$	$0,0,0$	$x,2x-y,z; \bar{x}+y,y,z+\frac{1}{4}$	$\infty^2\cdot 2\cdot 4$
9	$I11b$	General	P^2112/m	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0; 0,s,0$	$0,0,0$		$\infty^2\cdot 2\cdot 1$
		$a<b, \gamma=90°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0; 0,s,0$	$0,0,0$	$\bar{x},y,z$	$\infty^2\cdot 2\cdot 2$
		$\cos\gamma=-a/b, 90<\gamma<180°$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r,0,0; 0,s,0$	$0,0,0$	$\bar{x}+2y,y,z$	$\infty^2\cdot 2\cdot 2$
		$a=b, 90<\gamma<180°$	P^2ccm	$\varepsilon_1(\mathbf{a}-\mathbf{b}), \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r,0,0; 0,s,0$	$0,0,0$	$y,x,z+\frac{1}{4}$	$\infty^2\cdot 2\cdot 2$
		$a=b, \gamma=90°$	P^24_2/mmc	$\varepsilon\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r,0,0; 0,s,0$	$0,0,0$	$\bar{x},y,z; y,x,z+\frac{1}{4}$	$\infty^2\cdot 2\cdot 4$
10	$P12/m1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
		$a>c, \beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x},y,z$	$8\cdot 1\cdot 2$
		$2\cos\beta=-c/a, 90<\beta<120°$	$Bmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$x,y,x-z$	$8\cdot 1\cdot 2$
		$a=c, 90<\beta<120°$	$Bmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		z,y,x	$8\cdot 1\cdot 2$
		$a=c, \beta=90°$	$P4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x},y,z; z,y,x$	$8\cdot 1\cdot 4$
		$a=c, \beta=120°$	$P6/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$z,y,x; \bar{x}+z,y,z$	$8\cdot 1\cdot 6$
10	$P112/m$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
		$a<b, \gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x},y,z$	$8\cdot 1\cdot 2$
		$2\cos\gamma=-a/b, 90<\gamma<120°$	$Cmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x}+y,y,z$	$8\cdot 1\cdot 2$
		$a=b, 90<\gamma<120°$	$Cmmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		y,x,z	$8\cdot 1\cdot 2$
		$a=b, \gamma=90°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x},y,z; y,x,z$	$8\cdot 1\cdot 4$
		$a=b, \gamma=120°$	$P6/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$y,x,z; x,x-y,z$	$8\cdot 1\cdot 6$
11	$P12_1/m1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
		$a>c, \beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x},y,z$	$8\cdot 1\cdot 2$
		$2\cos\beta=-c/a, 90<\beta<120°$	$Bmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$x,y,x-z$	$8\cdot 1\cdot 2$
		$a=c, 90<\beta<120°$	$Bmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		z,y,x	$8\cdot 1\cdot 2$
		$a=c, \beta=90°$	$P4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x},y,z; z,y,x$	$8\cdot 1\cdot 4$
		$a=c, \beta=120°$	$P6/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$z,y,x; \bar{x}+z,y,z$	$8\cdot 1\cdot 6$
11	$P112_1/m$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
		$a<b, \gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x},y,z$	$8\cdot 1\cdot 2$
		$2\cos\gamma=-a/b, 90<\gamma<120°$	$Cmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x}+y,y,z$	$8\cdot 1\cdot 2$
		$a=b, 90<\gamma<120°$	$Cmmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		y,x,z	$8\cdot 1\cdot 2$
		$a=b, \gamma=90°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x},y,z; y,x,z$	$8\cdot 1\cdot 4$
		$a=b, \gamma=120°$	$P6/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$y,x,z; x,x-y,z$	$8\cdot 1\cdot 6$
12	$C12/m1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
		$\beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$		$\bar{x},y,z$	$4\cdot 1\cdot 2$
		$\cos\beta=-c/a, 90<\beta<135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$		$x,y,2x-z$	$4\cdot 1\cdot 2$
		$2\cos\beta=-a/c, 90<\beta<135°$	$Bmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a}+\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$		$\bar{x}+z,y,z$	$4\cdot 1\cdot 2$
		$a=c\sqrt{2}, \beta=135°$	$P4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$		$x,y,2x-z; \bar{x}+z,y,z$	$4\cdot 1\cdot 4$
12	$A12/m1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$			$4\cdot 1\cdot 1$
		$\beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x},y,z$	$4\cdot 1\cdot 2$

Table 15.2.1.3. *Euclidean normalizers of the monoclinic and orthorhombic space groups* (*cont.*)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
		$\cos\beta = -a/c, 90 < \beta < 135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}(\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}+2z, y, z$	$4\cdot1\cdot2$
		$2\cos\beta = -c/a, 90 < \beta < 135°$	$Bmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$x, y, x-z$	$4\cdot1\cdot2$
		$c = a\sqrt{2}, \beta = 135°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$x, y, x-z; \bar{x}+2z, y, z$	$4\cdot1\cdot4$
12	$I12/m1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$			$4\cdot1\cdot1$
		$a > c, \beta = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}, y, z$	$4\cdot1\cdot2$
		$\cos\beta = -c/a, 90 < \beta < 180°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$x, y, 2x-z$	$4\cdot1\cdot2$
		$a = c, 90 < \beta < 180°$	$Bmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		z, y, x	$4\cdot1\cdot2$
		$a = c, \beta = 90°$	$P4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}, y, z; z, y, x$	$4\cdot1\cdot4$
12	$A112/m$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$			$4\cdot1\cdot1$
		$\gamma = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}, y, z$	$4\cdot1\cdot2$
		$\cos\gamma = -a/b, 90 < \gamma < 135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}+2y, y, z$	$4\cdot1\cdot2$
		$2\cos\gamma = -b/a, 90 < \gamma < 135°$	$Cmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$x, x-y, z$	$4\cdot1\cdot2$
		$b = a\sqrt{2}, \gamma = 135°$	$P4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}+2y, y, z; x, x-y, z$	$4\cdot1\cdot4$
12	$B112/m$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$			$4\cdot1\cdot1$
		$\gamma = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}, y, z$	$4\cdot1\cdot2$
		$\cos\gamma = -b/a, 90 < \gamma < 135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$x, 2x-y, z$	$4\cdot1\cdot2$
		$2\cos\gamma = -a/b, 90 < \gamma < 135°$	$Cmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}+y, y, z$	$4\cdot1\cdot2$
		$a = b\sqrt{2}, \gamma = 135°$	$P4/mmm$	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$x, 2x-y, z; \bar{x}+y, y, z$	$4\cdot1\cdot4$
12	$I112/m$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$			$4\cdot1\cdot1$
		$a < b, \gamma = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}, y, z$	$4\cdot1\cdot2$
		$\cos\gamma = -a/b, 90 < \gamma < 180°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}+2y, y, z$	$4\cdot1\cdot2$
		$a = b, 90 < \gamma < 180°$	$Cmmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		y, x, z	$4\cdot1\cdot2$
		$a = b, \gamma = 90°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}, y, z; y, x, z$	$4\cdot1\cdot4$
13	$P12/c1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8\cdot1\cdot1$
		$\beta = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x}, y, z$	$8\cdot1\cdot2$
		$\cos\beta = -a/c, 90 < \beta < 135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}(\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x}+2z, y, z$	$8\cdot1\cdot2$
		$2\cos\beta = -c/a, 90 < \beta < 135°$	$Bmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$x, y, x-z$	$8\cdot1\cdot2$
		$c = a\sqrt{2}, \beta = 135°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$x, y, x-z; \bar{x}+2z, y, z$	$8\cdot1\cdot4$
13	$P12/n1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8\cdot1\cdot1$
		$a > c, \beta = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x}, y, z$	$8\cdot1\cdot2$
		$\cos\beta = -c/a, 90 < \beta < 180°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$x, y, 2x-z$	$8\cdot1\cdot2$
		$a = c, 90 < \beta < 180°$	$Bmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		z, y, x	$8\cdot1\cdot2$
		$a = c, \beta = 90°$	$P4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x}, y, z; z, y, x$	$8\cdot1\cdot4$
13	$P12/a1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8\cdot1\cdot1$
		$\beta = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x}, y, z$	$8\cdot1\cdot2$
		$\cos\beta = -c/a, 90 < \beta < 135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$x, y, 2x-z$	$8\cdot1\cdot2$
		$2\cos\beta = -a/c, 90 < \beta < 135°$	$Bmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a}+\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x}+z, y, z$	$8\cdot1\cdot2$
		$a = c\sqrt{2}, \beta = 135°$	$P4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$x, y, 2x-z; \bar{x}+z, y, z$	$8\cdot1\cdot4$

Table 15.2.1.3. *Euclidean normalizers of the monoclinic and orthorhombic space groups* (*cont.*)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
13	$P112/a$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$\gamma = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	$8 \cdot 1 \cdot 2$
		$\cos\gamma = -b/a, 90 < \gamma < 135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, 2x-y, z$	$8 \cdot 1 \cdot 2$
		$2\cos\gamma = -a/b, 90 < \gamma < 135°$	$Cmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}+y, y, z$	$8 \cdot 1 \cdot 2$
		$a = b\sqrt{2}, \gamma = 135°$	$P4/mmm$	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, 2x-y, z; \bar{x}+y, y, z$	$8 \cdot 1 \cdot 4$
13	$P112/n$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$a < b, \gamma = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	$8 \cdot 1 \cdot 2$
		$\cos\gamma = -a/b, 90 < \gamma < 180°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}+2y, y, z$	$8 \cdot 1 \cdot 2$
		$a = b, 90 < \gamma < 180°$	$Cmmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		y, x, z	$8 \cdot 1 \cdot 2$
		$a = b, \gamma = 90°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}, y, z; y, x, z$	$8 \cdot 1 \cdot 4$
13	$P112/b$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$\gamma = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	$8 \cdot 1 \cdot 2$
		$\cos\gamma = -a/b, 90 < \gamma < 135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}+2y, y, z$	$8 \cdot 1 \cdot 2$
		$2\cos\gamma = -b/a, 90 < \gamma < 135°$	$Cmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, x-y, z$	$8 \cdot 1 \cdot 2$
		$b = a\sqrt{2}, \gamma = 135°$	$P4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}+2y, y, z; x, x-y, z$	$8 \cdot 1 \cdot 4$
14	$P12_1/c1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$\beta = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	$8 \cdot 1 \cdot 2$
		$\cos\beta = -a/c, 90 < \beta < 135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}(\mathbf{a}+\mathbf{c})$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}+2z, y, z$	$8 \cdot 1 \cdot 2$
		$2\cos\beta = -c/a, 90 < \beta < 135°$	$Bmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, y, x-z$	$8 \cdot 1 \cdot 2$
		$c = a\sqrt{2}, \beta = 135°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, y, x-z; \bar{x}+2z, y, z$	$8 \cdot 1 \cdot 4$
14	$P12_1/n1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$a > c, \beta = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	$8 \cdot 1 \cdot 2$
		$\cos\beta = -c/a, 90 < \beta < 180°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, y, 2x-z$	$8 \cdot 1 \cdot 2$
		$a = c, 90 < \beta < 180°$	$Bmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		z, y, x	$8 \cdot 1 \cdot 2$
		$a = c, \beta = 90°$	$P4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}, y, z; z, y, x$	$8 \cdot 1 \cdot 4$
14	$P12_1/a1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$\beta = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	$8 \cdot 1 \cdot 2$
		$\cos\beta = -c/a, 90 < \beta < 135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, y, 2x-z$	$8 \cdot 1 \cdot 2$
		$2\cos\beta = -a/c, 90 < \beta < 135°$	$Bmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a}+\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}+z, y, z$	$8 \cdot 1 \cdot 2$
		$a = c\sqrt{2}, \beta = 135°$	$P4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, y, 2x-z; \bar{x}+z, y, z$	$8 \cdot 1 \cdot 4$
14	$P112_1/a$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$\gamma = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	$8 \cdot 1 \cdot 2$
		$\cos\gamma = -b/a, 90 < \gamma < 135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, 2x-y, z$	$8 \cdot 1 \cdot 2$
		$2\cos\gamma = -a/b, 90 < \gamma < 135°$	$Cmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}+y, y, z$	$8 \cdot 1 \cdot 2$
		$a = b\sqrt{2}, \gamma = 135°$	$P4/mmm$	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, 2x-y, z; \bar{x}+y, y, z$	$8 \cdot 1 \cdot 4$
14	$P112_1/n$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$a < b, \gamma = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	$8 \cdot 1 \cdot 2$
		$\cos\gamma = -a/b, 90 < \gamma < 180°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}+2y, y, z$	$8 \cdot 1 \cdot 2$

Table 15.2.1.3. *Euclidean normalizers of the monoclinic and orthorhombic space groups* (*cont.*)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
		$a = b, 90 < \gamma < 180°$	$Cmmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		y, x, z	$8 \cdot 1 \cdot 2$
		$a = b, \gamma = 90°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x}, y, z; y, x, z$	$8 \cdot 1 \cdot 4$
14	$P112_1/b$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$\gamma = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x}, y, z$	$8 \cdot 1 \cdot 2$
		$\cos\gamma = -a/b, 90 < \gamma < 135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x}+2y, y, z$	$8 \cdot 1 \cdot 2$
		$2\cos\gamma = -b/a, 90 < \gamma < 135°$	$Cmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$x, x-y, z$	$8 \cdot 1 \cdot 2$
		$b = a\sqrt{2}, \gamma = 135°$	$P4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		$\bar{x}+2y, y, z; x, x-y, z$	$8 \cdot 1 \cdot 4$
15	$C12/c1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$\beta = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$		$\bar{x}, y, z$	$4 \cdot 1 \cdot 2$
		$\cos\beta = -c/a, 90 < \beta < 135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$		$x, y, 2x-z$	$4 \cdot 1 \cdot 2$
		$2\cos\beta = -a/c, 90 < \beta < 135°$	$Bbmb\ (n2/mn)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a}+\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$		$\bar{x}+z+\frac{1}{4}, y+\frac{1}{4}, z$	$4 \cdot 1 \cdot 2$
		$a = c\sqrt{2}, \beta = 135°$	$P4_2/mmc\ (2/m2/mn)$	$-\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$		$x, y, 2x-z$; $\bar{x}+z+\frac{1}{4}, y+\frac{1}{4}, z$	$4 \cdot 1 \cdot 4$
15	$A12/n1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$			$4 \cdot 1 \cdot 1$
		$\beta = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}, y, z$	$4 \cdot 1 \cdot 2$
		$\cos\beta = -a/c, 90 < \beta < 135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}(\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}+2z, y, z$	$4 \cdot 1 \cdot 2$
		$2\cos\beta = -c/a, 90 < \beta < 135°$	$Bbmb\ (n2/mn)$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$x, y+\frac{1}{4}, x-z+\frac{1}{4}$	$4 \cdot 1 \cdot 2$
		$c = a\sqrt{2}, \beta = 135°$	$P4_2/mmc\ (2/m2/mn)$	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}+2z, y, z$; $x, y+\frac{1}{4}, x-z+\frac{1}{4}$	$4 \cdot 1 \cdot 4$
15	$I12/a1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$			$4 \cdot 1 \cdot 1$
		$a > c, \beta = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}, y, z$	$4 \cdot 1 \cdot 2$
		$\cos\beta = -c/a, 90 < \beta < 180°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$x, y, 2x-z$	$4 \cdot 1 \cdot 2$
		$a = c, 90 < \beta < 180°$	$Bbmb\ (n2/mn)$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$z+\frac{1}{4}, y+\frac{1}{4}, x+\frac{1}{4}$	$4 \cdot 1 \cdot 2$
		$a = c, \beta = 90°$	$P4_2/mmc\ (2/m2/mn)$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}, y, z; z+\frac{1}{4}, y+\frac{1}{4}, x+\frac{1}{4}$	$4 \cdot 1 \cdot 4$
15	$A112/a$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$			$4 \cdot 1 \cdot 1$
		$\gamma = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}, y, z$	$4 \cdot 1 \cdot 2$
		$\cos\gamma = -a/b, 90 < \gamma < 135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}+2y, y, z$	$4 \cdot 1 \cdot 2$
		$2\cos\gamma = -b/a, 90 < \gamma < 135°$	$Cccm\ (nn2/m)$	$\mathbf{a}+\frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$x, x-y+\frac{1}{4}, z+\frac{1}{4}$	$4 \cdot 1 \cdot 2$
		$b = a\sqrt{2}, \gamma = 135°$	$P4_2/mmc\ (2/m2/mn)$	$-\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}+2y, y, z; x, x-y+\frac{1}{4}$, $z+\frac{1}{4}$	$4 \cdot 1 \cdot 4$
15	$B112/n$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$			$4 \cdot 1 \cdot 1$
		$\gamma = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$x, \bar{y}, z$	$4 \cdot 1 \cdot 2$
		$\cos\gamma = -b/a, 90 < \gamma < 135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$x, 2x-y, z$	$4 \cdot 1 \cdot 2$
		$2\cos\gamma = -a/b, 90 < \gamma < 135°$	$Cccm\ (nn2/m)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}+y+\frac{1}{4}, y, z+\frac{1}{4}$	$4 \cdot 1 \cdot 2$
		$a = b\sqrt{2}, \gamma = 135°$	$P4_2/mmc\ (2/m2/mn)$	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$x, 2x-y, z$; $\bar{x}+y+\frac{1}{4}, y, z+\frac{1}{4}$	$4 \cdot 1 \cdot 4$
15	$I112/b$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$			$4 \cdot 1 \cdot 1$
		$a < b, \gamma = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}, y, z$	$4 \cdot 1 \cdot 2$

Table 15.2.1.3. *Euclidean normalizers of the monoclinic and orthorhombic space groups* (*cont.*)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
		$\cos\gamma = -a/b, 90 < \gamma < 180°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}+2y, y, z$	$4\cdot1\cdot2$
		$a = b, 90 < \gamma < 180°$	$Cccm$ $(nn2/m)$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$4\cdot1\cdot2$
		$a = b, \gamma = 90°$	$P4_2/mmc$ $(2/m2/mn)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$\bar{x}, y, z; y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$4\cdot1\cdot4$
16	$P222$	$a \neq b \neq c \neq a$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$	$0,0,0$		$8\cdot2\cdot1$
		$a = b \neq c$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$	$0,0,0$	y, x, z	$8\cdot2\cdot2$
		$a = b = c$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$	$0,0,0$	$z, x, y; y, x, z$	$8\cdot2\cdot6$
17	$P222_1$	$a \neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$	$0,0,0$		$8\cdot2\cdot1$
		$a = b$	$P4_2/mmc$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$	$0,0,0$	$y, x, z+\frac{1}{4}$	$8\cdot2\cdot2$
18	$P2_12_12$	$a \neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$	$0,0,0$		$8\cdot2\cdot1$
		$a = b$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$	$0,0,0$	y, x, z	$8\cdot2\cdot2$
19	$P2_12_12_1$	$a \neq b \neq c \neq a$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$	$0,0,0$		$8\cdot2\cdot1$
		$a = b \neq c$	$P4_2/mmc$ $(2/m2/mn)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$	$0,0,0$	$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$8\cdot2\cdot2$
		$a = b = c$	$Pm\bar{3}n$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$	$0,0,0$	$z, x, y; y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$8\cdot2\cdot6$
20	$C222_1$	$a \neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot2\cdot1$
		$a = b$	$P4_2/mmc$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$	$0,0,0$	$y, x, z+\frac{1}{4}$	$4\cdot2\cdot2$
21	$C222$	$a \neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot2\cdot1$
		$a = b$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$	$0,0,0$	y, x, z	$4\cdot2\cdot2$
22	$F222$	$a \neq b \neq c \neq a$	$Immm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$0,0,0$		$4\cdot2\cdot1$
		$a = b \neq c$	$I4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$0,0,0$	y, x, z	$4\cdot2\cdot2$
		$a = b = c$	$Im\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$0,0,0$	$z, x, y; y, x, z$	$4\cdot2\cdot6$
23	$I222$	$a \neq b \neq c \neq a$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$	$0,0,0$		$4\cdot2\cdot1$
		$a = b \neq c$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$	$0,0,0$	y, x, z	$4\cdot2\cdot2$
		$a = b = c$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$	$0,0,0$	$z, x, y; y, x, z$	$4\cdot2\cdot6$
24	$I2_12_12_1$	$a \neq b \neq c \neq a$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$	$0,0,0$		$4\cdot2\cdot1$
		$a = b \neq c$	$P4_2/mmc$ $(2/m2/mn)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$	$0,0,0$	$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$4\cdot2\cdot2$
		$a = b = c$	$Pm\bar{3}n$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$	$0,0,0$	$z, x, y; y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$4\cdot2\cdot6$
25	$Pmm2$	$a \neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,t$	$0,0,0$		$(4\cdot\infty)\cdot2\cdot1$
		$a = b$	P^14/mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,t$	$0,0,0$	y, x, z	$(4\cdot\infty)\cdot2\cdot2$
26	$Pmc2_1$		P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,t$	$0,0,0$		$(4\cdot\infty)\cdot2\cdot1$
27	$Pcc2$	$a \neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,t$	$0,0,0$		$(4\cdot\infty)\cdot2\cdot1$
		$a = b$	P^14/mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,t$	$0,0,0$	y, x, z	$(4\cdot\infty)\cdot2\cdot2$
28	$Pma2$		P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,t$	$0,0,0$		$(4\cdot\infty)\cdot2\cdot1$
29	$Pca2_1$		P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,t$	$0,0,0$		$(4\cdot\infty)\cdot2\cdot1$
30	$Pnc2$		P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,t$	$0,0,0$		$(4\cdot\infty)\cdot2\cdot1$
31	$Pmn2_1$		P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,t$	$0,0,0$		$(4\cdot\infty)\cdot2\cdot1$

Table 15.2.1.3. *Euclidean normalizers of the monoclinic and orthorhombic space groups* (*cont.*)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
32	*Pba*2	$a \neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, t$	0, 0, 0		$(4 \cdot \infty) \cdot 2 \cdot 1$
		$a = b$	P^14/mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, t$	0, 0, 0	y, x, z	$(4 \cdot \infty) \cdot 2 \cdot 2$
33	$Pna2_1$		P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, t$	0, 0, 0		$(4 \cdot \infty) \cdot 2 \cdot 1$
34	*Pnn*2	$a \neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, t$	0, 0, 0		$(4 \cdot \infty) \cdot 2 \cdot 1$
		$a = b$	P^14/mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, t$	0, 0, 0	y, x, z	$(4 \cdot \infty) \cdot 2 \cdot 2$
35	*Cmm*2	$a \neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, t$	0, 0, 0		$(2 \cdot \infty) \cdot 2 \cdot 1$
		$a = b$	P^14/mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, t$	0, 0, 0	y, x, z	$(2 \cdot \infty) \cdot 2 \cdot 2$
36	$Cmc2_1$		P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, t$	0, 0, 0		$(2 \cdot \infty) \cdot 2 \cdot 1$
37	*Ccc*2	$a \neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, t$	0, 0, 0		$(2 \cdot \infty) \cdot 2 \cdot 1$
		$a = b$	P^14/mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, t$	0, 0, 0	y, x, z	$(2 \cdot \infty) \cdot 2 \cdot 2$
38	*Amm*2		P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, t$	0, 0, 0		$(2 \cdot \infty) \cdot 2 \cdot 1$
39	*Aem*2		P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, t$	0, 0, 0		$(2 \cdot \infty) \cdot 2 \cdot 1$
40	*Ama*2		P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, t$	0, 0, 0		$(2 \cdot \infty) \cdot 2 \cdot 1$
41	*Aea*2		P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, t$	0, 0, 0		$(2 \cdot \infty) \cdot 2 \cdot 1$
42	*Fmm*2	$a \neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	0, 0, 0		$\infty \cdot 2 \cdot 1$
		$a = b$	P^14/mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	0, 0, 0	y, x, z	$\infty \cdot 2 \cdot 2$
43	*Fdd*2	$a \neq b$	P^1ban (222)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$\frac{1}{8}, \frac{1}{8}, 0$		$\infty \cdot 2 \cdot 1$
		$a = b$	P^14/nbm ($\bar{4}2m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$\frac{1}{8}, \frac{1}{8}, 0$	y, x, z	$\infty \cdot 2 \cdot 2$
44	*Imm*2	$a \neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, t$	0, 0, 0		$(2 \cdot \infty) \cdot 2 \cdot 1$
		$a = b$	P^14/mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, t$	0, 0, 0	y, x, z	$(2 \cdot \infty) \cdot 2 \cdot 2$
45	*Iba*2	$a \neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, t$	0, 0, 0		$(2 \cdot \infty) \cdot 2 \cdot 1$
		$a = b$	P^14/mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, t$	0, 0, 0	y, x, z	$(2 \cdot \infty) \cdot 2 \cdot 2$
46	*Ima*2		P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, t$	0, 0, 0		$(2 \cdot \infty) \cdot 2 \cdot 1$
47	*Pmmm*	$a \neq b \neq c \neq a$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$a = b \neq c$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		y, x, z	$8 \cdot 1 \cdot 2$
		$a = b = c$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$z, x, y; y, x, z$	$8 \cdot 1 \cdot 6$
48	*Pnnn* (both origins)	$a \neq b \neq c \neq a$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$a = b \neq c$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		y, x, z	$8 \cdot 1 \cdot 2$
		$a = b = c$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$z, x, y; y, x, z$	$8 \cdot 1 \cdot 6$
49	*Pccm*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$a = b$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		y, x, z	$8 \cdot 1 \cdot 2$
50	*Pban* (both origins)	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$a = b$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		y, x, z	$8 \cdot 1 \cdot 2$
51	*Pmma*		*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
52	*Pnna*		*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
53	*Pmna*		*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
54	*Pcca*		*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$

Table 15.2.1.3. *Euclidean normalizers of the monoclinic and orthorhombic space groups* (*cont.*)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
55	*Pbam*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$a = b$	*P4/mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		y, x, z	$8 \cdot 1 \cdot 2$
56	*Pccn*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$a = b$	*P4/mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		y, x, z	$8 \cdot 1 \cdot 2$
57	*Pbcm*		*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8 \cdot 1 \cdot 1$
58	*Pnnm*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$a = b$	*P4/mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		y, x, z	$8 \cdot 1 \cdot 2$
59	*Pmmn* (both origins)	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$a = b$	*P4/mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		y, x, z	$8 \cdot 1 \cdot 2$
60	*Pbcn*		*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8 \cdot 1 \cdot 1$
61	*Pbca*	$a \neq b$ or $b \neq c$ or $a \neq c$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$a = b = c$	$Pm\bar{3}$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$		z, x, y	$8 \cdot 1 \cdot 3$
62	*Pnma*		*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$			$8 \cdot 1 \cdot 1$
63	*Cmcm*		*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$			$4 \cdot 1 \cdot 1$
64	*Cmce*		*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$			$4 \cdot 1 \cdot 1$
65	*Cmmm*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$a = b$	*P4/mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$		y, x, z	$4 \cdot 1 \cdot 2$
66	*Cccm*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$a = b$	*P4/mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$		y, x, z	$4 \cdot 1 \cdot 2$
67	*Cmme*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$a = b$	*P4/mmm* (*mmm*)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$		$y+\frac{1}{4}, x-\frac{1}{4}, z$	$4 \cdot 1 \cdot 2$
68	*Ccce* (222)	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$a = b$	*P4/mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$		y, x, z	$4 \cdot 1 \cdot 2$
68	*Ccce* ($\bar{1}$)	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$a = b$	*P4/mmm* (*mmm*)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,0,\frac{1}{2}$		$y+\frac{1}{4}, x-\frac{1}{4}, z$	$4 \cdot 1 \cdot 2$
69	*Fmmm*	$a \neq b \neq c \neq a$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$			$2 \cdot 1 \cdot 1$
		$a = b \neq c$	*P4/mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$		y, x, z	$2 \cdot 1 \cdot 2$
		$a = b = c$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$		$z, x, y; y, x, z$	$2 \cdot 1 \cdot 6$
70	*Fddd* (222)	$a \neq b \neq c \neq a$	*Pnnn* (222)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$			$2 \cdot 1 \cdot 1$
		$a = b \neq c$	$P4_2/nnm$ ($\bar{4}2m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$		$\bar{y}, \bar{x}, z$	$2 \cdot 1 \cdot 2$
		$a = b = c$	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$		$z, x, y; y, x, z$	$2 \cdot 1 \cdot 6$
70	*Fddd* ($\bar{1}$)	$a \neq b \neq c \neq a$	*Pnnn* ($\bar{1}$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$			$2 \cdot 1 \cdot 1$
		$a = b \neq c$	$P4_2/nnm$ ($2/m$ at $0, \frac{1}{2}, 0$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$		y, x, z	$2 \cdot 1 \cdot 2$
		$a = b = c$	$Pn\bar{3}m$ ($\bar{3}m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$		$z, x, y; y, x, z$	$2 \cdot 1 \cdot 6$
71	*Immm*	$a \neq b \neq c \neq a$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$			$4 \cdot 1 \cdot 1$
		$a = b \neq c$	*P4/mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		y, x, z	$4 \cdot 1 \cdot 2$
		$a = b = c$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0; 0,\frac{1}{2},0$		$z, x, y; y, x, z$	$4 \cdot 1 \cdot 6$

Table 15.2.1.3. *Euclidean normalizers of the monoclinic and orthorhombic space groups* (*cont.*)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
72	*Ibam*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$			$4 \cdot 1 \cdot 1$
		$a = b$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		y, x, z	$4 \cdot 1 \cdot 2$
73	*Ibca*	$a \neq b \neq c \neq a$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$			$4 \cdot 1 \cdot 1$
		$a = b \neq c$	$P4_2/mmc$ $(2/m2/mn)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}$	$4 \cdot 1 \cdot 2$
		$a = b = c$	$Pm\bar{3}n$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		z, x, y; $y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}$	$4 \cdot 1 \cdot 6$
74	*Imma*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$			$4 \cdot 1 \cdot 1$
		$a = b$	$P4_2/mmc$ $(2/m2/mn)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$y + \frac{1}{4}, x - \frac{1}{4}, z + \frac{1}{4}$	$4 \cdot 1 \cdot 2$

combinations of matrices and vectors that originate from the specified pair(s) and from the restrictions on the coefficients. This set of matrix–vector pairs has of course to include the symmetry operations of $\mathcal{G}$ as well as of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$.

The relatively complicated group structure of these affine normalizers has to do with the fact that for the corresponding space groups the permissible basis transformations are more complicated than for space groups of higher crystal systems.

In contrast to orthorhombic space groups, the metric of a triclinic or monoclinic space group cannot be specialized in such a way that all elements of the affine normalizer simultaneously become isometries.

The affine normalizers of the oblique plane groups $p1$ and $p2$ can be described analogously. The corresponding unimodular matrix

$$\begin{pmatrix} n_{11} & n_{12} \\ n_{21} & n_{22} \end{pmatrix}$$

has to be combined with the vector

$$\begin{pmatrix} r \\ s \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{2}n_2 \end{pmatrix}$$

for the representation of $\mathcal{N}_{\mathcal{A}}(p1)$ and $\mathcal{N}_{\mathcal{A}}(p2)$, respectively. n stands for an integer number, r and s stand for real numbers.

Table 15.2.1.4. *Euclidean normalizers of the tetragonal, trigonal, hexagonal and cubic space groups*

The symbols in parentheses following a space-group symbol refer to the location of the origin ('origin choice' in Part 7).

Space group $\mathcal{G}$		Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
75	$P4$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$	y, x, z	$(2\cdot\infty)\cdot 2\cdot 2$
76	$P4_1$	P^1422	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, t$	/	$y, x, -z$	$(2\cdot\infty)\cdot 2$
77	$P4_2$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$	y, x, z	$(2\cdot\infty)\cdot 2\cdot 2$
78	$P4_3$	P^1422	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, t$	/	$y, x, -z$	$(2\cdot\infty)\cdot 2$
79	$I4$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$	y, x, z	$\infty\cdot 2\cdot 2$
80	$I4_1$	P^14/nbm ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$\frac{1}{4}, 0, 0$	$y, x, -z$	$\infty\cdot 2\cdot 2$
81	$P\bar{4}$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	y, x, z	$4\cdot 2\cdot 2$
82	$I\bar{4}$	$I4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, \frac{1}{4}$	$0, 0, 0$	y, x, z	$4\cdot 2\cdot 2$
83	$P4/m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		y, x, z	$4\cdot 1\cdot 2$
84	$P4_2/m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		y, x, z	$4\cdot 1\cdot 2$
85	$P4/n$ ($\bar{4}$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		y, x, z	$4\cdot 1\cdot 2$
85	$P4/n$ ($\bar{1}$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		y, x, z	$4\cdot 1\cdot 2$
86	$P4_2/n$ ($\bar{4}$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		y, x, z	$4\cdot 1\cdot 2$
86	$P4_2/n$ ($\bar{1}$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		y, x, z	$4\cdot 1\cdot 2$
87	$I4/m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		y, x, z	$2\cdot 1\cdot 2$
88	$I4_1/a$ ($\bar{4}$)	$P4_2/nnm$ ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		$y, x, -z$	$2\cdot 1\cdot 2$
88	$I4_1/a$ ($\bar{1}$)	$P4_2/nnm$ ($2/m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$2\cdot 1\cdot 2$
89	$P422$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
90	$P42_12$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
91	$P4_122$	$P4_222$ (222) origin at 4_212	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	/		$4\cdot 1$
92	$P4_12_12$	$P4_222$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	/		$4\cdot 1$
93	$P4_222$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
94	$P4_22_12$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
95	$P4_322$	$P4_222$ (222) origin at 4_212	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	/		$4\cdot 1$
96	$P4_32_12$	$P4_222$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	/		$4\cdot 1$
97	$I422$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$0, 0, 0$		$2\cdot 2\cdot 1$
98	$I4_122$	$P4_2/nnm$ ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$\frac{1}{4}, 0, \frac{1}{8}$		$2\cdot 2\cdot 1$
99	$P4mm$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
100	$P4bm$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
101	$P4_2cm$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
102	$P4_2nm$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
103	$P4cc$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
104	$P4nc$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
105	$P4_2mc$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
106	$P4_2bc$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
107	$I4mm$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$		$\infty\cdot 2\cdot 1$
108	$I4cm$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$		$\infty\cdot 2\cdot 1$
109	$I4_1md$	P^14/nbm ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$\frac{1}{4}, 0, 0$		$\infty\cdot 2\cdot 1$
110	$I4_1cd$	P^14/nbm ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$\frac{1}{4}, 0, 0$		$\infty\cdot 2\cdot 1$
111	$P\bar{4}2m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
112	$P\bar{4}2c$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
113	$P\bar{4}2_1m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
114	$P\bar{4}2_1c$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
115	$P\bar{4}m2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
116	$P\bar{4}c2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
117	$P\bar{4}b2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
118	$P\bar{4}n2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
119	$I\bar{4}m2$	$I4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, \frac{1}{4}$	$0, 0, 0$		$4\cdot 2\cdot 1$

Table 15.2.1.4. *Euclidean normalizers of the tetragonal, trigonal, hexagonal and cubic space groups* (*cont.*)

Space group $\mathcal{G}$		Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
120	$I\bar{4}c2$	$I4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, \frac{1}{4}$	$0, 0, 0$		$4\cdot 2\cdot 1$
121	$I\bar{4}2m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$0, 0, 0$		$2\cdot 2\cdot 1$
122	$I\bar{4}2d$	$P4_2/nnm$ $(\bar{4}2m)$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$\frac{1}{4}, 0, \frac{1}{8}$		$2\cdot 2\cdot 1$
123	$P4/mmm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
124	$P4/mcc$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
125	$P4/nbm$ (422)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
125	$P4/nbm$ $(2/m)$	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
126	$P4/nnc$ (422)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
126	$P4/nnc$ $(\bar{1})$	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
127	$P4/mbm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
128	$P4/mnc$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
129	$P4/nmm$ $(\bar{4}m2)$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
129	$P4/nmm$ $(2/m)$	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
130	$P4/ncc$ $(\bar{4})$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
130	$P4/ncc$ $(\bar{1})$	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
131	$P4_2/mmc$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
132	$P4_2/mcm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
133	$P4_2/nbc$ $(\bar{4})$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
133	$P4_2/nbc$ $(\bar{1})$	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
134	$P4_2/nnm$ $(\bar{4}2m)$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
134	$P4_2/nnm$ $(2/m)$	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
135	$P4_2/mbc$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
136	$P4_2/mnm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
137	$P4_2/nmc$ $(\bar{4}m2)$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
137	$P4_2/nmc$ $(\bar{1})$	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
138	$P4_2/ncm$ $(\bar{4})$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
138	$P4_2/ncm$ $(2/m)$	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4\cdot 1\cdot 1$
139	$I4/mmm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2\cdot 1\cdot 1$
140	$I4/mcm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2\cdot 1\cdot 1$
141	$I4_1/amd$ $(\bar{4}m2)$	$P4_2/nnm$ $(\bar{4}2m)$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2\cdot 1\cdot 1$
141	$I4_1/amd$ $(2/m)$	$P4_2/nnm$ $(2/m)$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2\cdot 1\cdot 1$
142	$I4_1/acd$ $(\bar{4})$	$P4_2/nnm$ $(\bar{4}2m)$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2\cdot 1\cdot 1$
142	$I4_1/acd$ $(\bar{1})$	$P4_2/nnm$ $(2/m)$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2\cdot 1\cdot 1$
143	$P3$	P^16/mmm	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, t$	$0, 0, 0$	$-x, -y, z; y, x, z$	$(3\cdot\infty)\cdot 2\cdot 4$
144	$P3_1$	P^1622	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, t$	/	$-x, -y, z; y, x, -z$	$(3\cdot\infty)\cdot 4$
145	$P3_2$	P^1622	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, t$	/	$-x, -y, z; y, x, -z$	$(3\cdot\infty)\cdot 4$
146	$R3$ (hexag.)	$P^1\bar{3}1m$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$	$-y, -x, z$	$\infty\cdot 2\cdot 2$
146	$R3$ (rhomboh.)	$P^1\bar{3}1m$	$\frac{2}{3}\mathbf{a}-\frac{1}{3}\mathbf{b}-\frac{1}{3}\mathbf{c}$, $-\frac{1}{3}\mathbf{a}+\frac{2}{3}\mathbf{b}-\frac{1}{3}\mathbf{c}, \varepsilon(\mathbf{a}+\mathbf{b}+\mathbf{c})$	r, r, r	$0, 0, 0$	y, x, z	$\infty\cdot 2\cdot 2$
147	$P\bar{3}$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		$-x, -y, z; y, x, z$	$2\cdot 1\cdot 4$
148	$R\bar{3}$ (hexag.)	$R\bar{3}m$ (hexag.)	$-\mathbf{a}, -\mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		$-y, -x, z$	$2\cdot 1\cdot 2$
148	$R\bar{3}$ (rhomboh.)	$R\bar{3}m$ (rhomboh.)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}), \frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2\cdot 1\cdot 2$
149	$P312$	$P6/mmm$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	$-x, -y, z$	$6\cdot 2\cdot 2$
150	$P321$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$0, 0, 0$	$-x, -y, z$	$2\cdot 2\cdot 2$
151	$P3_112$	$P6_222$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, \frac{1}{2}$	/	$-x, -y, z$	$6\cdot 2$
152	$P3_121$	$P6_222$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/	$-x, -y, z$	$2\cdot 2$
153	$P3_212$	$P6_422$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, \frac{1}{2}$	/	$-x, -y, z$	$6\cdot 2$
154	$P3_221$	$P6_422$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/	$-x, -y, z$	$2\cdot 2$
155	$R32$ (hexag.)	$R\bar{3}m$ (hexag.)	$-\mathbf{a}, -\mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$0, 0, 0$		$2\cdot 2\cdot 1$
155	$R32$ (rhomboh.)	$R\bar{3}m$ (rhomboh.)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}), \frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, 0$		$2\cdot 2\cdot 1$

Table 15.2.1.4. *Euclidean normalizers of the tetragonal, trigonal, hexagonal and cubic space groups* (*cont.*)

Space group $\mathcal{G}$		Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
156	$P3m1$	P^16/mmm	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, t$	$0, 0, 0$	$-x, -y, z$	$(3\cdot\infty)\cdot 2\cdot 2$
157	$P31m$	P^16/mmm	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$	$-x, -y, z$	$\infty\cdot 2\cdot 2$
158	$P3c1$	P^16/mmm	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, t$	$0, 0, 0$	$-x, -y, z$	$(3\cdot\infty)\cdot 2\cdot 2$
159	$P31c$	P^16/mmm	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$	$-x, -y, z$	$\infty\cdot 2\cdot 2$
160	$R3m$ (hexag.)	$P^1\bar{3}1m$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$		$\infty\cdot 2\cdot 1$
160	$R3m$ (rhomboh.)	$P^1\bar{3}1m$	$\frac{2}{3}\mathbf{a}-\frac{1}{3}\mathbf{b}-\frac{1}{3}\mathbf{c}$, $-\frac{1}{3}\mathbf{a}+\frac{2}{3}\mathbf{b}-\frac{1}{3}\mathbf{c}, \varepsilon(\mathbf{a}+\mathbf{b}+\mathbf{c})$	r, r, r	$0, 0, 0$		$\infty\cdot 2\cdot 1$
161	$R3c$ (hexag.)	$P^1\bar{3}1m$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$		$\infty\cdot 2\cdot 1$
161	$R3c$ (rhomboh.)	$P^1\bar{3}1m$	$\frac{2}{3}\mathbf{a}-\frac{1}{3}\mathbf{b}-\frac{1}{3}\mathbf{c}$, $-\frac{1}{3}\mathbf{a}+\frac{2}{3}\mathbf{b}-\frac{1}{3}\mathbf{c}, \varepsilon(\mathbf{a}+\mathbf{b}+\mathbf{c})$	r, r, r	$0, 0, 0$		$\infty\cdot 2\cdot 1$
162	$P\bar{3}1m$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		$-x, -y, z$	$2\cdot 1\cdot 2$
163	$P\bar{3}1c$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		$-x, -y, z$	$2\cdot 1\cdot 2$
164	$P\bar{3}m1$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		$-x, -y, z$	$2\cdot 1\cdot 2$
165	$P\bar{3}c1$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		$-x, -y, z$	$2\cdot 1\cdot 2$
166	$R\bar{3}m$ (hexag.)	$R\bar{3}m$ (hexag.)	$-\mathbf{a}, -\mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2\cdot 1\cdot 1$
166	$R\bar{3}m$ (rhomboh.)	$R\bar{3}m$ (rhomboh.)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}), \frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2\cdot 1\cdot 1$
167	$R\bar{3}c$ (hexag.)	$R\bar{3}m$ (hexag.)	$-\mathbf{a}, -\mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2\cdot 1\cdot 1$
167	$R\bar{3}c$ (rhomboh.)	$R\bar{3}m$ (rhomboh.)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}), \frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2\cdot 1\cdot 1$
168	$P6$	P^16/mmm	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$	y, x, z	$\infty\cdot 2\cdot 2$
169	$P6_1$	P^1622	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	/	$y, x, -z$	$\infty\cdot 2$
170	$P6_5$	P^1622	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	/	$y, x, -z$	$\infty\cdot 2$
171	$P6_2$	P^1622	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	/	$y, x, -z$	$\infty\cdot 2$
172	$P6_4$	P^1622	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	/	$y, x, -z$	$\infty\cdot 2$
173	$P6_3$	P^16/mmm	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$	y, x, z	$\infty\cdot 2\cdot 2$
174	$P\bar{6}$	$P6/mmm$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	y, x, z	$6\cdot 2\cdot 2$
175	$P6/m$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		y, x, z	$2\cdot 1\cdot 2$
176	$P6_3/m$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		y, x, z	$2\cdot 1\cdot 2$
177	$P622$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$0, 0, 0$		$2\cdot 2\cdot 1$
178	$P6_122$	$P6_222$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/		$2\cdot 1$
179	$P6_522$	$P6_422$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/		$2\cdot 1$
180	$P6_222$	$P6_422$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/		$2\cdot 1$
181	$P6_422$	$P6_222$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/		$2\cdot 1$
182	$P6_322$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$0, 0, 0$		$2\cdot 2\cdot 1$
183	$P6mm$	P^16/mmm	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$		$\infty\cdot 2\cdot 1$
184	$P6cc$	P^16/mmm	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$		$\infty\cdot 2\cdot 1$
185	$P6_3cm$	P^16/mmm	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$		$\infty\cdot 2\cdot 1$
186	$P6_3mc$	P^16/mmm	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$		$\infty\cdot 2\cdot 1$
187	$P\bar{6}m2$	$P6/mmm$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$6\cdot 2\cdot 1$
188	$P\bar{6}c2$	$P6/mmm$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$6\cdot 2\cdot 1$
189	$P\bar{6}2m$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$0, 0, 0$		$2\cdot 2\cdot 1$
190	$P\bar{6}2c$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$0, 0, 0$		$2\cdot 2\cdot 1$
191	$P6/mmm$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2\cdot 1\cdot 1$
192	$P6/mcc$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2\cdot 1\cdot 1$
193	$P6_3/mcm$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2\cdot 1\cdot 1$
194	$P6_3/mmc$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2\cdot 1\cdot 1$
195	$P23$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, 0$	y, x, z	$2\cdot 2\cdot 2$
196	$F23$	$Im\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$0, 0, 0$	y, x, z	$4\cdot 2\cdot 2$
197	$I23$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$		$0, 0, 0$	y, x, z	$1\cdot 2\cdot 2$

Table 15.2.1.4. *Euclidean normalizers of the tetragonal, trigonal, hexagonal and cubic space groups* (*cont.*)

Space group $\mathcal{G}$		Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$
198	$P2_13$	$Ia\bar{3}d$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, 0	$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$2\cdot2\cdot2$
199	$I2_13$	$Ia\bar{3}d$	**a**, **b**, **c**		0, 0, 0	$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$1\cdot2\cdot2$
200	$Pm\bar{3}$	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2\cdot1\cdot2$
201	$Pn\bar{3}$ (23)	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2\cdot1\cdot2$
201	$Pn\bar{3}$ ($\bar{3}$)	$Im\bar{3}m$ ($\bar{3}m$)	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2\cdot1\cdot2$
202	$Fm\bar{3}$	$Pm\bar{3}m$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2\cdot1\cdot2$
203	$Fd\bar{3}$ (23)	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2\cdot1\cdot2$
203	$Fd\bar{3}$ ($\bar{3}$)	$Pn\bar{3}m$ ($\bar{3}m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2\cdot1\cdot2$
204	$Im\bar{3}$	$Im\bar{3}m$	**a**, **b**, **c**			y, x, z	$1\cdot1\cdot2$
205	$Pa\bar{3}$	$Ia\bar{3}$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2\cdot1\cdot1$
206	$Ia\bar{3}$	$Ia\bar{3}d$	**a**, **b**, **c**			$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$1\cdot1\cdot2$
207	$P432$	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, 0		$2\cdot2\cdot1$
208	$P4_232$	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, 0		$2\cdot2\cdot1$
209	$F432$	$Pm\bar{3}m$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, 0		$2\cdot2\cdot1$
210	$F4_132$	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$		$2\cdot2\cdot1$
211	$I432$	$Im\bar{3}m$	**a**, **b**, **c**		0, 0, 0		$1\cdot2\cdot1$
212	$P4_332$	$I4_132$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	/		$2\cdot1$
213	$P4_132$	$I4_132$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	/		$2\cdot1$
214	$I4_132$	$Ia\bar{3}d$	**a**, **b**, **c**		0, 0, 0		$1\cdot2\cdot1$
215	$P\bar{4}3m$	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, 0		$2\cdot2\cdot1$
216	$F\bar{4}3m$	$Im\bar{3}m$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	0, 0, 0		$4\cdot2\cdot1$
217	$I\bar{4}3m$	$Im\bar{3}m$	**a**, **b**, **c**		0, 0, 0		$1\cdot2\cdot1$
218	$P\bar{4}3n$	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, 0		$2\cdot2\cdot1$
219	$F\bar{4}3c$	$Im\bar{3}m$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	0, 0, 0		$4\cdot2\cdot1$
220	$I\bar{4}3d$	$Ia\bar{3}d$	**a**, **b**, **c**		0, 0, 0		$1\cdot2\cdot1$
221	$Pm\bar{3}m$	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2\cdot1\cdot1$
222	$Pn\bar{3}n$ (432)	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2\cdot1\cdot1$
222	$Pn\bar{3}n$ ($\bar{3}$)	$Im\bar{3}m$ ($\bar{3}m$)	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2\cdot1\cdot1$
223	$Pm\bar{3}n$	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2\cdot1\cdot1$
224	$Pn\bar{3}m$ ($\bar{4}3m$)	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2\cdot1\cdot1$
224	$Pn\bar{3}m$ ($\bar{3}m$)	$Im\bar{3}m$ ($\bar{3}m$)	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2\cdot1\cdot1$
225	$Fm\bar{3}m$	$Pm\bar{3}m$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2\cdot1\cdot1$
226	$Fm\bar{3}c$	$Pm\bar{3}m$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2\cdot1\cdot1$
227	$Fd\bar{3}m$ ($\bar{4}3m$)	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2\cdot1\cdot1$
227	$Fd\bar{3}m$ ($\bar{3}m$)	$Pn\bar{3}m$ ($\bar{3}m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2\cdot1\cdot1$
228	$Fd\bar{3}c$ (23)	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2\cdot1\cdot1$
228	$Fd\bar{3}c$ ($\bar{3}$)	$Pn\bar{3}m$ ($\bar{3}m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2\cdot1\cdot1$
229	$Im\bar{3}m$	$Im\bar{3}m$	**a**, **b**, **c**				$1\cdot1\cdot1$
230	$Ia\bar{3}d$	$Ia\bar{3}d$	**a**, **b**, **c**				$1\cdot1\cdot1$

Table 15.2.2.1. *Affine normalizers of the triclinic and monoclinic space groups*

Space group $\mathcal{G}$		Matrix–vector pairs in Table 15.2.2.2
No.	Hermann–Mauguin symbol	
1	$P1$	$\boldsymbol{M}_1, \boldsymbol{v}_1$
2	$P\bar{1}$	$\boldsymbol{M}_1, \boldsymbol{v}_2$
3	$P121$	$\boldsymbol{M}_2, \boldsymbol{v}_3$
3	$P112$	$\boldsymbol{M}_3, \boldsymbol{v}_4$
4	$P12_11$	$\boldsymbol{M}_2, \boldsymbol{v}_3$
4	$P112_1$	$\boldsymbol{M}_3, \boldsymbol{v}_4$
5	$C121$	$\boldsymbol{M}_4, \boldsymbol{v}_3$
5	$A121$	$\boldsymbol{M}_5, \boldsymbol{v}_3$
5	$I121$	$\boldsymbol{M}_6, \boldsymbol{v}_3$; $\boldsymbol{M}_7, \boldsymbol{v}_3$
5	$A112$	$\boldsymbol{M}_8, \boldsymbol{v}_4$
5	$B112$	$\boldsymbol{M}_9, \boldsymbol{v}_4$
5	$I112$	$\boldsymbol{M}_{10}, \boldsymbol{v}_4$; $\boldsymbol{M}_{11}, \boldsymbol{v}_4$
6	$P1m1$	$\boldsymbol{M}_2, \boldsymbol{v}_5$
6	$P11m$	$\boldsymbol{M}_3, \boldsymbol{v}_6$
7	$P1c1$	$\boldsymbol{M}_5, \boldsymbol{v}_5$
7	$P1n1$	$\boldsymbol{M}_6, \boldsymbol{v}_5$; $\boldsymbol{M}_7, \boldsymbol{v}_5$
7	$P1a1$	$\boldsymbol{M}_4, \boldsymbol{v}_5$
7	$P11a$	$\boldsymbol{M}_9, \boldsymbol{v}_6$
7	$P11n$	$\boldsymbol{M}_{10}, \boldsymbol{v}_6$; $\boldsymbol{M}_{11}, \boldsymbol{v}_6$
7	$P11b$	$\boldsymbol{M}_8, \boldsymbol{v}_6$
8	$C1m1$	$\boldsymbol{M}_4, \boldsymbol{v}_5$
8	$A1m1$	$\boldsymbol{M}_5, \boldsymbol{v}_5$
8	$I1m1$	$\boldsymbol{M}_6, \boldsymbol{v}_5$; $\boldsymbol{M}_7, \boldsymbol{v}_5$
8	$A11m$	$\boldsymbol{M}_8, \boldsymbol{v}_6$
8	$B11m$	$\boldsymbol{M}_9, \boldsymbol{v}_6$
8	$I11m$	$\boldsymbol{M}_{10}, \boldsymbol{v}_6$; $\boldsymbol{M}_{11}, \boldsymbol{v}_6$
9	$C1c1$	$\boldsymbol{M}_6, \boldsymbol{v}_5$; $\boldsymbol{M}_{12}, \boldsymbol{v}_7$
9	$A1n1$	$\boldsymbol{M}_6, \boldsymbol{v}_5$; $\boldsymbol{M}_{13}, \boldsymbol{v}_7$
9	$I1a1$	$\boldsymbol{M}_6, \boldsymbol{v}_5$; $\boldsymbol{M}_7, \boldsymbol{v}_7$
9	$A11a$	$\boldsymbol{M}_{10}, \boldsymbol{v}_6$; $\boldsymbol{M}_{14}, \boldsymbol{v}_8$
9	$B11n$	$\boldsymbol{M}_{10}, \boldsymbol{v}_6$; $\boldsymbol{M}_{15}, \boldsymbol{v}_8$
9	$I11b$	$\boldsymbol{M}_{10}, \boldsymbol{v}_6$; $\boldsymbol{M}_{11}, \boldsymbol{v}_8$
10	$P12/m1$	$\boldsymbol{M}_2, \boldsymbol{v}_2$
10	$P112/m$	$\boldsymbol{M}_3, \boldsymbol{v}_2$
11	$P12_1/m1$	$\boldsymbol{M}_2, \boldsymbol{v}_2$
11	$P112_1/m$	$\boldsymbol{M}_3, \boldsymbol{v}_2$
12	$C12/m1$	$\boldsymbol{M}_4, \boldsymbol{v}_2$
12	$A12/m1$	$\boldsymbol{M}_5, \boldsymbol{v}_2$
12	$I12/m1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_7, \boldsymbol{v}_2$
12	$A112/m$	$\boldsymbol{M}_8, \boldsymbol{v}_2$
12	$B112/m$	$\boldsymbol{M}_9, \boldsymbol{v}_2$
12	$I112/m$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{11}, \boldsymbol{v}_2$
13	$P12/c1$	$\boldsymbol{M}_5, \boldsymbol{v}_2$
13	$P12/n1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_7, \boldsymbol{v}_2$
13	$P12/a1$	$\boldsymbol{M}_4, \boldsymbol{v}_2$
13	$P112/a$	$\boldsymbol{M}_9, \boldsymbol{v}_2$
13	$P112/n$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{11}, \boldsymbol{v}_2$
13	$P112/b$	$\boldsymbol{M}_8, \boldsymbol{v}_2$
14	$P12_1/c1$	$\boldsymbol{M}_5, \boldsymbol{v}_2$
14	$P12_1/n1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_7, \boldsymbol{v}_2$
14	$P12_1/a1$	$\boldsymbol{M}_4, \boldsymbol{v}_2$
14	$P112_1/a$	$\boldsymbol{M}_9, \boldsymbol{v}_2$
14	$P112_1/n$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{11}, \boldsymbol{v}_2$
14	$P112_1/b$	$\boldsymbol{M}_8, \boldsymbol{v}_2$
15	$C12/c1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_{12}, \boldsymbol{v}_9$
15	$A12/n1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_{13}, \boldsymbol{v}_{10}$
15	$I12/a1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_7, \boldsymbol{v}_{11}$
15	$A112/a$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{14}, \boldsymbol{v}_{10}$
15	$B112/n$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{15}, \boldsymbol{v}_{12}$
15	$I112/b$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{11}, \boldsymbol{v}_{11}$

Table 15.2.2.2. *Matrices and vectors used in Table 15.2.2.1 for the description of the affine normalizers of monoclinic and triclinic space groups*

n, g and u represent integer, even and odd numbers, respectively, r, s and t real numbers. For all matrices, $\det(\boldsymbol{M}_i) = \pm 1$ must hold.

$$\boldsymbol{M}_1 = \begin{pmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{pmatrix} \quad \boldsymbol{M}_2 = \begin{pmatrix} n_{11} & 0 & n_{13} \\ 0 & \pm 1 & 0 \\ n_{31} & 0 & n_{33} \end{pmatrix} \quad \boldsymbol{M}_3 = \begin{pmatrix} n_{11} & n_{12} & 0 \\ n_{21} & n_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad \boldsymbol{M}_4 = \begin{pmatrix} u_{11} & 0 & n_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{pmatrix} \quad \boldsymbol{M}_5 = \begin{pmatrix} u_{11} & 0 & g_{13} \\ 0 & \pm 1 & 0 \\ n_{31} & 0 & u_{33} \end{pmatrix}$$

$$\boldsymbol{M}_6 = \begin{pmatrix} u_{11} & 0 & g_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{pmatrix} \quad \boldsymbol{M}_7 = \begin{pmatrix} g_{11} & 0 & u_{13} \\ 0 & \pm 1 & 0 \\ u_{31} & 0 & g_{33} \end{pmatrix} \quad \boldsymbol{M}_8 = \begin{pmatrix} u_{11} & g_{12} & 0 \\ n_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad \boldsymbol{M}_9 = \begin{pmatrix} u_{11} & n_{12} & 0 \\ g_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad \boldsymbol{M}_{10} = \begin{pmatrix} u_{11} & g_{12} & 0 \\ g_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix}$$

$$\boldsymbol{M}_{11} = \begin{pmatrix} g_{11} & u_{12} & 0 \\ u_{21} & g_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad \boldsymbol{M}_{12} = \begin{pmatrix} u_{11} & 0 & u_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{pmatrix} \quad \boldsymbol{M}_{13} = \begin{pmatrix} u_{11} & 0 & g_{13} \\ 0 & \pm 1 & 0 \\ u_{31} & 0 & u_{33} \end{pmatrix} \quad \boldsymbol{M}_{14} = \begin{pmatrix} u_{11} & g_{12} & 0 \\ u_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad \boldsymbol{M}_{15} = \begin{pmatrix} u_{11} & u_{12} & 0 \\ g_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix}$$

$$\boldsymbol{v}_1 = \begin{pmatrix} r \\ s \\ t \end{pmatrix} \quad \boldsymbol{v}_2 = \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{2}n_2 \\ \frac{1}{2}n_3 \end{pmatrix} \quad \boldsymbol{v}_3 = \begin{pmatrix} \frac{1}{2}n_1 \\ s \\ \frac{1}{2}n_3 \end{pmatrix} \quad \boldsymbol{v}_4 = \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{2}n_2 \\ t \end{pmatrix} \quad \boldsymbol{v}_5 = \begin{pmatrix} r \\ \frac{1}{2}n_2 \\ t \end{pmatrix}$$

$$\boldsymbol{v}_6 = \begin{pmatrix} r \\ s \\ \frac{1}{2}n_3 \end{pmatrix} \quad \boldsymbol{v}_7 = \begin{pmatrix} r \\ \frac{1}{4}u_2 \\ t \end{pmatrix} \quad \boldsymbol{v}_8 = \begin{pmatrix} r \\ s \\ \frac{1}{4}u_3 \end{pmatrix} \quad \boldsymbol{v}_9 = \begin{pmatrix} \frac{1}{4}u_1 \\ \frac{1}{4}u_2 \\ \frac{1}{2}n_3 \end{pmatrix} \quad \boldsymbol{v}_{10} = \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{4}u_2 \\ \frac{1}{4}u_3 \end{pmatrix}$$

$$\boldsymbol{v}_{11} = \begin{pmatrix} \frac{1}{4}u_1 \\ \frac{1}{4}u_2 \\ \frac{1}{4}u_3 \end{pmatrix} \quad \boldsymbol{v}_{12} = \begin{pmatrix} \frac{1}{4}u_1 \\ \frac{1}{2}n_2 \\ \frac{1}{4}u_3 \end{pmatrix}$$

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15.3. Examples of the use of normalizers

BY E. KOCH AND W. FISCHER

15.3.1. Introduction

The Euclidean and the affine normalizers of a space group form the appropriate tool to define equivalence relationships on sets of objects that are not symmetrically equivalent in this space group but 'play the same role' with respect to this group. Two such objects referring to the same space group will be called Euclidean- or affine-equivalent if there exists a Euclidean or affine mapping that maps the two objects onto one another and, in addition, maps the space group onto itself.

15.3.2. Equivalent point configurations, equivalent Wyckoff positions and equivalent descriptions of crystal structures

In the crystal structure of copper, all atoms are symmetrically equivalent with respect to space group $Fm\overline{3}m$. The pattern of Cu atoms may be described equally well by Wyckoff position $4a$ 000 or $4b$ $\frac{1}{2}\frac{1}{2}\frac{1}{2}$. The Euclidean normalizer of $Fm\overline{3}m$ gives the relation between the two descriptions.

Two *point configurations* (crystallographic orbits)* of a space group $\mathcal{G}$ are called *Euclidean-* or *$\mathcal{N}_{\mathcal{E}}$-equivalent* (*affine-* or *$\mathcal{N}_{\mathcal{A}}$-equivalent*) if they are mapped onto each other by the Euclidean (affine) normalizer of $\mathcal{G}$.

Affine-equivalent point configurations play the same role with respect to the space-group symmetry, *i.e.* their points are embedded in the pattern of symmetry elements in the same way. Euclidean-equivalent point configurations are congruent and may be interchanged when passing from one description of a crystal structure to another.

Starting from any given point configuration of a space group $\mathcal{G}$, one may derive all Euclidean-equivalent point configurations and – except for monoclinic and triclinic space groups – all affine-equivalent ones by successive application of the 'additional generators' of the normalizer as given in Tables 15.2.1.3 and 15.2.1.4.

Examples

(1) A point configuration $F\overline{4}3m$ $16e$ xxx with $x_1 = 0.10$ may be visualized as a set of parallel tetrahedra arranged in a cubic face-centred lattice. The Euclidean and affine normalizer of $F\overline{4}3m$ is $Im\overline{3}m$ with $a' = \frac{1}{2}a$ (*cf.* Table 15.2.1.4). Since the index k_g of $\mathcal{G}$ in $\mathcal{K}(\mathcal{G})$ is 4, three additional equivalent point configurations exist, which follow from the original one by repeated application of the tabulated translation $t(\frac{1}{4}\frac{1}{4}\frac{1}{4})$: $16e$ xxx with $x_2 = 0.35, x_3 = 0.60, x_4 = 0.85$. $\mathcal{L}(\mathcal{G})$ differs from $\mathcal{K}(\mathcal{G})$ and an additional centre of symmetry is located at 000. Accordingly, the following four equivalent point configurations may be derived from the first four: $16e$ xxx with $x_5 = -0.10$, $x_6 = -0.35, x_7 = -0.60, x_8 = -0.85$. In this case, the index 8 of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ equals the number of Euclidean-equivalent point configurations.

(2) $F\overline{4}3m$ $4a$ 000 represents a face-centred cubic lattice. The additional translations of $\mathcal{K}(F\overline{4}3m)$ generate three equivalent point configurations: $4c$ $\frac{1}{4}\frac{1}{4}\frac{1}{4}$, $4b$ $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ and $4d$ $\frac{3}{4}\frac{3}{4}\frac{3}{4}$. Inversion through 000 maps $4a$ and $4b$ each onto itself and interchanges $4c$ and $4d$. Therefore, here the number of equivalent point configurations is four, *i.e.* only half the index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$.

The difference between the two examples is the following: The reference point 0.1, 0.1, 0.1 of the first example does not change its site symmetry $.3m$ when passing from $F\overline{4}3m$ to $Im\overline{3}m$. Point 000 of the second example, however, has site symmetry $\overline{4}3m$ in $F\overline{4}3m$, but $m\overline{3}m$ in $Im\overline{3}m$.

The following rule holds without exception: The number of point configurations equivalent to a given one is equal to the quotient i/i_s, with i being the subgroup index of $\mathcal{G}$ in its Euclidean or affine normalizer and i_s the subgroup index between the corresponding two site-symmetry groups of any point in the original point configuration.

As a necessary but not sufficient condition for $i_s \neq 1$ when referring to the Euclidean normalizer, the inherent symmetry (*eigensymmetry*) of the point configuration considered (*i.e.* the group of all motions that maps the point configuration onto itself) must be a proper supergroup of $\mathcal{G}$. If $\mathcal{D}$ designates the intersection group of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ with the inherent symmetry of the point configuration, the number of Euclidean-equivalent point configurations equals the index of $\mathcal{D}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$.

Example

The Euclidean and affine normalizer of $P2_13$ is $Ia\overline{3}d$ with index 8. Point configuration $4a$ xxx with $x_1 = 0$ forms a face-centred cubic lattice with inherent symmetry $Fm\overline{3}m$. The reference point 000 has site symmetry $.3.$ in $P2_13$ but $.\overline{3}.$ in $Ia\overline{3}d$. The number of equivalent point configurations, therefore, is $i/i_s = 8/2 = 4$. One additional point configuration is generated by the translation $t(\frac{1}{2}\frac{1}{2}\frac{1}{2})$: $4a$ xxx with $x_2 = \frac{1}{2}$, the two others by applying the d-glide reflection $y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$ to the first two point configurations: $4a$ xxx with $x_3 = \frac{1}{4}$ and $x_4 = \frac{3}{4}$. The intersection group $\mathcal{D}$ of the inherent symmetry $Fm\overline{3}m$ with the normalizer $Ia\overline{3}d$ is $Pa\overline{3}$. Its index 4 in $Ia\overline{3}d$ gives again the number of equivalent point configurations.

The set of equivalent point configurations is always infinite if the normalizer contains continuous translations but this set may be described by a finite number of subsets due to non-continuous translations.

Example

The Euclidean and affine normalizer of $P6_1$ is P^1622 (**a**, **b**, ε**c**). With the aid of the 'additional generators' given in Table 15.2.1.4, one can calculate two subsets of point configurations that are equivalent to a given general point configuration $6a$ xyz with $x = x_0$, $y = y_0$, $z = z_0$: $6a$ xyz with $x_0, y_0, z_0 + t$ and $y_0, x_0, -z_0 + t$. If, however, the coordinates for the original point configuration are specialized, *e.g.* to $x = y = x_1$, $z = z_1$ or to $x = y = 0$, $z = z_2$, only one subset exists, namely $x_1, x_1, z_1 + t$ or 0, 0, $z_2 + t$, respectively. The reduction of the number of subsets is a consequence of the enhancement of the site symmetry in the normalizer (.2. or 622, respectively), but the index i_s, as introduced above, does not necessarily give the reduction factor for the number of subsets.

It has to be noticed that for most space groups with a Euclidean normalizer containing continuous translations the index i_s is larger than 1 for *all* point configurations, *i.e.* the number of subsets of equivalent point configurations is necessarily reduced. The general Wyckoff position of such a space group does not belong to a

* For the use of the terms 'point configuration' and 'crystallographic orbit' see Koch & Fischer (1985).

characteristic type of Wyckoff sets (*cf.* Part 14) and the inherent symmetry of all corresponding point configurations is enhanced.

Example

The Euclidean and affine normalizer of $P6$ is P^16/mmm ($\mathbf{a}$, $\mathbf{b}$, $\varepsilon\mathbf{c}$). As a consequence of the continuous translations, the site symmetry of any point is at least $m..$ in P^16/mmm. With the aid of the 'additional generators', one calculates four subsets of point configurations that are equivalent to a given general point configuration $6d$ xyz with $x = x_0$, $y = y_0$, $z = z_0$: $x_0, y_0, z_0 + t$; $-x_0, -y_0, -z_0 + t$; $y_0, x_0, z_0 + t$; $-y_0, -x_0, -z_0 + t$. The first two and the second two subsets coincide, however.

According to the above examples, Euclidean- (affine-) equivalent point configurations may or may not belong to the same Wyckoff position. Consequently, normalizers also define equivalence relations on Wyckoff positions:

Two *Wyckoff positions* of a space group $\mathcal{G}$ are called *Euclidean-* or $\mathcal{N}_{\mathcal{E}}$-equivalent (*affine-* or $\mathcal{N}_{\mathcal{A}}$-*equivalent*) if their point configurations are mapped onto each other by the Euclidean (affine) normalizer of $\mathcal{G}$.

Euclidean-equivalent Wyckoff positions are important for the description or comparison of crystal structures in terms of atomic coordinates. Affine-equivalent Wyckoff positions result in *Wyckoff sets* (*cf.* Section 8.3.2 and Chapter 14.1) and form the necessary basis for the *definition of lattice complexes.* All site-symmetry groups corresponding to equivalent Wyckoff positions are conjugate in the respective normalizer.

Examples

The Euclidean and affine normalizer of $I\bar{4}m2$ is $I4/mmm$ ($\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$). It maps the point configurations $2a$ 000, $2b$ $00\frac{1}{2}$, $2c$ $0\frac{1}{2}\frac{1}{4}$ and $2d$ $0\frac{1}{2}\frac{3}{4}$ (body-centred tetragonal lattices) onto each other. Accordingly, Wyckoff positions a to d are affine-equivalent and together form a Wyckoff set. Analogous point configurations exist in subgroup $P\bar{4}n2$ of $I\bar{4}m2$ (again Wyckoff positions a to d). The Euclidean and affine normalizer of $P\bar{4}n2$, however, is $P4/mmm$ ($\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$), not containing $t(\frac{1}{2}0\frac{1}{4})$. Therefore, Wyckoff positions a and b form one Wyckoff set, c and d a different one. This is also reflected in the site-symmetry groups $\bar{4}..$ and 2.22.

The existence of Euclidean-equivalent point configurations results in different but *equivalent descriptions of crystal structures* (exception: crystal structures with symmetry $Im\bar{3}m$ or $Ia\bar{3}d$). All such equivalent descriptions are derived by applying the additional generators of the Euclidean normalizer of the space group $\mathcal{G}$ to all point configurations of the original description. Since an adequate description of a crystal structure always displays the full symmetry group of that structure, the number of equivalent descriptions must equal the index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$.

Example

Ag_3PO_4 crystallizes with symmetry $P\bar{4}3n$ (*cf.* Masse *et al.*, 1976): P at $2a$ 000, Ag at $6d$ $\frac{1}{4}0\frac{1}{2}$ and O at $8e$ xxx with $x = 0.1486$. $\mathcal{N}_{\mathcal{E}}(P\bar{4}3n) = Im\bar{3}m$ with index 4 gives rise to three additional equivalent descriptions: $t(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ yields P at $2a$ 000, Ag at $6c$ $\frac{1}{4}\frac{1}{2}0$ and O at $8e$ xxx with $x = 0.1486$; inversion through the origin results in P at $2a$ 000, Ag at $6d$ $\frac{1}{4}0\frac{1}{2}$, O at $8e$ xxx with $x = -0.1486$ and in P at $2a$ 000, Ag at $6c$ $\frac{1}{4}\frac{1}{2}0$ and O at $8e$ xxx with $x = -0.1486$. Although the phosphorus configuration is the same for all descriptions and the silver and oxygen atoms refer to only two configurations each, their combinations result in a total of four different equivalent descriptions of the structure.

If the Euclidean normalizer of a space group contains continuous translations, each crystal structure with that symmetry refers to an infinite set of equivalent descriptions. This set may be subdivided into a finite number of subsets in such a way that the descriptions of each subset vary according to the continuous translations. The number of these subsets is given by the product of the finite factors listed in the last column of Tables 15.2.1.3 and 15.2.1.4.

Example

The tetragonal form of $BaTiO_3$ has been described in space group $P4mm$ (*cf. e.g.* Buttner & Maslen, 1992): Ba at $1a$ $00z$ with $z = 0$, Ti at $1b$ $\frac{1}{2}\frac{1}{2}z$ with $z = 0.482$, O1 at $1b$ $\frac{1}{2}\frac{1}{2}z$ with $z = 0.016$, and O2 at $2c$ $\frac{1}{2}0z$ with $z = 0.515$. $\mathcal{N}_{\mathcal{E}}(P4mm) = P^14/mmm$ $(\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \varepsilon\mathbf{c})$ gives rise to $(2 \cdot \infty) \cdot 2 \cdot 1$ equivalent descriptions of this structure. The continuous translation with vector $(00t)$ yields a first infinite subset of equivalent descriptions: Ba at $1a$ $00z$ with $z = t$, Ti at $1b$ $\frac{1}{2}\frac{1}{2}z$ with $z = 0.482 + t$, O1 at $1b$ $\frac{1}{2}\frac{1}{2}z$ with $z = 0.016 + t$, and O2 at $2c$ $\frac{1}{2}0z$ with $z = 0.515 + t$. The translation with vector $(\frac{1}{2}\frac{1}{2}0)$ generates a second infinite subset: Ba at $1b$ $\frac{1}{2}\frac{1}{2}z$ with $z = t$, Ti at $1a$ $00z$ with $z = 0.482 + t$, O1 at $1a$ $00z$ with $z = 0.016 + t$, and O2 at $2c$ $\frac{1}{2}0z$ with $z = 0.515 + t$. Inversion through the origin causes two further infinite subsets of equivalent coordinate descriptions of $BaTiO_3$: first, Ba at $1a$ $00z$ with $z = t$, Ti at $1b$ $\frac{1}{2}\frac{1}{2}z$ with $z = 0.518 + t$, O1 at $1b$ $\frac{1}{2}\frac{1}{2}z$ with $z = -0.016 + t$, and O2 at $2c$ $\frac{1}{2}0z$ with $z = 0.485 + t$; second, Ba at $1b$ $\frac{1}{2}\frac{1}{2}z$ with $z = t$, Ti at $1a$ $00z$ with $z = 0.518 + t$, O1 at $1a$ $00z$ with $z = -0.016 + t$, and O2 at $2c$ $\frac{1}{2}0z$ with $z = 0.485 + t$.

More details on Euclidean-equivalent point configurations and descriptions of crystal structures have been given by Fischer & Koch (1983).

15.3.3. Equivalent lists of structure factors

All the different but equivalent descriptions of a crystal structure refer to different but equivalent lists of structure factors. These lists contain the same moduli of the structure factors $|F(\boldsymbol{h})|$, but they differ in their indices $\boldsymbol{h} = (h, k, l)$ and phases $\varphi(\boldsymbol{h})$.

In the previous section, the unit cell (basis and origin) of a space group $\mathcal{G}$ has been considered fixed, whereas the crystal structure or its enantiomorph was embedded into the pattern of symmetry elements at different but equivalent locations. In the present context, however, it is advantageous to regard the crystal structure as being fixed and to let $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ transform the basis and the origin with respect to which the crystal structure is described. This matches the usual approach to resolve the ambiguities in direct methods by fixing the origin and the absolute structure.

Each matrix–vector pair $(\boldsymbol{P}, \boldsymbol{p})$ representing an element of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ describes a unit-cell transformation of $\mathcal{G}$. According to Section 5.1.3 the following equations hold:

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}'),\ = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}, \qquad \begin{pmatrix} \mathbf{a}^{*\prime} \\ \mathbf{b}^{*\prime} \\ \mathbf{c}^{*\prime} \end{pmatrix} = \boldsymbol{P}^{-1} \begin{pmatrix} \mathbf{a}^{*} \\ \mathbf{b}^{*} \\ \mathbf{c}^{*} \end{pmatrix}, \qquad \boldsymbol{h}' = \boldsymbol{h}\,\boldsymbol{P}.$$

As a consequence, the phase $\varphi(\boldsymbol{h})$ of a certain structure factor also changes into $\varphi'(\boldsymbol{h}') = \varphi(\boldsymbol{h}) - 2\pi\boldsymbol{hp}$.

Similar to equivalent descriptions of a crystal structure, it is possible to derive all equivalent lists of structure factors: The additional generators of $\mathcal{K}(\mathcal{G})$ are pure translations that leave the indices $\boldsymbol{h}$ of all structure factors unchanged but transform their phases according to $\varphi'(\boldsymbol{h}) = \varphi(\boldsymbol{h}) - 2\pi\boldsymbol{hp}$. Therefore, the origin for the description of the crystal structure may be fixed by appropriate restrictions of some phases. The number of these phases equals the

Table 15.3.3.1. *Changes of structure-factor phases for the equivalent descriptions of a crystal structure in F222*

	$h+k+l=$			
$F222$	$4n$	$4n+2$	$4n+1$	$4n+3$
$t(000)$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$
$t(\frac{1}{4}\frac{1}{4}\frac{1}{4})$	$\varphi(\boldsymbol{h})$	$\pi+\varphi(\boldsymbol{h})$	$\frac{3}{2}\pi+\varphi(\boldsymbol{h})$	$\frac{1}{2}\pi+\varphi(\boldsymbol{h})$
$t(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$	$\pi+\varphi(\boldsymbol{h})$	$\pi+\varphi(\boldsymbol{h})$
$t(\frac{3}{4}\frac{3}{4}\frac{3}{4})$	$\varphi(\boldsymbol{h})$	$\pi+\varphi(\boldsymbol{h})$	$\frac{1}{2}\pi+\varphi(\boldsymbol{h})$	$\frac{3}{2}\pi+\varphi(\boldsymbol{h})$
$\bar{1}(000)$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$
$\bar{1}(\frac{1}{8}\frac{1}{8}\frac{1}{8})$	$-\varphi(\boldsymbol{h})$	$\pi-\varphi(\boldsymbol{h})$	$\frac{1}{2}\pi-\varphi(\boldsymbol{h})$	$\frac{3}{2}\pi-\varphi(\boldsymbol{h})$
$\bar{1}(\frac{1}{4}\frac{1}{4}\frac{1}{4})$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$	$\pi-\varphi(\boldsymbol{h})$	$\pi-\varphi(\boldsymbol{h})$
$\bar{1}(\frac{3}{8}\frac{3}{8}\frac{3}{8})$	$-\varphi(\boldsymbol{h})$	$\pi-\varphi(\boldsymbol{h})$	$\frac{3}{2}\pi-\varphi(\boldsymbol{h})$	$\frac{1}{2}\pi-\varphi(\boldsymbol{h})$

number of additional generators of $\mathcal{K}(\mathcal{G})$, given in Table 15.2.1.3 or 15.2.1.4. These generators [together with the inversion that generates $\mathcal{L}(\mathcal{G})$, if present] also determine the parity classes of the structure factors and the ranges for the phase restrictions.

The inversion that generates $\mathcal{L}(\mathcal{G})$ changes the handedness of the coordinate system in direct space and in reciprocal space and, therefore, gives rise to different absolute crystal structures. The indices of a given structure factor change from $\boldsymbol{h}$ to $\boldsymbol{h}'=-\boldsymbol{h}$, whereas the phase is influenced only if the symmetry centre is not located at 000.

If no anomalous scattering is observed, Friedel's rule holds and the moduli of any two structure factors with indices $\boldsymbol{h}$ and $-\boldsymbol{h}$ are equal. As a consequence, different absolute crystal structures result in lists of structure factors and indices that differ only in their phases. Therefore, one phase may be restricted to an appropriate range of length π to fix the absolute structure. This is not possible if anomalous scattering has been observed.

If $\mathcal{L}(\mathcal{G})$ differs from $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$, *i.e.* if $\mathcal{G}$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ belong to different Laue classes, the further generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ always change the orientation of the basis in direct and in reciprocal space. Therefore, the indices of the structure factors are permuted, but their phases are transformed only if $\boldsymbol{p}\neq\boldsymbol{0}$. The choice between these equivalent descriptions of the crystal structure is made when indexing the reflection pattern. In the case of anomalous scattering, the similar choice between the absolute structures is also combined with the indexing procedure.

Example

According to Table 15.2.1.3, eight equivalent descriptions exist for each crystal structure with symmetry $F222$. Four of them differ only by an origin shift and the other four are enantiomorphic to the first four. $t(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ transforms all phases according to $\varphi'(\boldsymbol{h})=\varphi(\boldsymbol{h})-(\pi/2)(h+k+l)$, which gives rise to four parity classes of structure factors: $h+k+l=4n, 4n+1, 4n+2$ and $4n+3$ (n integer). As $t(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ generates all additional translations of $\mathcal{K}(F222)$, restriction of one phase $\varphi(\boldsymbol{h}_1)$ to a range of length $\pi/2$ fixes the origin. Restriction of a second phase $\varphi(\boldsymbol{h}_2)$ to an appropriately chosen range of length π discriminates between pairs of enantiomorphic descriptions in the absence of anomalous scattering. For $\bar{1}(000)$, the corresponding change of phases is $\varphi'(\boldsymbol{h})=-\varphi(\boldsymbol{h})$. Table 15.3.3.1 shows, for structure factors from all parity classes, how their phases depend on the chosen description of the crystal structure. Only phases from parity classes $h+k+l=4n+1$ or $4n+3$ determine the origin in a unique way. The phase $\varphi(\boldsymbol{h}_2)$ that fixes the absolute structure may be chosen from any parity class but the appropriate range for its restriction depends on the parity classes of $\varphi(\boldsymbol{h}_1)$ *and* $\varphi(\boldsymbol{h}_2)$ and, moreover, on the range chosen for $\varphi(\boldsymbol{h}_1)$. If, for instance, $\varphi(\boldsymbol{h}_1)$ with $h+k+l=4n+1$ is restricted to $\pi/2\leq\varphi(\boldsymbol{h}_1)<\pi$, one of the following restrictions may be chosen for $\varphi(\boldsymbol{h}_2): 0<\varphi(\boldsymbol{h}_2)<\pi$ for $h+k+l=4n$; $-\pi/2<\varphi(\boldsymbol{h}_2)<\pi/2$ for $h+k+l=4n+2$; $-\pi/4<\varphi(\boldsymbol{h}_2)<3\pi/4$ for $h+k+l=4n+1$; $-3\pi/4<\varphi(\boldsymbol{h}_2)<\pi/4$ for $h+k+l=4n+3$. If, however, the phase $\varphi(\boldsymbol{h}_1)$ of the same first reflection was restricted to $-\pi/4\leq\varphi(\boldsymbol{h}_1)<3\pi/4$, the possible restrictions for the second phase change to: $0<\varphi(\boldsymbol{h}_2)<\pi$ for $h+k+l=4n$ or $4n+2$; $-\pi/2<\varphi(\boldsymbol{h}_2)<\pi/2$ for $h+k+l=4n+1$ or $4n+3$ (for further details, *cf.* Koch, 1986).

15.3.4. Euclidean- and affine-equivalent sub- and supergroups

The Euclidean or affine normalizer of a space group $\mathcal{G}$ maps any subgroup or supergroup of $\mathcal{G}$ either onto itself or onto another subgroup or supergroup of $\mathcal{G}$. Accordingly, these normalizers define equivalence relationships on the sets of subgroups and supergroups of $\mathcal{G}$ (Koch, 1984*b*):

Two *subgroups* or *supergroups* of a space group $\mathcal{G}$ are called *Euclidean-* or $\mathcal{N}_{\mathcal{E}}$*- equivalent* (*affine-* or $\mathcal{N}_{\mathcal{A}}$*- equivalent*) if they are mapped onto each other by an element of the Euclidean (affine) normalizer of $\mathcal{G}$, *i.e.* if they are conjugate subgroups of the Euclidean (affine) normalizer.

In the following, the term 'equivalent subgroups (supergroups)' is used if a statement is true for Euclidean-equivalent *and* affine-equivalent subgroups (supergroups), and $\mathcal{N}(\mathcal{G})$ is used to designate the Euclidean as well as the affine normalizer.

The knowledge of Euclidean-equivalent subgroups is necessary in connection with the possible deformations of a crystal structure due to subgroup degradation. Affine-equivalent subgroups play an important role for the derivation and classification of black-and-white groups (magnetic groups) and of colour groups (*cf.* for example Schwarzenberger, 1984). Information on equivalent supergroups is useful for the determination of the idealized type of a crystal structure.

For any pair of space groups $\mathcal{G}$ and $\mathcal{H}$ with $\mathcal{H}<\mathcal{G}$, the relation between the two normalizers $\mathcal{N}(\mathcal{G})$ and $\mathcal{N}(\mathcal{H})$ controls the subgroups of $\mathcal{G}$ that are equivalent to $\mathcal{H}$ and the supergroups of $\mathcal{H}$ equivalent to $\mathcal{G}$. The intersection group of both normalizers, $\mathcal{M}(\mathcal{G},\mathcal{H})=\mathcal{N}(\mathcal{G})\cap\mathcal{N}(\mathcal{H})\geq\mathcal{H}$ may or may not coincide with $\mathcal{N}(\mathcal{G})$ and/or with $\mathcal{N}(\mathcal{H})$. The following two statements hold generally:

(i) The index i_g of $\mathcal{M}(\mathcal{G},\mathcal{H})$ in $\mathcal{N}(\mathcal{G})$ equals the number of subgroups of $\mathcal{G}$ which are equivalent to $\mathcal{H}$. Each coset of $\mathcal{M}(\mathcal{G},\mathcal{H})$ in $\mathcal{N}(\mathcal{G})$ maps $\mathcal{H}$ onto another equivalent subgroup of $\mathcal{G}$.

(ii) The index i_h of $\mathcal{M}(\mathcal{G},\mathcal{H})$ in $\mathcal{N}(\mathcal{H})$ equals the number of supergroups of $\mathcal{H}$ equivalent to $\mathcal{G}$. Each coset of $\mathcal{M}(\mathcal{G},\mathcal{H})$ in $\mathcal{N}(\mathcal{H})$ maps $\mathcal{G}$ onto another equivalent supergroup of $\mathcal{H}$.

Equivalent subgroups are *conjugate* in $\mathcal{G}$ if and only if $\mathcal{G}\cap\mathcal{N}(\mathcal{H})\neq\mathcal{G}$. In this case, $\mathcal{G}$ contains elements not belonging to $\mathcal{N}(\mathcal{H})$ and the cosets of $\mathcal{G}\cap\mathcal{N}(\mathcal{H})$ in $\mathcal{G}$ refer to the different conjugate subgroups.

Examples

(1) $\mathcal{G}=Cmmm$ has four monoclinic subgroups of type $P2/m$ with the same orthorhombic metric and the same basis as $Cmmm$: $\mathcal{H}_1=P2/m11$, $\mathcal{H}_2=P12/m1$, $\mathcal{H}_3=P112/m$ ($\bar{1}$ at 000), $\mathcal{H}_4=P112/m$ ($\bar{1}$ at $\frac{1}{4}\frac{1}{4}0$). According to Table 15.2.1.3, the

Euclidean normalizer of $\mathcal{G}$ is $Pmmm(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$. Because of the orthorhombic metric of all four subgroups, their Euclidean normalizers $\mathcal{N}_{\mathcal{E}}(\mathcal{H}_1)$, $\mathcal{N}_{\mathcal{E}}(\mathcal{H}_2)$, $\mathcal{N}_{\mathcal{E}}(\mathcal{H}_3)$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{H}_4)$ are enhanced in comparison with the general case and coincide with $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$. Hence, no two of the four subgroups are Euclidean-equivalent.

(2) $\mathcal{G} = I\overline{4}m2(\mathbf{a},\mathbf{b},\mathbf{c})$, $\mathcal{H} = P\overline{4}(\mathbf{a},\mathbf{b},\mathbf{c})$.
$\mathcal{N}(\mathcal{G}) = I4/mmm(\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ is a supergroup of index 2 of $\mathcal{N}(\mathcal{H}) = P4/mmm(\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}) = \mathcal{M}(I\overline{4}m2, P\overline{4})$. Therefore, $I\overline{4}m2$ has two equivalent subgroups $P\overline{4}$ that are mapped onto another by a centring translation of $\mathcal{N}(\mathcal{G})$, *e.g.* by $t(0\frac{1}{2}\frac{1}{4})$. Both subgroups are not conjugate in $I\overline{4}m2$ because $\mathcal{G} \cap \mathcal{N}(\mathcal{H})$ equals $\mathcal{G}$. As $\mathcal{N}(\mathcal{H})$ coincides with $\mathcal{M}(\mathcal{G},\mathcal{H})$, no further supergroups of $P\overline{4}$ equivalent to $I\overline{4}m2$ exist.

(3) $\mathcal{G} = Fm\overline{3}(\mathbf{a},\mathbf{b},\mathbf{c})$, $\mathcal{H} = F23(\mathbf{a},\mathbf{b},\mathbf{c})$.
$\mathcal{N}(\mathcal{H}) = Im\overline{3}m(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ is a supergroup of index 2 of $\mathcal{N}(\mathcal{G}) = Pm\overline{3}m(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}) = \mathcal{M}(Fm\overline{3}, F23)$. Therefore, $F23$ has two equivalent supergroups $Fm\overline{3}$ that differ in their locations with site symmetry $m\overline{3}$ by a centring translation of $Im\overline{3}m(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$, *e.g.* by $t(\frac{1}{4}\frac{1}{4}\frac{1}{4})$. As $\mathcal{N}(\mathcal{G})$ coincides with $\mathcal{M}(\mathcal{G},\mathcal{H})$, no further subgroups of $Fm\overline{3}$ equivalent to $F23$ exist.

(4) $\mathcal{G} = Pmma(\mathbf{a},\mathbf{b},\mathbf{c})$, $\mathcal{H} = Pmmn(\mathbf{a}, 2\mathbf{b}, \mathbf{c})$.
The intersection of $\mathcal{N}_{\mathcal{A}}(Pmma) = Pmmm(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ and $\mathcal{N}_{\mathcal{A}}(Pmmn) = P4/mmm(\frac{1}{2}\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c})$ is the group $\mathcal{M}(Pmma, Pmmn) = Pmmm(\frac{1}{2}\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c})$, which is a proper subgroup of both normalizers. As i_g equals 2, $Pmma$ has two affine-equivalent subgroups of type $Pmmn$ that are mapped onto each other by the additional translation $t(0\frac{1}{2}0)$ of the normalizer of $\mathcal{G}$. As i_h also equals 2, $Pmmn$ has two affine-equivalent supergroups, $Pmma$ and $Pmmb$, that are mapped onto each other, *e.g.* by the affine 'reflection' at a diagonal 'mirror plane' of $\mathcal{N}_{\mathcal{A}}(\mathcal{H})$.

15.3.5. Reduction of the parameter regions to be considered for geometrical studies of point configurations

Each point configuration with space-group symmetry $\mathcal{G}$ may be described by its metrical and coordinate parameters. To cover all point configurations belonging to a certain space-group type exactly once, the metrical parameters of $\mathcal{G}$ have to be varied without restrictions, whereas the coordinate parameters x, y and z must be restricted to one asymmetric unit of $\mathcal{G}$. For the study of the geometrical properties of point configurations (*e.g.* sphere-packing conditions or types of Dirichlet domains, *etc.*), the Euclidean normalizers (*cf. e.g.* Laves, 1931; Fischer, 1971, 1991; Koch, 1984*a*) as well as the affine normalizers (*cf.* Fischer, 1968) of the space groups allow a further reduction of the parameter regions that have to be considered.

Examples

(1) $\mathcal{G} = P4/m$ with asymmetric unit $0 \le x \le \frac{1}{2}$, $0 < y < \frac{1}{2}$, $0 \le z \le \frac{1}{2}$: A geometrical consideration may be restricted to one asymmetric unit of $\mathcal{N}_{\mathcal{E}}(\mathcal{G}) = \mathcal{N}_{\mathcal{A}}(\mathcal{G}) = P4/mmm(\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$, *i.e.* to the region $0 \le x \le \frac{1}{2}$, $y \le \min(x, \frac{1}{2} - x)$, $0 \le z \le \frac{1}{4}$. All metrical parameters are unrestricted.

(2) $\mathcal{G} = P4$ with asymmetric unit $0 \le x \le \frac{1}{2}$, $0 < y < \frac{1}{2}$, $0 \le z < 1$: The normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G}) = \mathcal{N}_{\mathcal{A}}(\mathcal{G}) = P^1 4/mmm(\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c})$ restricts the parameter region to be considered to $0 \le x \le \frac{1}{2}$, $y \le \min(x, \frac{1}{2} - x)$, $z = 0$. Again, no restriction exists for the metrical parameters.

(3) $\mathcal{G} = Pmmm$ with asymmetric unit $0 \le x \le \frac{1}{2}$, $0 \le y \le \frac{1}{2}$, $0 \le z \le \frac{1}{2}$: The Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G}) = Pmmm(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ reduces the parameter region to be considered to $0 \le x \le \frac{1}{4}$, $0 \le y \le \frac{1}{4}$, $0 \le z \le \frac{1}{4}$. All metrical parameters are unrestricted. The affine normalizer $\mathcal{N}_{\mathcal{A}}(\mathcal{G}) = Pm\overline{3}m(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ enables a further reduction of the parameter region that has to be studied. For this, two different possibilities exist:

(i) the metrical parameters remain unrestricted but the coordinate parameters are limited to one asymmetric unit of $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$, *i.e.* to $0 \le x \le \frac{1}{4}$, $0 \le y \le x$, $0 \le z \le y$;

(ii) the coordinate parameters are not further restricted, but the metrical parameters have to obey *e.g.* the relation $a \le b \le c$, *i.e.* $a/c \le b/c \le 1$.

(4) $\mathcal{G} = P112/m$ with asymmetric unit $0 \le x < 1, 0 \le y \le \frac{1}{2}$, $0 \le z \le \frac{1}{2}$. The Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G}) = P112/m(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ reduces the region that has to be considered for the coordinate parameters to $0 \le x < \frac{1}{2}$, $0 \le y \le \frac{1}{4}$, $0 \le z \le \frac{1}{4}$, but it does not impose restrictions on the metrical parameters. These may be restricted, however, to the range $a/b \le 1$ and $0 \le 2\cos\gamma \le -a/b$ (as shown in Fig. 15.2.1.1) by means of the affine normalizer $\mathcal{N}_{\mathcal{A}}(P112/m)$.

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15.4. Normalizers of point groups

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Normalizers with respect to the Euclidean or affine group may be defined for any group of isometries (*cf.* Gubler, 1982*a*,*b*). For a point group, however, it seems inadequate to use a supergroup that contains transformations that do not map a fixed point of that point group onto itself. Appropriate supergroups for the definition of normalizers of point groups are the full isometry groups of the sphere, $m\overline{\infty}$, and of the circle, ∞m, in three-dimensional and two-dimensional space (*cf.* Galiulin, 1978).

These normalizers are listed in Tables 15.4.1.1 and 15.4.1.2. It has to be noticed that the normalizer of a crystallographic point group may contain continuous rotations, *i.e.* rotations with infinitesimal rotation angle, or noncrystallographic rotations (∞m; $m\overline{\infty}, \infty/mm, 8mm, 12mm$; $8/mmm, 12/mmm$). In analogy to space groups, these normalizers define equivalence relationships on the 'Wyckoff positions' of the point groups (*cf.* Section 10.1.2). They give also the relation between the different but equivalent morphological descriptions of a crystal.

Table 15.4.1.1. *Normalizers of the two-dimensional point groups with respect to the full isometry group of the circle*

The upper part refers to the crystallographic, the lower part to the noncrystallographic point groups as listed in Table 10.1.4.1.

Normalizer	Point groups
∞m	1, 2, 4, 3, 6
$12mm$	$6mm$
$8mm$	$4mm$
$6mm$	$3m$
$4mm$	$2mm$
$2mm$	m
∞m	$n, \infty, \infty m$
$(2n)mm$	nmm, nm

Table 15.4.1.2. *Normalizers of the three-dimensional point groups with respect to the full isometry group of the sphere*

The upper part refers to the crystallographic, the lower part to the noncrystallographic point groups as listed in Table 10.1.4.2.

Normalizer	Point groups
$m\overline{\infty}$	$1, \bar{1}$
$m\bar{3}m$	$222, mmm, 23, m\bar{3}, 432, \bar{4}3m, m\bar{3}m$
∞/mm	$2, m, 2/m, 4, \bar{4}, 4/m, 3, \bar{3}, 6, \bar{6}, 6/m$
$12/mmm$	$622, 6mm, 6/mmm$
$8/mmm$	$422, 4mm, 4/mmm$
$6/mmm$	$32, 3m, \bar{3}m, \bar{6}2m$
$4/mmm$	$mm2, \bar{4}2m$
$m\overline{\infty}$	$2\infty, m\overline{\infty}$
$m\overline{35}$	$235, m\overline{35}$
∞/mm	$n, \bar{n}, n/m, \infty, \infty/m, \infty 2, \infty m, \infty/mm$
$(2n)/mmm$	$n22, nmm, n/mmm, n2, nm, \bar{n}m$
n/mmm	$\bar{n}2m$

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