INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY

Volume A

SPACE-GROUP SYMMETRY

Edited by

THEO HAHN

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Contents

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.

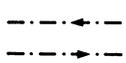
The electronic preparation of the plane- and space-group tables was carried out on various Unix and Windows-based computers in Sofia, Bilbao and Karlsruhe. The development of the computer programs and the layout macros in the package file was done in parallel by different members of the team, which included 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.

SAMPLE PAGES

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

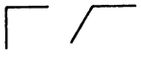
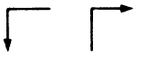
BY TH. HAHN

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.

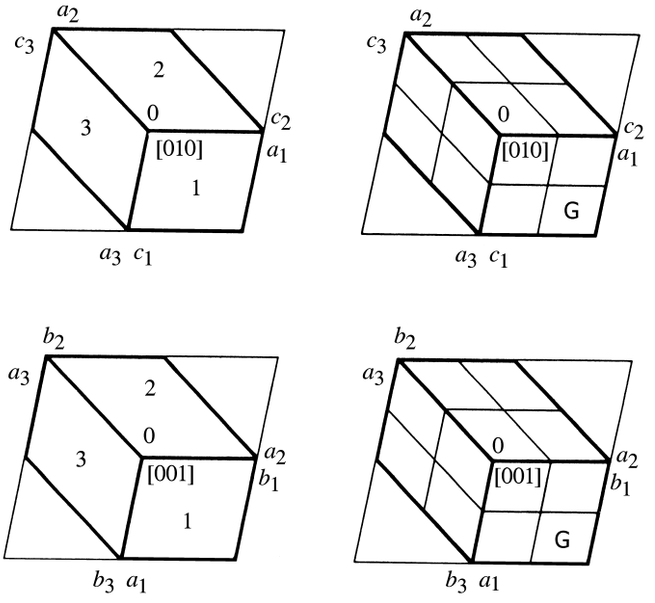


Fig. 2.2.6.4. Monoclinic space groups, cell choices 1, 2, 3. Upper pair of diagrams: setting with unique axis *b*. Lower pair of diagrams: setting with unique axis *c*. The numbers 1, 2, 3 within the cells and the subscripts of the labels of the axes indicate the cell choice (*cf.* Section 2.2.16). The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

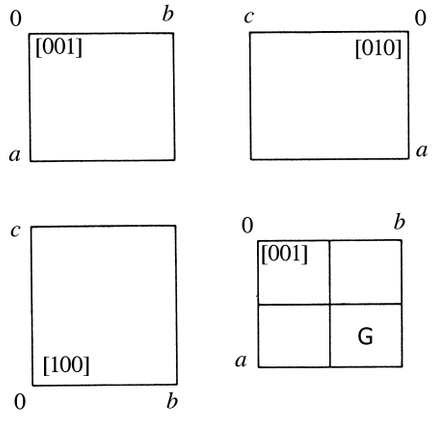


Fig. 2.2.6.5. Orthorhombic space groups. Diagrams for the 'standard setting' as described in the space-group tables (G = general-position diagram).

* 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**, $\mathbf{ab\bar{c}}$, $\mathbf{\bar{a}b\bar{c}}$, $\mathbf{\bar{a}bc}$ and the left-handed systems $\mathbf{\bar{a}\bar{b}c}$, $\mathbf{\bar{a}b\bar{c}}$, $\mathbf{a\bar{b}\bar{c}}$.

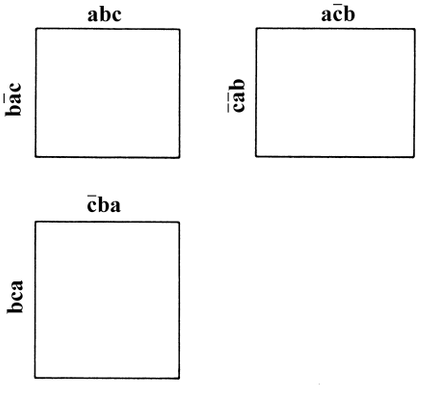


Fig. 2.2.6.6. Orthorhombic space groups. The three projections of the symmetry elements with the six setting symbols (see text). For setting symbols printed vertically, the page has to be turned clockwise by 90° or viewed from the side. Note that in the actual space-group tables instead of the setting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

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: p*3*m*1 (14)

The symbol of this plane group, described by the triple cell *h,* is *h*31*m,* where the symmetry elements of the secondary and tertiary positions are interchanged. 'Decentring' the *h* cell gives rise to maximal non-isomorphic *k* subgroups *p*31*m* of index [3], with lattice parameters $a\sqrt{3}, a\sqrt{3}$ (*cf.* Section 4.3.5).

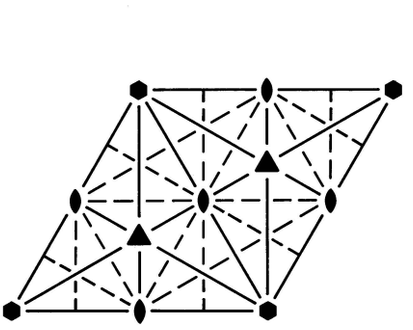
Table 4.2.1.1. *Index of symbols for plane groups*

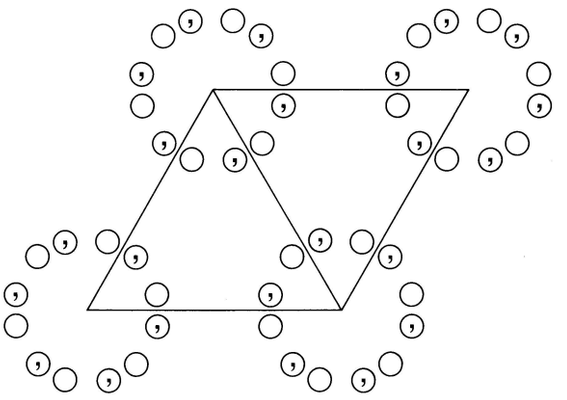
System and lattice symbol	Point group	No. of plane group	Hermann–Mauguin symbol			Full symbol for other setting	Multiple cell
			Short	Full	Extended		
Oblique *p*	1 2	1 2		*p*1 *p*2			
Rectangular *p*, *c*	*m* 2*mm*	3 4 5 6 7 8 9	*pm* *pg* *cm*	*p*1*m*1 *p*1*g*1 *c*1*m*1 *p*2*mm* *p*2*mg* *p*2*gg* *c*2*mm*	 *c*1*m*1 *g* *c*2*mm* *g g*	*p*11*m* *p*11*g* *c*11*m* *p*2*mm* *p*2*gm* *p*2*gg* *c*2*mm*	
Square *p*	4 4*mm*	10 11 12		*p*4 *p*4*mm* *p*4*gm*	 *p*4*mm* *g* *p*4*gm* *g*		*c*4 *c*4*mm* *g* *c*4*mg* *g*
Hexagonal *p*	3 3*m* 6 6*mm*	13 14 15 16 17		*p*3 *p*3*m*1 *p*31*m* *p*6 *p*6*mm*	 *p*3*m*1 *g* *p*31*m* *g* *p*6*mm* *g g*		*h*3 *h*31*m* *g* *h*3*m*1 *g* *h*6 *h*6*mm* *g g*

*p*6*mm* 6*mm* Hexagonal

No. 17 *p*6*mm*

Patterson symmetry *p*6*mm*





Origin at 6*mm*

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

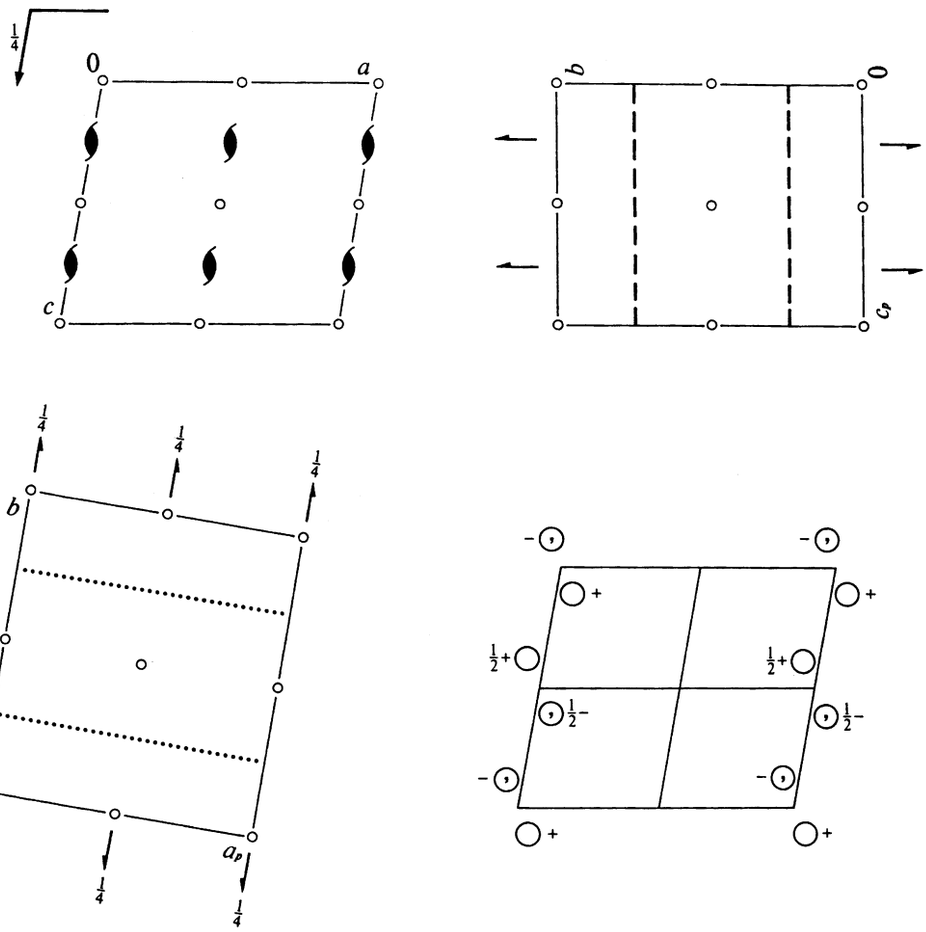
I none

II none

No. 14 $P12_1/c1$

Patterson symmetry $P12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (3) $\bar{1}$ $0,0,0$ (4) c $x,\frac{1}{4},z$

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)

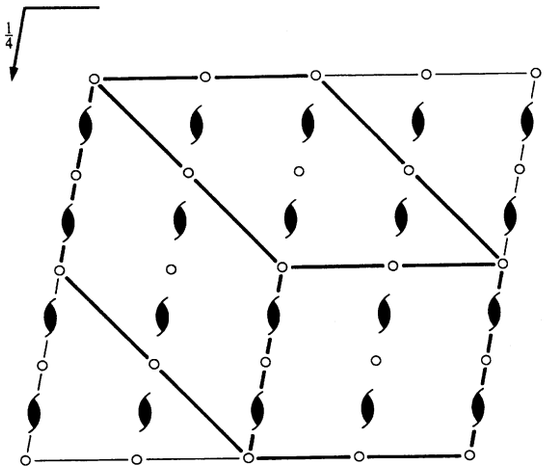
Minimal non-isomorphic supergroups

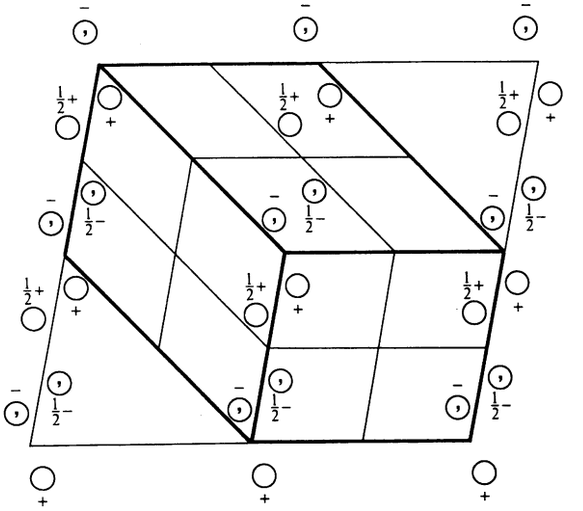
I [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pbam$ (55); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pnnm$ (58); [2] $Pbcn$ (60); [2] $Pbca$ (61); [2] $Pnma$ (62); [2] $Cmce$ (64)

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)

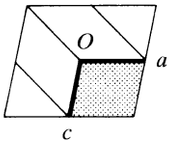
No. 14

UNIQUE AXIS b, DIFFERENT CELL CHOICES





$P12_1/c1$



UNIQUE AXIS b, CELL CHOICE 1

Origin at $\bar{1}$

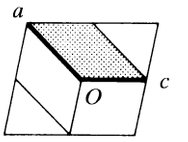
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

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) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(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 : $k+l=2n$

$P12_1/n1$



UNIQUE AXIS b, CELL CHOICE 2

Origin at $\bar{1}$

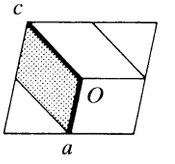
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

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 : $h+k+l=2n$

$P12_1/a1$



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 : $h+k=2n$

8.2. Classifications of space groups, point groups and lattices

BY H. WONDRATSCHEK

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

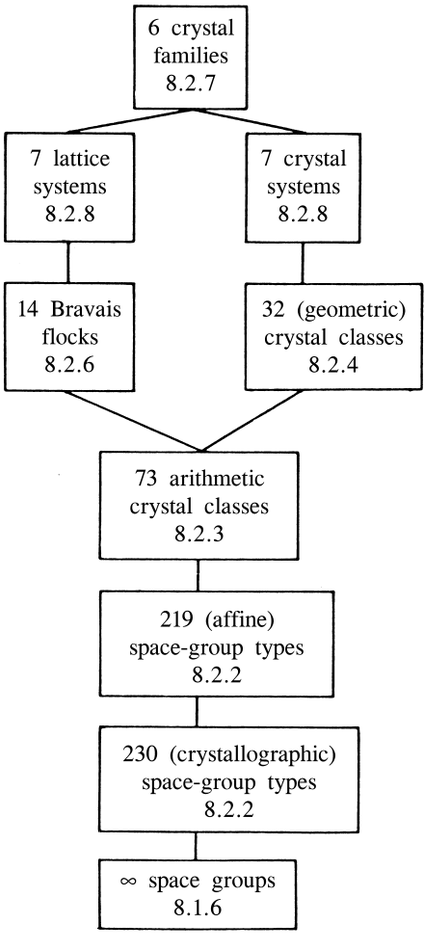
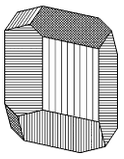
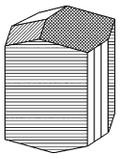
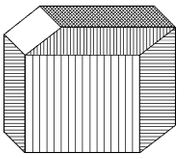
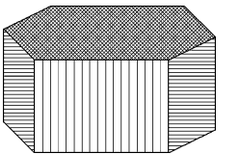
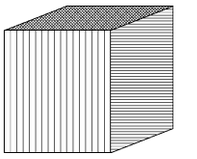


Fig. 8.2.1.1. Classifications of space groups. In each box, the number of classes, *e.g.* 32, and the section in which the corresponding term is defined, *e.g.* 8.2.4, are stated.

* 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).

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

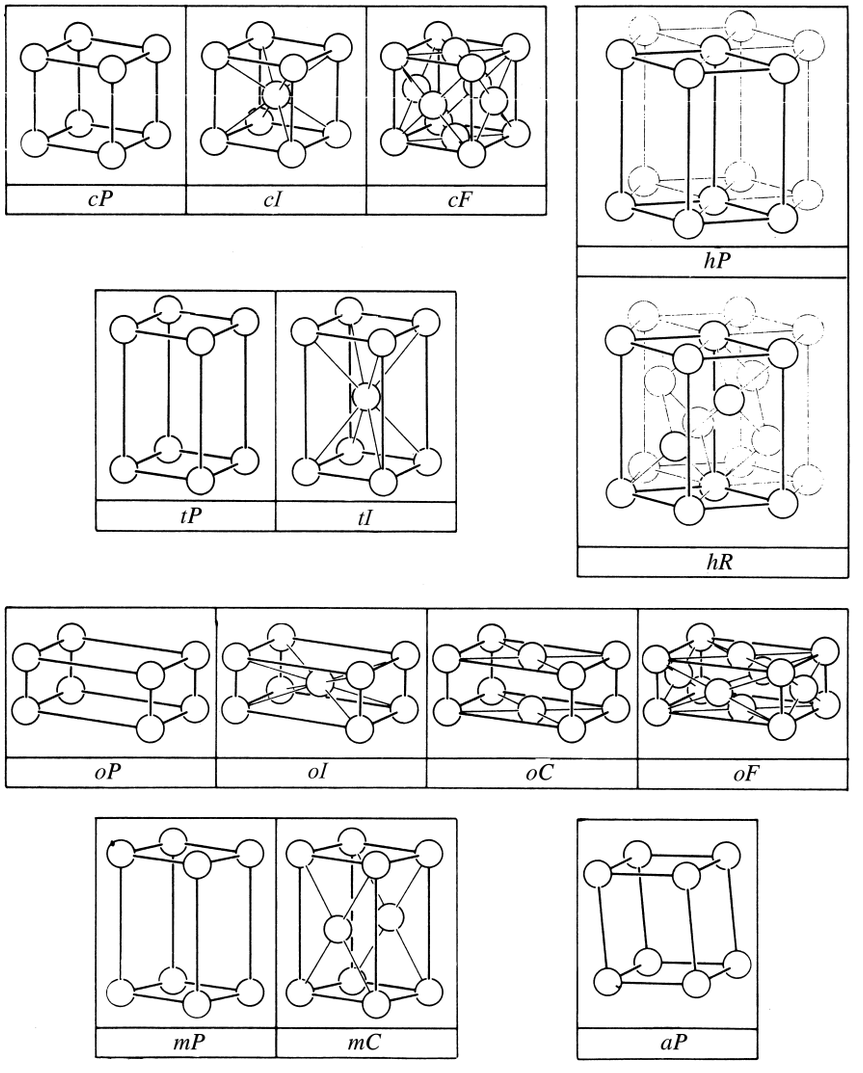
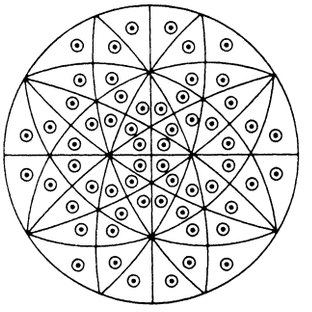


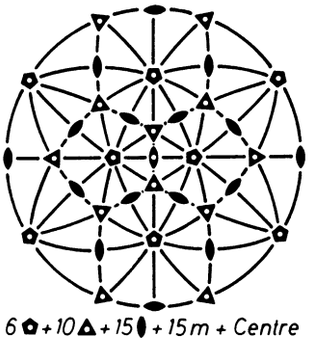
Fig. 9.1.7.1. Conventional cells of the three-dimensional Bravais lattices (for symbols see Table 9.1.7.2).

Table 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 $\|l\| < 0.382\|k\|$ $0, y, z$ *with* $\|z\| < 0.382\|y\|$
			Deltoid-hexecontahedron *Rhomb-triacontahedron & pentagon-dodecahedron & icosahedron* (poles between axes $\bar{3}$ and $\bar{5}$)	$(0kl)$ with $0.382\|k\| < \|l\| < 1.618\|k\|$ $0, y, z$ *with* $0.382\|y\| < \|z\| < 1.618\|y\|$
			Pentakisdodecahedron *Icosahedron truncated by pentagon-dodecahedron* (poles between axes $\bar{5}$ and 2)	$(0kl)$ with $\|l\| > 1.618\|k\|$ $0, y, z$ *with* $\|z\| > 1.618\|y\|$
30	*c*	2*mm*..	Rhomb-triacontahedron *Icosadodecahedron* (= *pentagon-dodecahedron & icosahedron*)	(100) *x*, 0, 0
20	*b*	3*m* (*m*3.)	Regular icosahedron *Regular pentagon-dodecahedron*	(111) *x*, *x*, *x*
12	*a*	5*m* (*m*.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 [1τ0]
2*mm*	6*mm*	10*mm*

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.

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 $\mathcal{N}_E(\mathcal{G})$ 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: $C12/m1$,

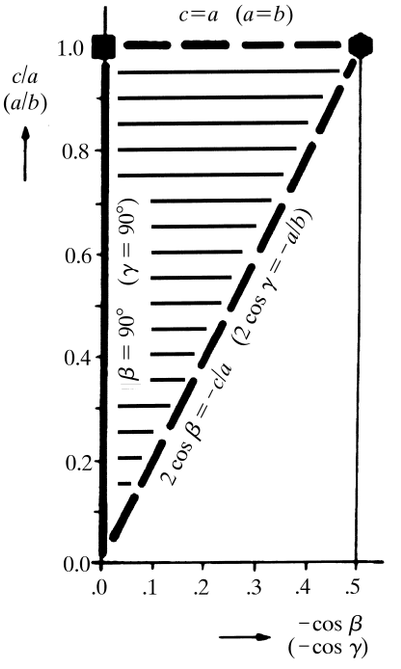


Fig. 15.2.1.1. Parameter range for space groups of types $P2$, $P2_1$, Pm, $P2/m$ and $P2_1/m$ (plane groups of types $p1$ and $p2$). The information in parentheses refers to unique axis *c*.

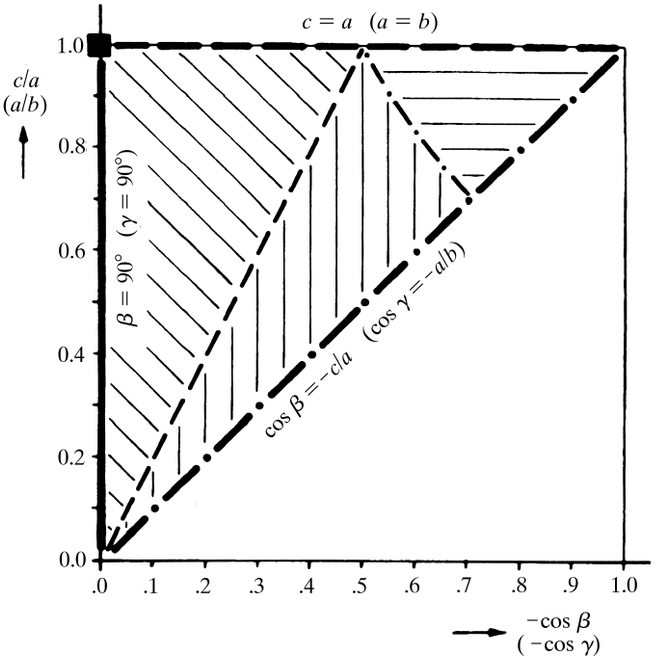


Fig. 15.2.1.2. Parameter range for space groups of types $C2$, Pc, Cm, Cc, $C2/m$, $P2/c$, $P2_1/c$ and $C2/c$:
unique axis *b*, cell choice 2: $P1n1$, $P12/n1$, $P12_1/n1$;
unique axis *b*, cell choice 3: $I121$, $I1m1$, $I1a1$, $I12/m1$, $I12/a1$;
unique axis *c*, cell choice 2: $P11n$, $P112/n$, $P112_1/n$;
unique axis *c*, cell choice 3: $I112$, $I11m$, $I11b$, $I112/m$, $I112/b$.
The information in parentheses refers to unique axis *c*.