INTERNATIONAL TABLES for CRYSTALLOGRAPHY

Volume

A

Space-group symmetry

Edited by Th. Hahn

Fifth edition

INTERNATIONAL TABLES
FOR
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SPACE-GROUP SYMMETRY

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THEO HAHN

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† Deceased.

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. Ibers (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

* 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}$2*m* (121), *I*4/*mmm* (139), *I*4/*mcm* (140);
Cubic:	*Fm*$\bar{3}$ (202), *Fm*$\bar{3}$*m* (225), *Fm*$\bar{3}$*c* (226), *I*$\bar{4}$3*m* (217), *Im*$\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

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.

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