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In 1919, Paul Niggli (1888–1953) published the first compilation of space groups in a form that has been the basis for all later space-group tables, in particular for the first volume of the trilingual series *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935), for *International Tables for X-ray Crystallography* Volume I (1952) and for *International Tables for Crystallography* Volume A (1983). The tables in his book *Geometrische Kristalographie des Diskontinuums* (1919) contained lists of the *Punktlagen*, now known as Wyckoff positions. He was a great universal geoscientist, his work covering all fields from crystallography to petrology.

Carl Hermann (1899–1963) published among his seminal works four famous articles in the series *Zur systematischen Strukturtheorie* I to IV in *Z. Kristallogr.* 68 (1928) and 69 (1929). The first article contained the background to the Hermann–Mauguin space-group symbolism. The last article was fundamental to the theory of subgroups of space groups and forms the basis of the maximal-subgroup tables in the present volume. In addition, he was the editor of the first volume of the trilingual series *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935) and one of the founders of *n*-dimensional crystallography, $n > 3$. 
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Acknowledgments

Work on Parts 1 and 2 of this volume was spread out over a long period of time and there have been a number of colleagues and friends who have helped us in the preparation of this book. We are particularly grateful to Professor Th. Hahn, RWTH Aachen, Germany, not only for providing the initial impetus for this work but also for his constant interest and support. His constructive proposals on the arrangement and layout of the tables of Part 2 improved the presentation of the data and his stimulating comments contributed considerably to the content and the organization of Part 1, particularly Chapter 1.2.

Chapter 1.1 contains a contribution by Professor Y. Billiet, Bourg-Blanc, France, concerning isomorphic subgroups.

Nearly all contributors to this volume, but particularly Professors J. Neubüser and W. Plesken, RWTH Aachen, Germany, and Professor M. I. Aroyo, Universidad del País Vasco, Bilbao, Spain, commented on Chapter 1.2, correcting the text and giving valuable advice. Section 1.2.7 was completely reworked after intensive discussions with Professor V. Janovec, University of Liberec, Czech Republic, making use of his generously offered expertise in the field of domains.

In the late 1960s and early 1970s, J. Neubüser and his team at RWTH Aachen, Germany, calculated the basic lattices of non-isomorphic subgroups by computer. The results now form part of the content of the tables of Chapters 2.2 and 2.3. The team provided a great deal of computer output which was used for the composition of earlier versions of the present tables and for their checking by hand. The typing and checking of the original tables was done with great care and patience by Mrs R. Henke and many other members of the Institut für Kristallographie, Universität Karlsruhe, Germany.

The graphs of Chapters 2.4 and 2.5 were drawn and checked by Professor W. E. Klee, Dr R. Cruse and numerous students and technicians at the Institut für Kristallographie, Universität Karlsruhe, Germany, around 1970. M. I. Aroyo recently rechecked the graphs and transformed the hand-drawn versions into computer graphics.

We are grateful to Dr L. L. Boyle, University of Kent, Canterbury, England, who read, commented on and improved all parts of the text, in particular the English. We thank Professors J. M. Perez-Mato and G. Madariaga, Universidad del País Vasco, Bilbao, Spain, for many helpful discussions on the content and the presentation of the data. M. I. Aroyo would like to note that most of his contribution to this volume was made during his previous appointment in the Faculty of Physics, University of Sofia, Bulgaria, and he is grateful to his former colleagues, especially Drs J. N. Kotzev and M. Mikhov, for their interest and encouragement during this time.

We are indebted to Dr G. Nolze, Bundesanstalt für Materialforschung, Berlin, Germany, for checking the data of Chapter 3.2 using his computer program POWDER CELL. We also thank Mrs S. Funke and Mrs H. Sippel, Universität Kassel, Germany, who rechecked a large part of the relations of the Wyckoff positions in this chapter.

MRS S. E. BARNES, DR N. J. ASHCROFT and the rest of the staff of the International Union of Crystallography in Chester took care of the successful technical production of this volume. In particular, we wish to thank Dr Ashcroft for her tireless help in matters of English style and her guidance in shaping the volume to fit the style of the International Tables series.

We gratefully acknowledge the financial support received from various organizations which helped to make this volume possible: in the early stages of the project from the Deutsche Forschungsgemeinschaft, Germany, and more recently from the Alexander von Humboldt-Stiftung, Germany, the International Union for Crystallography, the Sofia University Research Fund, Bulgaria, and the Universidad del País Vasco, Bilbao, Spain.
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Symmetry and periodicity are among the most fascinating and characteristic properties of crystals by which they are distinguished from other forms of matter. On the macroscopic level, this symmetry is expressed by point groups, whereas the periodicity is described by translation groups and lattices, and the full structural symmetry of crystals is governed by space groups.

The need for a rigorous treatment of space groups was recognized by crystallographers as early as 1935, when the first volume of the trilingual series *Internationale Tabellen zur Bestimmung von Kristallstrukturen* appeared. It was followed in 1952 by Volume I of *International Tables for X-ray Crystallography* and in 1983 by Volume A of *International Tables for Crystallography* (fifth edition 2002). As the depth of experimental and theoretical studies of crystal structures and their properties increased, particularly with regard to comparative crystal chemistry, polymorphism and phase transitions, it became apparent that not only the space group of a given crystal but also its ‘descent’ and ‘ascent’, i.e. its sub- and supergroups, are of importance and have to be derived and listed.

This had already been done in a small way in the 1935 edition of *Internationale Tabellen zur Bestimmung von Kristallstrukturen* with the brief inclusion of the *translationengleiche* subgroups of the space groups (see the first volume, pp. 82, 86 and 90). The 1952 edition of *International Tables for X-ray Crystallography* did not contain sub- and supergroups, but in the 1983 edition of *International Tables for Crystallography* the full range of maximal subgroups was included (see Volume A, pp. 35–38): *translationengleiche* (type I) and *klassengleiche* (type II), the latter subdivided into ‘decentred’ (IIa), ‘enlarged unit cell’ (IIb) and ‘isomorphic’ (IIc) subgroups. For types I and IIa, all subgroups were listed individually, whereas for IIb only the *subgroup types* and for IIc only the *subgroups of lowest index* were given.

All these data were presented in the form known in 1983, and this involved certain omissions and shortcomings in the presentation, e.g. no Wyckoff positions of the subgroups and no conjugacy relations were given. Meanwhile, both the theory of subgroups and its application have made considerable progress, and the present Volume A1 is intended to fill the gaps left in Volume A and present the ‘complete story’ of the sub- and supergroups of space groups in a comprehensive manner. In particular, all maximal subgroups of types I, IIa and IIb are listed individually with the appropriate transformation matrices and origin shifts, whereas for the infinitely many maximal subgroups of type IIc expressions are given which contain the complete characterization of all isomorphic subgroups for any given index.

In addition, the relations of the Wyckoff positions for each group–subgroup pair of space groups are listed for the first time in the tables of Part 3 of this volume.

Volume A1 is thus a companion to Volume A, and the editors of both volumes have cooperated closely on problems of symmetry for many years. I wish Volume A1 the same acceptance and success that Volume A has enjoyed.
Group–subgroup relations between space groups, the subject of this volume, are an important tool in crystallographic, physical and chemical investigations. In addition to listing these relations, the corresponding relations between the Wyckoff positions of the group–subgroup pairs are also listed here.

The basis for these tables was laid by the pioneering papers of Carl Hermann in the late 1920s. Some subgroup data were made available in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935), together with a graph displaying the symmetry relations between the crystallographic point groups.

Since then, the vast number of crystal structures determined and improvements in experimental physical methods have directed the interest of crystallographers, physicists and chemists to the problems of structure classification and of phase transitions. Methods of computational mathematics have been developed and applied to the problems of crystallographic group theory and group–subgroup relations.

When the new series *International Tables for Crystallography* began to appear in 1983, the subgroup data that were then available were included in Volume A. However, these data were incomplete and their description was only that which was available in the late 1970s. This is still the case in the present (fifth) edition of Volume A.

The subgroup data for the space groups are now complete and form the basis of this volume. After introductory chapters on group-theoretical aspects of space groups, group–subgroup relations between space groups and the underlying mathematical background, this volume provides the reader (in many cases for the first time) with:

1. complete listings of all maximal non-isomorphic subgroups for each space group, not just by type but individually, including their general positions or their generators, their conjugacy relations and transformations to conventional settings;
2. listings of the maximal isomorphic subgroups with index 2, 3 or 4 individually in the same way as for non-isomorphic subgroups;
3. listings of all maximal isomorphic subgroups as members of infinite series, but with the same information as for non-isomorphic subgroups;
4. data for non-isomorphic supergroups for all space groups (these are already in Volume A) such that the subgroup data may be reversed for problems that involve supergroups of space groups;
5. two kinds of graphs for all space groups displaying their types of translationengleiche subgroups and their types of non-isomorphic klassengleiche subgroups;
6. listings of the splittings of all Wyckoff positions for each space group if its symmetry is reduced to that of a subgroup. These data include the corresponding coordinate transformations such that the coordinates in the subgroup can be obtained easily from the coordinates in the original space group;
7. examples explaining how the data in this volume can be used.

The subgroup data in this volume are indispensable for a thorough analysis of phase transitions that do not involve drastic structural changes: the group–subgroup relations indicate the possible symmetry breaks that can occur during a phase transition and they are essential for determining the symmetry of the driving mechanism and the related symmetry of the resulting phase. The group–subgroup graphs describing the symmetry breaks provide information on the possible symmetry modes taking part in the transition and allow a detailed analysis of domain structures and twins. The subgroup relations between the space groups also determine the possible symmetries of intermediate phases that may be involved in the transition pathway in reconstructive phase transitions.

The data in this volume are invaluable for the construction of graphs of group–subgroup relations which visualize in a compact manner the relations between different polymorphic modifications involved in phase transitions and which allow the comparison of crystal structures and their classification into crystal-structure types. Particularly transparent graphs are the family trees that relate crystal structures in the manner developed by Bärnighausen (1980) (also called Bärnighausen trees), which also take into account the relations of the Wyckoff positions of the crystal structures considered. Such family trees display the additional degrees of freedom for the structural parameters of the low-symmetry phases, the possibilities of adapting to different kinds of distortions by reduction of site symmetries and the chemical variations (atomic substitutions) allowed for atomic positions that have become symmetry-independent.

The data on supergroups of space groups are useful for the prediction of high-temperature phase transitions, including the search for new ferroelectric and/or ferroelastic materials, for the treatment of the problem of overlooked symmetry in structure determination and for the study of phase transitions in which a hypothetical parent phase plays an important role.
Computer production of Parts 2 and 3

By Preslav Konstantinov, ASEN KIROV, ELI B. KROUMOVA, MOIS I. AROYO and ULRICH MÜLLER

The text and tables of this volume were produced electronically using the \LaTeX\ typesetting system (Lamport, 1994), which has the following advantages:

1. correcting and modifying the text, the layout and the data is easy;
2. correcting or updating all of the above for future editions of this volume should also be simple;
3. the cost of production for this first edition and for later editions should be kept low.

At first, sample input files for generating the tables of Part 2 for a few space groups were written which contained \LaTeX\ instructions for creating both the page layout and the subgroup information. However, these files turned out to be rather complex and difficult to write and to adapt. It proved practically impossible to make changes in the layout. In addition, it could be foreseen that there would be many different layouts for the different space groups. Therefore, this method was abandoned. Instead, a separate data file was created for every space group in each setting listed in the tables. These files contained only the information about the subgroups and supergroups, encoded using specially created \LaTeX\ commands and macros. These macros were defined in a separate package file which essentially contained the algorithm for the layout. Keeping the formatting information separate from the content as much as possible allowed us to change the layout by redefining the macros without changing the data files. This was done several times during the production of the tables.

The data files are relatively simple and only a minimal knowledge of \LaTeX\ is required to create and revise them should it be necessary later. A template file was used to facilitate the initial data entry by filling blank spaces and copying pieces of text in a text editor. It was also possible to write computer programs to extract the information from the data files directly. Such programs were used for checking the data in the files that were used to typeset the volume. The data prepared for Part 2 were later converted into a more convenient, machine-readable format so that they could be used in the database of the Bilbao crystallographic server at http://www.cryst.ehu.es/.

The final composition of all plane-group and space-group tables of maximal subgroups and minimal supergroups was done by a single computer job. References in the tables from one page to another were automatically computed. The run takes 1 to 2 minutes on a modern workstation. The result is a PostScript file which can be fed to most laser printers or other modern printing/typesetting equipment.

The resulting files were also used for the preparation of the fifth edition of \textit{International Tables for Crystallography} Volume A (2002) (abbreviated as \textit{IT} A). Sections of the data files of Part 2 of the present volume were transferred directly to the data files for Parts 6 and 7 of \textit{IT} A to provide the subgroup and supergroup information listed there. The formatting macros were rewritten to achieve the layout used in \textit{IT} A.

The different types of data in the \LaTeX\ files were either keyed by hand or computer-generated. The preparation of the data files of Part 2 can be summarized as follows:

- Headline, origin: hand-keyed.
- Generators: hand-keyed.
- General positions: created by a program from a set of generators. The algorithm uses the well known generating process for space groups based on their solvability property, cf. Section 8.3.5 of \textit{IT} A.
- Minimal supergroups: hand-keyed. The data for the subgroup generators (or general-position representatives for the cases of translationengleiche subgroups and klassengleiche subgroups with ‘loss of centring translations’), for transformation matrices and for conjugacy relations between subgroups were checked by specially designed computer programs.
- Maximal subgroups: created automatically from the data for maximal subgroups.

The electronic preparation of the subgroup tables and the text of Part 2 was carried out on various Unix- and Windows-based computers in Sofia, Bilbao, Stuttgart 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. Th. Hahn (Aachen) contributed to the final arrangement of the data.

The tables of Part 3 have a different layout, and a style file of their own was created for their production. Again, separate data files were prepared for every space group, containing only the information concerning the subgroups. The macros of the style file were developed by U. Müller, who also hand-keyed all files over the course of seven years.

Most of the data of Part 2 were checked using computer programs developed by F. Gähler (cf. Chapter 1.4) and A. Kirov. The relations of the Wyckoff positions (Part 3) were checked by G. Nolze (Berlin) with the aid of his computer program \textit{POWDER CELL} (Nolze, 1996). In addition, all relations were cross-checked with the program \textit{WYCKSPLOT} by Kroumova \textit{et al.} (1998), with the exception of the positions of high multiplicities of some cubic space groups with subgroup indices $> 50$, which could not be handled by the program.
List of symbols and abbreviations used in this volume

(1) Points and point space

- \( P, Q, R \): points
- \( O \): origin
- \( A_n, A_m, P_n \): \( n \)-dimensional affine space
- \( E_n, E_m \): \( n \)-dimensional Euclidean point space
- \( x, y, z, x_i \): point coordinates
- \( x \): column of point coordinates
- \( \tilde{X} \): image point
- \( \tilde{x} \): column of coordinates of an image point
- \( \tilde{x}_i \): coordinates of an image point
- \( x' \): column of coordinates in a new coordinate system (after basis transformation)
- \( x'_i \): coordinates in a new coordinate system

(2) Vectors and vector space

- \( a, b, c; a_i \): basis vectors of the space
- \( r, x \): vectors, position vectors
- \( o \): zero vector (all coefficients zero)
- \( a, b, c \): lengths of basis vectors
- \( \alpha, \beta, \gamma; \alpha_j \): angles between basis vectors
- \( r \): column of vector coefficients
- \( r_i \): vector coefficients
- \( (a)^T \): row of basis vectors
- \( V_n \): \( n \)-dimensional vector space

(3) Mappings and their matrices and columns

- \( A, W \): \( (3 \times 3) \) matrices
- \( A^T \): matrix \( A \) transposed
- \( I \): \( (3 \times 3) \) unit matrix
- \( A_{ik}, W_{ik} \): matrix coefficients
- \( (A, a), (W, w) \): matrix–column pairs
- \( \tilde{W} \): augmented matrix
- \( x, \tilde{x}, \tilde{u} \): augmented columns
- \( P, P \): transformation matrices
- \( A, I, W \): mappings
- \( w \): column of the translation part of a mapping
- \( w_i \): coefficients of the translation part of a mapping
- \( G, G_{ik} \): fundamental matrix and its coefficients
- \( \det(\ldots) \): determinant of a matrix
- \( \text{tr}(\ldots) \): trace of a matrix

(4) Groups

- \( \mathcal{G} \): group; space group
- \( \mathcal{R} \): space group (Chapter 1.5)
- \( \mathcal{H}, \mathcal{U} \): subgroups of \( \mathcal{G} \)
- \( \mathcal{M} \): maximal subgroup of \( \mathcal{G} \) (Chapter 1.5)
- \( \mathcal{M} \): Hermann’s group (Chapter 1.2)
- \( \mathcal{P}, \mathcal{S}, \mathcal{V}, \mathcal{Z} \): groups
- \( T(\mathcal{G}), T(\mathcal{R}) \): group of all translations of \( \mathcal{G}, \mathcal{R} \)
- \( \mathcal{A} \): group of all affine mappings = affine group
- \( \mathcal{E} \): group of all isometries (motions)
- \( \mathcal{F} \): factor group
- \( \mathcal{I} \): trivial group, consisting of the unit element
- \( e \): only
- \( \mathcal{N} \): normal subgroup
- \( \mathcal{O} \): group of all orthogonal mappings
- \( \mathcal{N}(\mathcal{H}) \): normalizer of \( \mathcal{H} \) in \( \mathcal{G} \)
- \( \mathcal{N}(\mathcal{H}) \): Euclidean normalizer of \( \mathcal{H} \)
- \( \mathcal{N}(\mathcal{A}(\mathcal{H})) \): affine normalizer of \( \mathcal{H} \)
- \( \mathcal{P}(\mathcal{G}), \mathcal{P}(\mathcal{H}) \): point groups of the space groups \( \mathcal{G}, \mathcal{H} \)
- \( \mathcal{S}(\mathcal{G}(X)), \mathcal{S}(\mathcal{H}(X)) \): site-symmetry groups of point \( X \) in the space groups \( \mathcal{G}, \mathcal{H} \)
- \( a, b, c, h, m, t \): group elements
- \( e \): unit element
- \( i \) or \( [i] \): index of \( \mathcal{H} \) in \( \mathcal{G} \)

(5) Symbols used in the tables

- \( p \): prime number
- \( n, n' \): arbitrary positive integer numbers
- \( q, r, u, v, w \): arbitrary integer numbers in the given range
- \( a, b, c \): basis vectors of the space group
- \( a', b', c' \): basis vectors of the subgroup or supergroup
- \( x, y, z \): site coordinates in the space group
- \( t(1, 0, 0), t(0, 1, 0), \ldots \): generating translations

(6) Abbreviations

- HM symbol: Hermann–Mauguin symbol
- \( ITA \): International Tables for Crystallography
- Volume A
- PCA: parent-clamping approximation
- \( k \)-subgroup: \( \text{klassengleiche} \) subgroup
- \( t \)-subgroup: \( \text{translationengleiche} \) subgroup