Preface

Like its predecessors, this new sixth edition of *International Tables for Crystallography*, Volume A (referred to as *IT*A 6) treats the symmetries of two- and three-dimensional space groups and point groups in direct space. It is the reference work for crystal symmetry and provides standard symmetry data which are indispensable for any crystallographic or structural study. The text and data in *IT*A 6 fall into three main parts: Part 1 serves as a didactic introduction to space-group symmetry; Part 2 contains the authoritative tabulations of plane and space groups, and a guide to the tabulated data; and Part 3 features articles on more specialized, advanced topics.

Apart from new topics and developments, this sixth edition includes important modifications of the contents and of the arrangement of the text and the tabulated material of the previous (fifth) edition (*IT*A 5). The most salient feature of this edition is the introductory material in Part 1, which offers a homogeneous text of educational and teaching nature explaining the different kinds of symmetry information found in the tables. Although the first part is designed to provide a didactic introduction to symmetry in crystallography, suitable for advanced undergraduate and postgraduate students and for researchers from other fields, it is not meant to serve as an elementary textbook: readers are expected to have a basic understanding of the subject. The following aspects of symmetry theory are dealt with in Part 1:

Chapter 1.1 (Souvignier) offers a general introduction to group theory, which provides the mathematical background for considering symmetry properties. Starting from basic principles, those properties of groups are discussed that are of particular interest in crystallography. Essential topics like group–subgroup relationships, homomorphism and isomorphism, group actions and Wyckoff positions, conjugacy and equivalence relations or group normalizers are treated in detail and illustrated by crystallographic examples.

Chapter 1.2 (Wondratschek and Aroyo) deals with the types of crystallographic symmetry operations and the application of the matrix formalism in their description. The procedure for the geometric interpretation of a matrix–column pair of a symmetry operation is thoroughly explained and demonstrated by several instructive examples. The last section of the chapter provides a detailed discussion of the key concepts of a symmetry element and its constituents, a geometric element and an element set.

Chapter 1.3 (Souvignier) presents an introduction to the structure and classification of crystallographic space groups. Fundamental concepts related to translation lattices, such as the metric tensor, the unit cell and the distinction into primitive and centred lattices are rigorously defined. The action of point groups on translation lattices and the interplay between point groups and lattices is discussed in detail and, in particular, the distinction between symmorphic and non-symmorphic groups is explained. The final part of this chapter deals with various classification schemes of crystallographic space groups, including the classification into space-group types, geometric crystal classes and Bravais types of lattices.

Chapter 1.4 (Souvignier, Wondratschek, Aroyo, Chapuis and Glazer) handles various crystallographic terms used for the presentation of the symmetry data in the space-group tables. It starts with a detailed introduction to Hermann–Mauguin symbols for space, plane and crystallographic point groups, and to their Schoenflies symbols. A description is given of the symbols used for symmetry operations, and of their listings in the general-position and in the symmetry-operations blocks of the space-group tables. The Seitz notation for symmetry operations adopted by the Commission on Crystallographic Nomenclature as the standard convention for Seitz symbolism of the International Union of Crystallography [Glazer *et al.* (2014). *Acta Cryst.* A**70**, 300–302] is described and the Seitz symbols for the plane- and space-group symmetry operations are tabulated. The so-called additional symmetry operations of space groups resulting from the combination of the generating symmetry operations with lattice translations are introduced and illustrated. The classification of points in direct space into general and special Wyckoff positions, and the study of their site-symmetry groups and Wyckoff multiplicities are presented in detail. The final sections of the chapter offer a helpful introduction to two-dimensional sections and projections of space groups and their symmetry properties.

Chapter 1.5 (Wondratschek, Aroyo, Souvignier and Chapuis) introduces the mathematical tools necessary for performing coordinate transformations. The transformations of crystallographic data (point coordinates, space-group symmetry operations, metric tensors of direct and reciprocal space, indices of reflection conditions *etc.*) under a change of origin or a change of the basis are discussed and demonstrated by examples. More than 40 different types of coordinate-system transformations representing the most frequently encountered cases are listed and illustrated. Finally, synoptic tables of the space and plane groups show a large selection of alternative settings and their Hermann–Mauguin symbols covering most practical cases. It is worth pointing out that, in contrast to *IT*A 5, the extended Hermann–Mauguin symbols shown in the synoptic tables follow their original definition according to which the characters of the symbols indicate symmetry operations, and not symmetry elements.

Chapter 1.6 (Shmueli, Flack and Spence) offers a detailed presentation of methods of determining the symmetry of single-domain crystals from diffraction data, followed by a brief discussion of intensity statistics and their application to real intensity data from a $P\bar{1}$ crystal structure. The theoretical background for the derivation of the possible general reflections is introduced along with a brief discussion of special reflection conditions. An extensive tabulation of general reflection conditions and possible space groups is presented. The chapter concludes with a description and illustration of symmetry determination based on electron-diffraction methods, principally using convergent-beam electron diffraction.

Chapter 1.7 (Wondratschek, Müller, Litvin and Kopský) gives a short outline of the content of *International Tables for Crystallography* Volume A1, which is devoted to symmetry relations between space groups, and also of the content of *International Tables for Crystallography* Volume E, in which two- and three-dimensional subperiodic groups are treated. The chapter starts with a brief introduction to the different kinds of maximal subgroups and minimal supergroups of space groups. The relations between the Wyckoff positions for group–subgroup-related space groups and their crystallographic applications are discussed. Illustrative examples of the application of the relationship between a crystal space group and the subperiodic-group symmetry of planes that transect the crystal in the determination of the layer-group symmetry of such planes and of domain walls are also given.

The essential data in Volume A are the diagrams and tables of the 17 types of plane groups and of the 230 types of space groups shown in Chapters 2.2 and 2.3 of Part 2. For each group type the following symmetry data are presented: a headline block with the relevant group symbols; diagrams of the symmetry elements and of the general positions; specifications of the origin and of the asymmetric unit; symmetry operations; generators; general and special Wyckoff positions with multiplicities, site symmetries, coordinate triplets and reflection conditions; and symmetries of special projections (for the space-group types). Compared to the tabulated symmetry data in *IT*A 5, two important differences are to be noted:

(i) The subgroups and supergroups of the space groups were listed as part of the space-group tables in the first to fifth editions of Volume A (from 1983 to 2005), but the listing was incomplete and lacked additional information on any basis transformations and origin shifts that may be involved. A complete listing of all maximal subgroups and minimal supergroups of all plane and space groups is now given in Volume A1 of *International Tables for Crystallography*, and to avoid repetition of the data tabulated there, the maximal-subgroup and minimal-supergroup data are omitted from the plane-group and space-group tables of *IT*A 6.

(ii) To improve the visualization and to aid interpretation of the complicated general-position diagrams of the cubic space groups, the stereodiagrams that were used for them in the previous editions of Volume A have been replaced by orthogonal-projection diagrams of the type given in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935). In the new diagrams the points of the general position are shown as vertices of transparent polyhedra whose origins are chosen at special points of highest site symmetry. To provide a clearer three-dimensional style overview of the arrangements of the polyhedra, additional general-position diagrams in perspective projection are shown for all the cubic space groups in the online version of the volume, and for each of the ten space groups of the $m\bar{3}m$ crystal class in the print version in a new four-page arrangement of the data for each of these space groups. The general-position diagrams of the cubic groups in both orthogonal and perspective projections were generated using the program *VESTA* [Momma & Izumi (2011). *J. Appl. Cryst.* **44**, 1272–1276].

There are further modifications of the symmetry data in the space-group tables, some of which deserve special mention:

(iii) To simplify the use of the symmetry-element diagrams for the three different projections of the orthorhombic space groups, the corresponding origins and basis vectors are explicitly labelled, as in the tables of the monoclinic space groups.

(iv) Modifications to the tabulated data and diagrams of the seven trigonal space groups of the rhombohedral lattice system (the so-called *rhombohedral* space groups) include: (*a*) changes in the sequence of coordinate triplets of some special Wyckoff positions of five rhombohedral groups [namely $R\bar{3}$ (148): Wyckoff positions 3*d* and 3*e*; *R*32 (155): 3*d* and 3*e*; *R*3*m* (160): 3*b*; $R\bar{3}m$ (166): 3*d*, 3*e* and 6*h*; $R\bar{3}c$ (167): 6*d*] in the rhombohedral-axes settings in order to achieve correspondence between the sequences of coordinate triplets of the rhombohedral and hexagonal descriptions; (*b*) labelling of the basis vectors (cell edges) of the primitive rhombohedral cell in the general-position diagrams of the rhombohedral-axes setting descriptions of all rhombohedral space groups.

The diagrams and tables of the plane and space groups in Part 2 are preceded by a guide to their use, which includes lists of the symbols and terms used in them. In general, this guide (Chapter 2.1) follows the presentation of the material in *IT*A 5 but with several important exceptions related to the modifications of the content and the rearrangement of the material as discussed above. The improvements include new sections on: (i) symmetry elements (Hahn and Aroyo), explaining the important modifications of the tables of symbols of symmetry elements; (ii) Patterson symmetry (Flack), with tables of Patterson symmetries and symmetries of Patterson functions for all space and plane groups; and (iii) the general-position diagrams of the cubic groups (Momma and Aroyo). An extended section on the computer preparation of *IT*A 6 (Konstantinov and Momma) discusses the specific features of the computer programs and layout macros applied in the preparation of the set of diagrams and tables for this new edition.

Advanced and more specialized topics on space-group symmetry are treated in Part 3 of the volume. Most of the articles are substantially revised, upgraded and extended with respect to the versions in *IT*A 5. The major changes can be briefly described as follows:

In Chapter 3.1 on crystal lattices and their properties, the discussion of the Delaunay reduction procedure and the resulting classification of lattices into 24 Delaunay sorts ('*Symmetrische Sorten*') by Burzlaff and Zimmermann is supplemented by illustrative examples and a new table of data. Gruber and Grimmer broaden the description of conventional cells, showing that the conditions characterizing the conventional cells of the 14 Bravais types of lattices are only necessary and to make them sufficient they have to be extended to a more comprehensive system.

Chapter 3.2 on point groups and crystal classes (Hahn, Klapper, Müller and Aroyo) is substantially revised and new material has been added. The new developments include: (i) graphical presentations of the 47 face and point forms; (ii) enhancement of the tabulated Wyckoff-position data of the 10 two-dimensional and the 32 three-dimensional crystallographic point groups by the inclusion of explicit listings of the coordinate triplets of symmetry-equivalent points, and (iii) a new section on molecular symmetry (Müller), which treats noncrystallographic symmetries, the symmetry of polymeric molecules, and symmetry aspects of chiral molecules and crystal structures.

The revised text of Chapter 3.4 (Fischer and Koch) on lattice complexes is complemented by a thorough discussion of the concepts of orbit types, characteristic and non-characteristic orbits, and their comparison with the concepts of lattice complexes and limiting complexes.

Chapter 3.5 (Koch, Fischer and Müller) introduces and fully tabulates for the first time the chirality-preserving Euclidean normalizers of plane and space groups. Illustrative examples demonstrate the importance of the chirality-preserving Euclidean normalizers in the treatment of chiral crystal structures.

The new Chapter 3.6 (Litvin) on magnetic groups addresses the revival of interest in magnetic symmetry. The magnetic groups considered are the magnetic point groups, the two- and three-dimensional magnetic subperiodic groups, *i.e.* the magnetic frieze, rod and layer groups, and the one-, two- and three-dimensional magnetic space groups. After an introduction to magnetic symmetry groups, the existing nomenclatures for magnetic space groups are discussed and compared. The structure, symbols and properties of the magnetic groups and their maximal subgroups as listed in the electronic book by Litvin [*Magnetic Group Tables* (2014). IUCr: Chester. http://www.iucr.org/publ/978-0-9553602-2-0] are presented and illustrated.

Work on this sixth edition extended over the last eight years and many people have contributed to the successful completion of this complicated project. My acknowledgements should start with H. Wondratschek (Universität, Karlsruhe) and Th. Hahn (RWTH, Aachen), to whose memory this volume is dedicated. Their constant interest, support and sometimes hard but always constructive criticism were decisive during the preparation of this volume.

It is my great pleasure to thank all the authors of *IT*A 6 who have contributed new material or have updated and substantially revised articles from the previous edition. Also, I should like to express my gratitude to B. Gruber and V. Kopský for their important contributions to *IT*A 6; unfortunately, and to my deep regret, they both passed away in 2016. My sincere thanks go to P. Konstantinov (INRNE, Sofia) and K. Momma (National Museum of Nature and Science, Tsukuba) for their hard work and the effort they invested in the computer production of the plane- and space-group tables of the volume. This sixth edition is a result of numerous discussions (some of them difficult and controversial, but always stimulating and fruitful) with different people: H. Wondratschek, B. Souvignier (Radboud University, Nijmegen), H. Flack (University of Geneva), M. Nespolo (Université de Lorraine, Nancy), U. Shmueli (Tel Aviv University), Th. Hahn, M. Glazer (Oxford University), U. Müller (Phillipps-Universität, Marburg), D. Schwarzenbach (École Polytechnique Fédérale, Lausanne), C. Lecomte (Université de Lorraine, Nancy) and many others. I gratefully acknowledge their constructive comments, helpful recommendations and improvements, and I apologize if not all their specific proposals have been included in this edition.

I am particularly grateful to my colleagues and friends J. M. Perez-Mato, G. Madariaga and F. J. Zuñiga (Universidad del País Vasco, Bilbao) for their constant support and understanding during the work on *IT*A 6, and for motivating discussions on the content and presentation of the crystallographic data. It is also my great pleasure to thank the useful comments and assistance provided by our PhD students and post-doctoral researchers, especially E. Kroumova, C. Capillas, D. Orobengoa, G. de la Flor and E. S. Tasci.

My particular thanks are due to C. P. Brock (University of Kentucky, Lexington), and P. R. Strickland and N. J. Ashcroft (IUCr Editorial Office, Chester) for their sage advice and encouragement, especially during the difficult moments of the work on the volume. I am deeply indebted to Nicola Ashcroft for the careful and dedicated technical editing of this volume, for her patient and careful checking and tireless proofreading, and for the invaluable suggestions for improvements of the manuscript. Nicola's support and cooperation were essential for the successful completion of this project.

Financial support by different institutions permitted the production of this volume and, in particular, my acknowledgements are due to the International Union of Crystallography, Universidad del País Vasco (UPV/EHU), the Government of the Basque Country, the Spanish Ministry of Science and Innovation, the Spanish Ministry of Economy and Competitiveness and FEDER funds.

Mois I. Aroyo
Editor, *International Tables for Crystallography* Volume A