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.