

## Foreword to the Sixth Edition

Standardizing the space-group tables has been a priority for crystallographers since at least 1929. The 1935 publication of the first set of such tables predated the founding of the International Union of Crystallography (IUCr) by 12 years. That book was one of the two volumes of *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (or *International Tables for the Determination of Crystal Structures*). It established conventions so fundamental to the field that it is hard to imagine the confusion they prevented.

Major revisions of the space-group tables were published by the IUCr in 1952 (*International Tables for X-ray Crystallography Volume I: Symmetry Groups*) and 1983 (*International Tables for Crystallography Volume A: Space-Group Symmetry*). The considerably revised fifth edition of Volume A was made available online in 2006 at <http://it.iucr.org/> along with the other seven volumes of the series as *International Tables Online*, which features many links within and between the electronic versions of the volumes. In 2011 the online series was complemented by the addition of the *Symmetry Database*, which provides more extensive symmetry information than do the volumes themselves.

Over the decades the information about space-group symmetry has been expanded so greatly that no single volume can contain it all. Some information about group–subgroup relationships was present in the 1935 volume but was left out of the 1952 edition. That information, augmented by some group–supergroup relationships, reappeared in the 1983 book. A full treatment of the subject was published in 2004 as the new Volume A1: *Symmetry Relations Between Space Groups*. The ability to follow electronic links back and forth between the online versions of Volumes A and A1 makes their combination very powerful.

In 2002 the new Volume E, *Subperiodic Groups*, was published. It contains the tables for the space groups of two-dimensional patterns that are periodic in only one dimension (the frieze groups) and three-dimensional patterns that are periodic in only one dimension (the rod groups) or two dimensions (the layer groups). The distinction between the 80 layer groups and the 17 plane groups is important. The latter had been included since 1952 along with the 230 space groups because the plane groups are so useful for teaching; they do not, however, allow for layer thickness. Layer groups may have more symmetry elements than are allowed for a plane group, *i.e.* inversion centers, a mirror plane within the layer, and 2 and  $2_1$  axes within the layer.

The new Volume C: *Mathematical, Physical and Chemical Tables* appeared in 1992 as a successor to Volume II of *Internationale Tabellen zur Bestimmung von Kristallstrukturen*, which had grown to Volumes II–IV of the series *International Tables for X-ray Crystallography*; Volume C includes a section on the

symmetry descriptions of commensurately and incommensurately modulated structures. Since then, that field has grown so much that the material is currently being expanded and relocated to the next edition of Volume B, *Reciprocal Space*.

Symmetry descriptions of magnetic structures are still under development. The number of magnetic groups is so large that any volume of *International Tables* listing them will have to be electronic only. In 2014, as an interim step, the IUCr published an e-book by D. B. Litvin (*Magnetic Group Tables*) that is available for downloading from the IUCr website at <http://www.iucr.org/publ/978-0-9553602-2-0>.

Because Volume A is usually the first volume of *International Tables* encountered by non-experts, an important aim of this edition has been to make its contents more accessible. The text sections have been completely reorganized and new introductory chapters have been written by authors experienced in teaching crystallography at all levels. Many explanatory examples have been added, and the terms and symbols used have been made consistent throughout. Diagrams for the cubic space groups have been redrawn so that they are easier to comprehend and axis labels have been added for the orthorhombic groups. Introductions to the topics covered in Volumes A1 and E, as well as to magnetic symmetry, have been added.

Volume A continues to evolve; this new edition, the sixth, is a major revision intended to meet the needs of scientists in the Electronic Age: users of the online version will also have access to the *Symmetry Database*, which is under continuous development and contains far more data than can be presented in print. The database can be used to calculate, among other things, the symmetry operations and Wyckoff positions for nonstandard settings in order to facilitate the tracking of symmetry relationships through a series of phase transitions or chemical substitutions.

We are all greatly indebted to Mois Aroyo, the Editor of this edition, for having had the vision for this revision of Volume A and for then having seen the project through. Getting experts to write for a wide group of readers and to agree on consistent terminology required erudition, tact and patience, all of which Mois has displayed in abundance.

Those who have been involved with this sixth edition are also indebted to all the crystallographers who contributed to previous editions. Two of the longtime architects of Volumes A and A1, Theo Hahn and Hans Wondratschek, recently passed on, but not before making very significant contributions towards the preparation of this new edition. It is an honor to acknowledge their many contributions.

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