Acta Crystallographica Section A

Foundations of Crystallography

ISSN 0108-7673

International tables for crystallography.

Vol. A. 5th edition. Edited by Th. Hahn. Pp. xx + 911. Dordrecht: Kluwer Academic Publishers, 2002. Price EUR 242, GBP 142, USD 225. ISBN 0-7923-6590-9.

Since its first appearance in 1983, Volume A of International Tables for Crystallography (hereafter ITA) has served 'consumers' of symmetry-group data for about 20 years and has experienced, during a permanent dialog with the readers, four more or less major revisions. ITA is the first in a series of International Tables for Crystallography and treats one-, two- and three-dimensional crystallographic space groups. Extensions to 'generalized symmetry' are beyond the scope of this volume. A salient point of ITA is the adoption of an advanced level of symmetry theory, which is strictly compatible with the demands of computerization of crystallographic problems. The Editor's goal to provide data that are useful for all aspects of crystallography as well as text to satisfy the needs of those interested in the theoretical reasons behind these tables has led to a fruitful combination of tables for practical use in the first part and a high-level textbook in the second. ITA succeeded in proposing a compromise between competing view points. I mention issues such as the hexagonal/trigonal versus rhombohedral subdivision and the so-called 'monoclinic monster', which, for the convenience of the reader, is a summary of all settings and cell choices of the monoclinic space groups.

Because symmetry is the basis of crystallography, previous editions of ITA had to be reissued several times: 1st edition 1983, reprinted with corrections 1984, 2nd revised edition 1987, 2nd revised edition reprinted with corrections 1989, 3rd revised edition 1992, 4th revised edition 1995, 4th revised edition reprinted with corrections 1996, 4th edition reprinted 1998, 5th revised edition 2002. The volume has increased from xv + 854 pages in 1983 to xx + 911 pages in 2002. This 5th edition (ITA5) is more extensively revised than any of the preceding editions. While the number of parts (15) is maintained in ITA5, the number of authors has increased.

book reviews

Works intended for this column should be sent direct to the Book-Review Editor, whose address appears in this issue. All reviews are also available from **Crystallography Journals Online**, supplemented where possible with direct links to the publisher's information.

The first edition of ITA was reviewed by Stadnicka *et al.* [Acta Cryst. (1987), A43, 156–159]. They concluded, after assessing all sections individually, that ITA is a clearly, thoroughly and coherently written book that has been prepared carefully and is of good technical quality.

The reader of ITA5 will first notice a new white (red)-green hard cover differing from the blue (gold) predecessors, this time without a book jacket. Although it looks more attractive at first glance, the white part might lose its beauty more quickly. Then, looking at the layout of the interior, a smaller font attracts the reader's attention which makes the arrangement of the text more concise, because the number of lines per page is approximately maintained. Hence, more space between the subsections along with an in-depth four-digit decimal classification facilitates browsing ITA5 considerably. The table of contents now covers 6 pages instead of 4 of the previous edition. The plain rearrangement of the text of the fourth edition is a noteworthy achievement of ITA5 in itself. One component of that is bringing tables or figures closer to the place where they are quoted first. Moreover, instead of the creamy paper previously utilized, for the current edition white paper has been used. Again this makes reading easier, apart from proper fractions which, due to the smaller font, appear a bit faint now. However, the general quality of print is excellent.

Then a hidden change in ITA5 should be mentioned, which will certainly become a great advantage for future application compared to editions 1–4. It is the computer-based production of ITA5, accomplished by M. I. Aroyo and P. B. Konstantinov. All space-group tables were reprogrammed, whereas the space-group diagrams were scanned from the existing presentations, which in turn had been improved several times over the years. One promising future option of this computerization is the linking of ITA5 to other volumes of this series.

Because ITA is published for the International Union of Crystallography (IUCr), its content has been the subject of permanent attention by Commissions of the IUCr, in particular by the Commission on International Tables and the Commission on

Nomenclature. Hence, unlike common texts or tables, ITA is being continuously improved by a well organized and competent community, whose recommendations, after thorough discussion, are taken as input for subsequent editions. One example was an inconsistency in the concept of 'symmetry element' [H. D. Flack *et al.* (2000). *Acta Cryst.* **A56**, 96–98], which has been removed by defining the geometric element as a labelled geometric item. Hence corrigenda and addenda became necessary. Those of the third edition were summarized in *Acta Cryst.* (1995), **A51**, 592–595.

Turning to changes of the crystallographic information supplied by ITA5 as compared to the previous edition, it should first be mentioned that the incorporation of the double-glide-plane symbol 'e' into spacegroup symbols has been completed throughout the volume. This means that, in addition to glide planes a, b, c, d, n used before 1995, a sixth symmetry element appears in all parts (in centred cells only). Secondly, subgroup and supergroup data have been changed by adding space-group numbers and rearranging the group symbols according to rising index and falling spacegroup number. This applies particularly to Part 7 as the main part of ITA and facilitates dealing with the various symbols. It is recommended for future editions to obey these rules in the examples of subgroups given in Chapter 4.3 (by E. F. Bertaut), too. Thirdly, there are several improvements that apply to individual groups only, such as changes in the sequence of the positions and symmetry operations for the 'rhombohedral axes' descriptions of certain R groups. While changes of Parts 1, 3–6, 11–13 (by Th. Hahn, A. Looijenga-Vos, M. J. Buerger, E. F. Bertaut, H. Arnold, W. Fischer, E. Koch, H. Burzlaff, H. Zimmermann, Y. Billiet) are mainly of formal character, substantial revisions and reorganizations of the text have been carried out in the remaining parts. They can in most cases be considered successful in expressing the fundamentals more clearly, apparently stimulated by the feedback from students, and in taking new developments into account.

Examples are the presentation of general and special reflection conditions (Section 2.2.13) and the way monoclinic space groups

Acta Cryst. (2004). A60, 641–642

book reviews

are treated (Section 2.2.16), both by Th. Hahn & A. Looijenga-Vos. The text of Part 8 (by H. Wondratschek) has been updated to bridge the gap to topics that are not the subject of ITA but are of current interest to crystallographers, like symmetry in spaces of dimension >3 and incommensurate structures, as well as to topics which have now been dealt with comprehensively in subsequent volumes of the International Tables series, like subperiodic groups. The concept of a 'lattice system of space groups' and its relationship to Bravais flocks and the concept of 'normalizers of space groups' has been worked out in a much clearer manner in the revised formulation. With regard to normalizers, 'special topics' have been removed in view of the extended Part 15.

Part 9 on crystal lattices has been enlarged by a new chapter on the Delaunay reduction (by H. Burzlaff & H. Zimmermann) and by a chapter on 'further properties of lattices', where B. Gruber deals with Buerger cells, lattice characters and sublattices of n-dimensional lattices. The former authors contribute also a list of the 24 'Symmetrische Sorten'. In Part 14 on lattice complexes (by W. Fischer & E. Koch), the list of assignment of Wyckoff positions to lattice complexes has been slightly extended (oriented site symmetry added) and changed. Then more examples are given to illustrate the concept of the lattice complex. The new chapter on the application of the lattice-complex concept will certainly also be appreciated by the reader. The final Part 15, dealing with normalizers (by E. Koch, W. Fischer & U. Müller), has also experienced extension and revision. The most striking changes are figures of the parameter range of monoclinic space groups, showing the borders of the metric, and the greatly expanded (from 3 to 13 pages) table of normalizers of the monoclinic and orthorhombic space groups.

References at the end of each part have been updated, if appropriate, and are now listed for each 2-digit chapter separately. Finally, the number of entries in the subject index has more than doubled.

To sum up, ITA is not only the first and the most frequently edited volume in this series of a new generation of crystallographic references, it sets standards for the subject of crystallography in general as a 'hard' and far-reaching branch of science. Thanks to the availability of this reference, supported by the IUCr, there is nowadays an international consensus on key concepts of crystallography. ITA is a book of symbols relevant for symmetry properties of crystals. While many other books are using the

relevant symbols, ITA delivers not only the complete listings but also a comprehensive explanation of the theory behind them and detailed instructions for use. Hence, it is indispensable for people dealing with the symmetry of crystals. The present revised edition, ITA5, is another step towards minimization of inaccuracies and improvement of readability. Chapters of different authors of ITA5 have become more homogeneous by cross references and due to the rearrangement of topics between them. I have been strikingly unsuccessful in the search for errors. Minor flaws (some mentioned above) may readily be corrected. Being published in the 21st century, historic remarks like 'something is known since the last century' (e.g. on p. 738) should now better read '... since the 19th century' to avoid further corrections in 2102. I feel personal indebtedness to the Editor and to the other authors of this useful volume and the huge work that has been done.

Peter Paufler

Chair of Crystallography
Department of Physics
Dresden University of Technology
D-01062 Dresden
Germany
E-mail: paufler@physik.tu-dresden.de

books received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works either because of difficulty in finding a suitable reviewer without great delay or in order to inform readers prior to publication of the full review.

Orientations and rotations. Computations in crystallographic textures. By Adam Morawiec. Pp. X + 200. Berlin, Heidelberg, New York: Springer-Verlag, 2004. Price EUR 59.95, GBP 46.00, USD 79.95. ISBN 3 540 40734 0.

Essentially, *Orientations and rotations* treats the mathematical and computational foundations of texture analysis. It contains an extensive and thorough introduction to parameterizations and geometry of the rotation space. Since the notions of orientations and rotations are of primary importance for science and engineering, the book can be useful for a very broad audience using rotations in other fields.

Crystal structure determination. By Werner Massa. Second completely updated edition. Pp. XI + 210. Berlin,

updated edition. Pp. XI + 210. Berlin, Heidelberg, New York: Springer-Verlag, 2004. Price EUR 48.10. ISBN 3 540 20644 2.

A review of the first edition of this book was published in the May 2001 issue of *Acta Cryst.* A**57**, page 368. The second edition has been considerably updated, especially the chapter on experimental methods, which is now mainly concerned with modern data collection using area detectors. Many tips and insights help readers to recognise and avoid possible errors and traps, and to judge the quality of results.

Mathematical techniques in crystallography and materials science. By Edward Prince. 3rd ed. Pp. XI + 224. Berlin, Heidelberg, New York: Springer-Verlag, 2004. Price (softcover) EUR 42.75. ISBN 3 540 21111 X.

This book brings together common and less familiar mathematical procedures used in studies of the structures and physical properties of solids. A review of the second edition of this book was published in the July 1995 issue of *Acta Cryst.* A**51**, page 590. The third edition further clarifies key points, as well as offering new sections on two topics: the projection matrix and the fast Fourier transform.

642 Acta Cryst. (2004). A**60**, 641–642