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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.

Crystal structure determination. By Werner Massa. (English translation by R. O. Gould.) Heidelberg: Springer-Verlag. Pp. xi + 206. Price (soft cover) DM 69.00. ISBN 3-540-65970-6.

This book provides a nice balance between describing the mathematical fundamentals and offering practical advice on how to solve a crystal structure. It is a very good translation of the original German text. The book is appropriate for an undergraduate audience (particularly in chemistry) and for graduate students or researchers who find they need a better grasp of the subject. Students seeking a rigorous treatment of the theoretical basis of many concepts in crystallography will need to supplement this book with other sources, some of which are listed in a useful bibliography. Students whose main interest is macromolecular crystallography will find it inadequate in certain places. For instance, the sections describing crystallization experiments and on preparing the crystal sample for data collection make no mention of standard procedures for dealing with macromolecular crystals. To keep the size of the book small, there is no mention of the accumulated results of diffraction experiments – the many interesting known structures and what we can learn from them. However, the various small-molecule databases are mentioned, together with some useful Internet addresses, in a short chapter towards the end of the book.

The first six chapters deal with geometric fundamentals of lattices, symmetry and X-ray diffraction. One of the strengths of the text is that the author tries to clarify many of the topics that frequently cause confusion to the new student of crystallography. For example, he gives a clear explanation of the differences between the trigonal, hexagonal and rhombohedral crystal systems when initially defining lattice symmetry in Chapter 2. From my perspective in teaching, Chapter 5, on structure factors, might be better placed if it came immediately before Chapter 8, on structure solution. Chapter 7, one of the lengthiest, describes the various experimental methods and is quite complete and very readable. The next three chapters, devoted to structure solution, refinement and the determination of absolute configuration, include definitions of a variety of terms used by commonly available software programs. The description of how hydrogen atoms are treated is useful – particularly for a novice who may not be aware of the different ways used to report their positions. There are also hints and advice on how to deal with problem structures. The use of the Rietveld method for structure refinement based on powder data (as opposed to single-crystal data) is also briefly described. The book is clearly a useful reference to have around when performing an X-ray diffraction experiment.

Another strength of the book is Chapter 11 entitled 'Errors and Pitfalls'. The content is self-explanatory from the title and Massa points out potential errors in the interpretation of crystal data and experimental results. It covers important topics such as disorder, twinning and quasicrystals.

Chapter 12 discusses the results obtained from a structure determination. It contains equations for calculating bond distances, angles, torsion angles and best planes. Also useful for a novice is a description of the different types of structural diagrams used to display the results, including the polyhedral drawings used for inorganic and materials science applications. These three-dimensional drawings are usually incomprehensible when seen for the first time by a chemistry undergraduate student. To my way of thinking, this chapter should precede Chapter 9, on structure refinement. Given that it describes the important results of the experiment, its placement after the 'Errors and Pitfalls' chapter seems a bit pessimistic!

Chapter 14 offers a useful and fairly detailed outline of the various stages of a crystal structure determination with references to the appropriate section in the text where the particular topic is discussed. Chapter 15 includes a worked and annotated crystal structure determination, using *SHELX*, that is very useful for the new student. I only wish that the space group of the example had not been chosen as $I2/a$, which is a non-standard space group in the monoclinic system. However, Chapter 2, on crystal lattices, has an illustration showing the relationship between the monoclinic I and C centering. A bibliography lists other crystallography texts and a score of software packages, though none relating to macromolecular applications.

Overall, the book is a helpful addition to the collection of introductory texts in X-ray crystallography, especially for its treatment of common errors in the collection of intensity data and in the interpretation of results. This feature is particularly important in a book directed at non-specialist users of this powerful method.

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books received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally, a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

Modern crystallography. Vol. 2. **Structure of crystals.** (Third edition). Edited by B. K. Vainshtein, V. M. Fridkin and V. L. Indenbom. Heidelberg: Springer-Verlag, 2000. Pp. xx + 520. Price DM 198. ISBN 3-540-67474-8. A review of this book, by Robert F. Bryan, has been published in the February 2001 issue of *Acta Cryst.* Section B, page 112.

Synchrotron radiation (Production and properties). By P. J. Duke. Oxford: Oxford University Press, 2000. Pp. xiv + 251. Price £70.00. ISBN 0 19 85178 0. A review of this book, by J. C. Grossman, R. W. Strange & V. P. Suller has been published in the January 2001 issue of *J. Synchrotron Rad.*, page 38.