Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, USA). As far as practicable, books will be reviewed in a country different from that of publication.

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Fundamentals of crystallography. By C. GIACOVAZZO, H. L. MONACO, D. VITERBO, F. SCORDARI, G. GILLI, G. ZANOTTI and M. CATTI. (**IUCr Texts on Crystallography** No. 2.) Pp. xv + 654. Oxford: International Union of Crystallography/Oxford University Press, 1992. Price £27.50 (paperback), £62.00 (hardback). ISBN 0-19-855578-4 (p/b), 0-19-85579-2 (h/b).

For this book, the second of the new IUCr Texts on Crystallography, Carmelo Giacovazzo has edited, revised, expanded and brought up to date in English translation *Introduzione alla Cristallografia Moderna*, first published in 1985. The stated aim of the book is to provide a compact comprehensive account of modern crystallographic subjects that should be useful as a text for university courses that cover crystallography, fully or only partially, but that should also be of use at the doctoral or research level. I believe that this book more than adequately meets these goals and the high quality of the translation should ensure it a significantly wider audience than that reached by the original.

Recognizing the interdisciplinary character of modern crystallography, the editor realized that a book of this kind would need to be written by several authors and that the various contributions would have to be 'carefully harmonized in order to conform them to a unified plan'. The result is a text that can be used with profit in its entirety but from which instructors and students can select according to their particular interests. There are three core chapters. Chapter 1 (Giacovazzo, 60 pp.) is a concise treatment of symmetry in crystals. The first half covers symmetry elements, lattices, point groups, Laue classes, crystal systems, Bravais lattices, and plane, line and space groups. This material is fundamental for audiences at all levels. For the more advanced student, the second half of the chapter consists of appendices dealing with isometric transformations, combinations of movements, Wigner–Seitz cells, space-group rotation matrices, symmetry groups and generalized symmetry with an introduction to G groups and color symmetry. Very usefully, in this last case, actual structural arrangements are used as illustrations. The second core chapter (Chapter 3, Giacovazzo, 86 pp.) covers the diffraction of X-rays by crystals. The same division between fundamental and more advanced topics is adopted here. The treatment is kinematic, with a progression from scattering by electrons to that by atoms, molecules and crystals. There are good treatments of symmetry in reciprocal space and of anomalous dispersion, and a short introduction to modulated structures. The appendices here deal with the mathematics of Fourier transforms and convolution operations, and with more subtle aspects of scattering such as Compton scattering, the anisotropic temperature factor, the Renninger effect and electron and neutron scattering. Scattering by non-crystalline materials such as gases, liquids and amorphous solids is covered, as is small-angle scattering. Two final appendices deal with electron-density mapping and a more advanced look at modulated structures and quasicrystals.

For the newcomer to crystallography, the third core chapter (Chapter 5, Viterbo, 79 pp.) deals with the solution and refinement of crystal structures. After a general introduction come sections dealing with the statistical analysis of structure amplitudes, the use of the Patterson method and direct methods, and refinement by least-squares and difference Fourier methods, with a short discussion of the determination of absolute configuration. For the more experienced reader, the appendices deal with structure-factor and triplet-invariant probability distributions, Patterson vector methods, pseudotranslational symmetry, magic integers and newer multisolution methods and procedures for completing a partial model. As is the case for the other core chapters, the references here are particularly helpful and cover the literature into 1990.

For the practicing crystallographer, these three core chapters may be supplemented by two others. Chapter 4 (Monaco, 85 pp.) deals with experimental methods. X-ray sources, both conventional and synchrotron, are discussed with respect to the production, monochromatization, collimation and focusing of X-rays. Data collection for single crystals by both film and diffractometer methods is considered in detail, including the use of area detectors and densitometers. A comparable treatment is given for polycrystalline materials but not for fibers or less-ordered systems such as liquid crystals. The chapter concludes with a discussion of data reduction and corrections for absorption and radiation damage. The chapter provides a good overview but, unlike the core chapters, there is no real division here between introductory and advanced material, and any potential film users might wish to supplement the treatment offered by consulting such classic works as Buerger's *X-ray Crystallography* and *The Precession Method*. The appendix to this chapter deals with the determination of the number of molecules in the unit cell for both small and large molecules. Chapter 2 (Giacovazzo, 77 pp.) is really the second of the two supplementary chapters. It is eccentrically placed from the standpoint of the newcomer and perhaps even from that of the advanced reader. The chapter title is 'Crystallographic Computing' but the material is really a mathematical treatment of a variety of topics beginning with the metric matrix, the reciprocal lattice, lattice transformations and rotations, and the application of these results to such problems as the Niggli reduced cell, sub- and superlattices, coincidence-site lattices and twinning. The calculation of bond lengths, bond angles, least-squares mean planes and torsion angles is included, even before fractional coordinates have been defined. (Indeed, the index does not even include that term!) This is followed by the mathematics of the structure factor, the electron-density function and the least-squares method. Rietveld refinement and the analysis of thermal motion and its effect on bond lengths and angles are next treated and the chapter appendices deal principally with transformation matrices, the derivation of normal equations, variance–covariance matrices, M_x, and the FFT algorithm. Finally, and to my mind oddly, the chapter concludes with some fine illustrations of twin laws in the various crystal systems. Giacovazzo the mathematician shows through in this chapter. The treatment relies heavily upon matrix methodology, though expanded forms useful for actual calculation are generously provided in the earlier stages.

The remaining four chapters integrate crystallography with aspects of chemistry, biology and physics. Chapter 6 (Scordari, 62 pp.) deals with ionic crystals, introducing basic concepts in bonding and lattice energy using both Born and CFT theory. The application of radius-ratio rules is treated well, as are Pauling's rules. The fundamental binary and ternary structure types are described, as is Liebau's classification of silicate structures. Appendices deal with the application of the concept of the packing coefficient and structural inferences from crystallochemical parameters. Chapter 7 (Gilli, 70 pp.) provides a comparable treatment for molecular crystals. There is a comprehensive discussion of the various types of intermolecular forces and a short overview of the thermodynamics of molecular crystals. This is followed by a useful discussion of elements of classical stereochemistry, including conformational isomerism, with a group-theoretical approach to ring conformations. A treatment of covalent bonding is followed by a short treatment of molecular mechanics. The chapter concludes with a useful overview of molecular hermeneutics – the interpretation of molecular structures – including the use of correlative methods in the study of nucleophilic additions, conformational rearrangement and resonance-assisted hydrogen bonding. Chapter 8 (Zanotti, 63 pp.) offers an introductory review of protein crystallography, beginning with the preparation of protein crystals and culminating in a classification of protein structures. In between, every aspect of structure determination, interpretation and refinement is beautifully and comprehensively covered, including a discussion of the latest advances in the application of the maximum-entropy principle in phase determination. This chapter alone is worth the price of the paperback version! With a comparable treatment of nucleic acid crystallography included, this book would have few competitors as an introductory text in the biological structural crystallography market. The final chapter (Catti, 44 pp.) deals with the physical properties of crystals. An introduction to tensor algebra is followed by an overview of the principal electrical and elastic properties of crystals. Defects and the means to examine them are well covered, with a discussion of their thermal distribution and diffusion. The diagrams illustrating the various defects are particularly helpful.

This is a remarkable text. It is a tribute at once to the wide reach of crystallography over many branches of science and to the contemporary vigor and vitality of Italian crystallography and crystallographers. As its editor hoped, it can well form the foundation of a curriculum in crystallography at the undergraduate level or a means to introduce crystallographic ideas into courses in other disciplines and much of the material is suited to more advanced and more specialized courses. The flavor of the book is quite contemporary and its emphases are on current areas of research. The many references to the primary literature offer entry points for further study. The book contains a wealth of information, easily accessible through the use of boldface for key terms in the main text, and there is a high level of mathematical rigor in the treatment of the core topics. Errors and typographical slips are few, though on p. 23 there is an obvious example in the figure and on p. 147 less obvious ones in both the figure and the caption. In his introduction to Chapter 3, Giacovazzo attributes a share in the solutions of the structures of the alkali halides to von Laue. Bragg did use Laue photographs but that marked the extent of von Laue's participation. Also, Friedrich, who is identified as Röntgen's student, had been appointed Sommerfeld's second assistant by the time of the first famous experiment. No matter; all of the pioneers of 1912 would be properly astonished at the range of developments in crystallography and its applications recorded and distilled in this text for presentation to the student 80 years later.

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