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.

Acta Cryst. (1997). B53, 737

Elements of inorganic structural chemistry. Selected efforts to predict structural features, 2nd English ed. By ERWIN PARTHÉ. Pp. xii + 169 (computer program disk included). Geneva: K. Sutter Parthe, 1996. Price US $60. ISBN 2-9504924-2-8.

This book starts with the sentence 'Definition: Two structures are called configurationally isotopic if they have the same space group, the same number of atoms in the unit cell on the same Wyckoff sites with the same or similar positional coordinates (x,y,z) and the same or similar values of the unit cell axial ratios (c/a, a/b, b/c) and cell angles (α, β, γ)'. The sentence gives a good indication of what the reader can expect, a book rich in definitions, in which a familiarity with *International Tables for Crystallography* (1992, Vol. A) is assumed, despite a disclaimer to the contrary in the preface. The subtitle 'Selected efforts to predict structural features' better describes the book's contents, which strongly reflect the author's lifelong interest in the classification and prediction of tetrahedral structures, *i.e.* structures in which at least some of the atoms are tetrahedrally coordinated. This is a category which, by the author's own admission, contains only $\sim 20\%$ of known inorganic compounds. Those for whom the term 'inorganic chemistry' means 'transition metal complexes' will find little of interest here as compounds with organic components are explicitly excluded from consideration.

Developed from notes to accompany a course given by the author, the book shows how electron counting rules can be used to predict the likely tetrahedral structure of a wide range of compounds. Given the difficulty of remembering the 32 specially defined variables that appear in these rules, a glossary would have been more helpful than the index that gives only the page number on which each term is defined. Fortunately for a user who might be confused by the complexity of the rules, they are all coded into the DOS program *VEC* that comes with the book. *VEC* is easy to install and use and, when given a chemical formula, it applies the rules and presents the user with a possible structural diagram. The disk also contains a database of the nearly 400 structures described in the book. A rotatable picture of each structure would have been helpful, but the addition of graphics would probably have rendered the database much less portable.

The first two chapters contain mostly definitions and Chapters 3–9 show how the electron counting rules can be used to predict the structures of a range of different substances such as elements, normal valence compounds, compounds with adamantane structures and compounds containing tetrahedral anions. The text of the book, which is published privately, has some weaknesses. Germanic constructions, persistent spelling mistakes (*e.g.* 'differenciate') and some inexplicably large spaces between words in mid-sentence tend to interrupt the flow. However, the meaning is clear and the language easy to understand. There are excellent figures that make it easier to visualize the many structures that are described and their numbering makes them easy to find when they are referred to in other parts of the book. A number of exercises, with solutions, are provided for students. Experienced crystallographers will appreciate the appendix of unit-cell transformations, but its inclusion is surprising and may reflect the author's frustration in dealing with the large number of different space-group settings found in the literature.

While the crystal chemist will find much of interest in the book, not least the definitions of different systems of systematic labelling (*e.g.* Pearson codes, Ramsden notation), the neophyte will find the book heavy going. As the opening quotation indicates, a considerable background knowledge of crystal chemistry and of crystallography is assumed. The text would undoubtedly be a helpful supplement to a postgraduate course of the kind given by the author, but this is not a book that a novice could use without direction.

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Acta Cryst. (1997). B53, 737–738

Designing the molecular world: chemistry at the frontier. Edited by PHILIP BALL. Pp. vii + 376. Princeton, NJ: Princeton University Press, 1994. Price $16.95 (paperback). ISBN 0-691-02900-8.

Philip Ball has written an excellent summary of the state of the art of structural chemistry for the nonspecialist. He covers a broad range of topics, including basic principles of X-ray crystallography, NMR spectroscopy and kinetics, and describes advances in chemistry, biochemistry and materials sciences. He writes knowledgeably and, for the most part, accurately about all these topics in a way that should be comprehensible to all. His writing is lucid and entertaining, and the book is amply and excellently illustrated. Most chemists, physicists and biochemists could benefit from reading it; although there may be little in the book of which they are not already aware, this balanced overview of the many facets of structural chemistry illuminates links and patterns of interaction that give the reader a valuable, popular, integrated summary.

Besides reviewing all the currently fashionable topics, such as quasicrystals, fullerenes, molecular sieves, supramolecular assemblies and self assembly, self replication, chaos, fractals, the origin of life and global warming, Ball offers speculations on future applications and developments. His comments on the reconciliation of science and spirituality with respect to

the origin of life are well balanced and articulate, as is his thorough treatment of current theory and opinion on the topic. He concludes that the evidence in support of any of the various ideas is inadequate to allow an unequivocal choice among them.

Experts in any given topic who quibble about the details of coverage of their own specialty are, often justifiably, accused of failing to see the wood for the trees. It is not to detract from the overall value of the work that I offer a crystallographer's quibbles. Ball refers to the techniques of X-ray crystallography as bouncing beams of X-rays off crystals and as providing only static information on molecules frozen in place. In light of this shortcoming, he asserts that spectroscopy is 'perhaps the chemist's primary investigative tool'. True enough, and it is certainly too much to expect him to be aware of the subtleties of the study of thermal motion, atomic displacement parameters and structure correlation, or the use of rapid data collection using synchrotron sources and Laue techniques to follow the dynamic details of enzyme reactions in the solid state. Something for a later edition, perhaps?

More fundamentally, his description of the process of structure determination by X-ray diffraction is muddled and inaccurate (pp. 120–121). Ball states 'If the unit cell contains a large number of atoms, the task of indexing the peaks is far from straightforward'. It isn't clear what he means by 'indexing the peaks'. Clearly, indexing the diffracted intensities is trivial and identifying which peaks correspond to which atoms may or may not be straightforward, depending upon the resolution of the map and the accuracy of the phasing. He also has the following remarkable interpretation of the use of electron density maps: 'The advantage of treating the structure in terms of an electron density map is that it allows one to bring to bear some mathematical tools that cannot be applied to a discrete "atomic" picture. Rather than pushing atoms about in order to match a calculated diffraction pattern to the measured one, a continuous map of electron density can be "molded" like clay to the right shape, using a mathematical procedure derived from the work of the nineteenth century French mathematician Joseph Fourier.' Equally fuzzy is his lack of distinction between the heavy atom method and isomorphous replacement as phasing tools, and his total disregard of the existence of direct methods. We should, however, take heart from Ball's assertion that 'Today huge and complex biological structures, such as that of the virus responsible for foot-and-mouth disease, can be solved more or less routinely'.

Such superficiality is perhaps inescapable in a popular work such as this, though one may point to such honorable exceptions as *The Eighth Day of Creation*, and does make one wonder what misconceptions one may acquire about areas with which one is less familiar. However, such misgivings must be balanced against the good that results from introducing students of all ages to an overview of current hot topics in structural science that, at least, catches the excitement of the 'new chemistry'.

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Acta Cryst. (1997). B**53**, 738

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.

Crystallography in modern chemistry. By THOMAS C. W. MAK AND GONG-DU ZHOU. Pp. xiii + 1323. Chichester: John Wiley & Sons, Ltd, 1997. Price £55.00, US $76.95 (paperback). ISBN 0-471-18438-1. This is a paperback reprint of the original 1992 publication of this book, reviewed in this journal by J. P. Glusker [*Acta Cryst.* (1993), B**49**, 576–578]. It meets, at least in part, Dr Glusker's criticism that the high price of the original 'puts the book out of reach of a student audience and may deter scientists who would benefit from owning this splendid work from acquiring it for their personal libraries'.

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Collected works of Dorothy Crowfoot Hodgkin. Vol. I. **Insulin.** Vol. II. **Cholesterol, penicillin and other antibiotics.** Vol. III. **General crystallography and essays.** Edited by G. G. DODSON, J. P. GLUSKER, S. RAMASESHAN and K. VENKATESAN. Pp. cxliii + 2230. Bangalore: Indian Academy of Sciences, 1996. Price US $120 (Individual vols. US $40). ISBN 81-7296-020-4. A review of this book, by Edward Baker, has been published in the July 1997 issue of *Acta Crystallographica Section A*, pages 528–530.