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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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Organic crystal chemistry. (IUCr Crystallographic Symposia No. 4.) Edited by J. B. GARBARCZYK and D. W. JONES. Pp. xi + 203. Oxford University Press, 1991. Price £30.00, US \$55.00. ISBN 0-19-855383-8.

This book contains a cross-section of the papers presented at the Seventh Symposium on Organic Crystal Chemistry, organized by Professor Z. Kałuski of the Faculty of Chemistry at Adam Mickiewicz University, and held at Poznań-Rydzyna, Poland, 14–17 August 1989. These symposia have provided a forum for interaction between the sizable Polish chemical crystallographic community and a significant number of chemical crystallographers from other countries. The field of organic crystal chemistry has moved beyond the basic experimental determination of molecular dimensions to consideration of the chemical, biological and physical properties of both molecules and the crystals in which they find themselves. The papers in this volume deal with a wide range of current topics in crystal chemistry, including the arrangement of molecules in crystals (studies of polymorphism and crystal engineering), analysis and prediction of intermolecular interactions, studies of the properties of solid solutions, and identification of structural trends - found by surveying the wealth of data available from crystallographic databases.

This book is an excellent introduction to these various applications of crystallographic studies and should be placed in the hands of any young person considering a career in crystal chemistry. It is an admirable refutation of the misperception of many scientists that crystallography is a service rather than a scientific study.

A strong theme in the volume is the study, analysis and control of intermolecular interactions. The book begins with J. Bernstein's elegant presentation of polymorphism and its implications for the properties of crystalline materials, and of molecules, that depend strongly on conformation. D. Paukstza and coworkers present a cleverly designed device for growing crystals in an electric field and thereby affecting polymorphism. A chapter on controlling crystal growth through solvent-surface interactions (by L. Shimon, M. Vaida, L. Addadi, M. Lahav and L. Leiserowitz) continues the emphasis on intermolecular interactions and their role in determining crystal properties. T. Krygowski's paper provides mathematical tools helpful in the analysis of interactions, and examples of such

interactions are presented by A. Katrusiak in a study of β -diketoalkanes.

The chemistry or biology of molecules is another theme in the book and is represented in articles on the steroid hormone receptor (W. Duax and J. Griffin), Werner clathrates (Z. Lipkowska), cycloannulated aromatic systems (R. Boese and coworkers), S \rightarrow O hypervalent bonds (A. Kálmán) and aryl oxide-aluminium π -bonding (A. Barron). These papers demonstrate the power of a study that joins detailed analysis of individual structure determinations to the analysis of a large number of similar structures to identify chemical properties or predict biological actions.

The volume is carefully prepared and edited in all but one respect. The exception relates to the linkage between text and illustrations. As is often the case with papers prepared from oral presentations, although the papers are clear and well illustrated, the illustrations are often not explained adequately in the text, or are captioned unclearly. However, overall this volume is important reading for anyone working in the field of crystal chemistry.

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Crystallography in modern chemistry. A resource book of crystal structures. By THOMAS C. W. MAK and GONG-DU ZHOU. Pp. xiii + 1323. New York: John Wiley, 1992. Price \$136.00. ISBN 0-471-54702-6.

This book is based on lectures of the authors at the Chinese University of Hong Kong, the University of Western Ontario and Peking University over the past 25 years. It is a tribute to the richness of structural data obtained by X-ray crystallographic studies. The first 20 pages consist of a historical review of crystal structure determinations. Then follow details of structure determinations and discussions of their significance

for 27 'fundamental structures', many inorganic structures (of which 43 are compounds of main-group elements and 23 involve compounds of transition elements), 23 organic compounds including vitamin B₁₂ coenzyme and valinomycin, together with 16 organometallic compounds and nine inclusion compounds. These fill nearly 1300 pages. Because the authors provide space groups, unit-cell dimensions and atomic coordinates for approximately 140 crystal structures, together with detailed commentary, conformational descriptions, diagrams and references, the reader may examine the structures in the most comfortable manner, either on a graphics terminal or from the book.

So much for the statistics. This book is a gem of a reference book on structural chemistry, useful for anyone who wishes to learn about the subject. It is like an annotated selection from scientific journals since the science of crystal structure analysis started. It is difficult to give a detailed analysis of such a hefty book, so I have selected a few descriptions that I personally found interesting in order to give readers an overall flavor of the book. There is no other volume that I know of that covers such a wide range of structures together with so much discussion.

Of current interest is the section on buckminsterfullerene and the quest for all-carbon molecules. The descriptions of the crystal structures of benzene and hexamethylbenzene contain a discussion of disordered Kekule-type structures (two D_{3h} models), and the limitations of X-ray studies in resolving this problem, noting that spectroscopic studies favor a D_{6h} structure. Cyclooctatetraene and its valence isomers, its benz-annulated derivatives and its silver adducts are also described. The description of the crystal structures of the allotropes of boron includes some elegant diagrams of the icosahedral structures found in the various forms. This is followed by information on borides and the structures of the boron hydrides – also derived from icosahedral structures.

General descriptions of structures each highlight some chemical principles. Copper sulfate, the first crystal studied by X-ray diffraction, has a crystal structure that illustrates many points. Neutron-diffraction data give good H-atom coordinates and show the increased H—O—H angle of water on coordination to the copper ion. The Jahn–Teller effect has been studied by charge density studies in $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ and compared to that in isomorphous $\text{CrSO}_4 \cdot 5\text{H}_2\text{O}$. The cube-shaped iron–sulfur tetranuclear clusters contain some fascinating chemistry, demonstrated by a variation in Fe—S distances along edges in one direction of the cube. This is described in the context of the various enzymes that contain this cluster, and is interesting with respect to the structure of nitrogenase just reported (since the book was published) and containing an Fe–Mo cluster.

Several examples of crystal structures that lead to descriptions of hydrogen bonding are described. Hydrochloric acid dihydrate, which is $\text{H}_3\text{O}_2^+ \cdot \text{Cl}^-$, contains very short hydrogen bonds (2.4 Å). The description of hydrogen bonds that follows at this point lists many compounds containing such an H_5O_2^+ ion, and the analogous protonated water structures found in other acid hydrates. Hydrogen peroxide and its torsion angles are described in the crystal and in the gas phase, together with the sensitivity of the dihedral angle to the surroundings in the crystal.

Perdeutero- α -glycylglycine provides an excellent introduction to peptide stereochemistry both with respect to protein structure (α -helices and β -sheets) and the conformations of

cyclic polypeptides. The description ends with details of the three-dimensional structures of hemoglobin and insulin.

The absolute configurations of crystal structures are also described. Potassium dihydrogen isocitrate provides a forum for discussion of absolute configuration, the measurement of Friedel pairs, and details of the method of determining absolute configuration. For α -quartz, the authors provide a description of its absolute configuration, and of deformation density studies leading to the determinations of atomic charges. I was sorry that the authors did not display a crystal morphology of α -quartz with hemihedral faces, the absolute structure and the sense of rotation of plane-polarized light for one of the two possible forms.

Several organometallic compounds of interest are included in this volume. Grignard's reagent (ethylmagnesium bromide), the Mg—C bond and the structures of other alkyl magnesium complexes are described. There follows a discussion of the crystal structure of triethylaluminum and the Al—C bond. In Zeise's salt $\text{K}[\text{H}_2\text{C}=\text{CH}_2]\text{PtCl}_3 \cdot \text{H}_2\text{O}$, the platinum is 2.02 Å from the carbon–carbon double bond and the hydrogen atoms are bent away from the metal. Dimanganese decacarbonyl, $\text{Mn}_2(\text{CO})_{10}$, has an Mn—Mn bond and has been the subject of deformation density studies. The nature of bonding in such compounds is discussed in detail. This leads on to well referenced information on the cluster structures of a variety of metals. The crystal structure of ferrocene, a molecule with two five-membered rings sandwiching an iron atom, is complicated by disorder problems. A detailed molecular orbital analysis follows descriptions of this type of structure. Cobaloximes – cobalt derivatives of dimethylglyoxime that bind an aromatic base and alkyl groups in axial positions – are of interest with respect to the stability and reactivity of the Co—C bond. In the crystalline state they can undergo a photochemical reaction leading to racemization if there is room in the crystal for the necessary movement of functional groups. The electronic effects of the axial ligands on each other are also of interest. These complexes are used as models for the action of vitamin B₁₂.

Molecular packing is well illustrated. Phase diagrams and crystal structures are presented for eight or more forms of normal ice and its high-pressure polymorphs. The prostaglandins have long alkyl side chains and their various conformations and the mode of packing of alkanes are well described. The crystal structure of methyl *p*-bromocinnamate provides an example of another compound that undergoes a solid-state reaction. In this structure the distance between C=C bonds in adjacent molecules in the crystal structure is 4.1 Å. A photochemical reaction leads to cyclization to a truxillic acid derivative.

There is a most interesting section on dehydrated zeolite 4A (Linde molecular sieve type 4A), a structure determined in 1977, leading into a description of framework structures and polyhedral cages in zeolites. Inclusion compounds, such as the cyclodextrins, are discussed because they provide a framework not only for molecular binding but also for reactions (cyclodextrin-based artificial enzymes).

The aim of the authors is to teach structural chemistry, so that the book should appeal to both students and teachers. The compounds chosen for description were selected with care to illustrate a point in chemistry or stereochemistry. The choices are excellent. The authors have not always chosen standard examples, but have selected those that illustrate some good chemical principles. They show a deep appreciation of the

overall literature in this field. With this book a teacher can introduce the student to the entire field of structural chemistry. The various publishers who have allowed their figures to be published are to be complimented. The stereodiagrams are very helpful in providing three-dimensional views of the crystal structures and the overall choice of illustrations is very good.

This is a book that should be lying in every chemical and biochemical laboratory. It is excellent to refer to for lecturing and illustrates well the power of structural studies with much useful data, diagrams and commentaries. The high price is unfortunate as it 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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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.

Structural and chemical analysis of materials. X-ray, electron, and neutron diffraction; X-ray, electron, and ion spectrometry; electron microscopy. By J. P. EBERHART. Pp. xxx + 545. Chichester (UK): John Wiley, 1991. Price £95.00. ISBN 0-471-92977-8. A review of this book, by Noel W. Thomas, has been published in the February 1993 issue of *Journal of Applied Crystallography*, page 145.

Protein structure – new approaches to disease and therapy. By MAX PERUTZ. Pp. 326. Oxford, New York: W. H. Freeman, 1992. Price £32.95 (hardcover), £21.95 (paperback). ISBN 0-7167-7021-0 (hardcover), 0-7167-7022-9 (paperback). A review of this book, by Charles M. Grisham, has been published in the May 1993 issue of *Acta Crystallographica* Section D, page 355.

International tables for crystallography. Vol. C. Mathematical, physical and chemical tables. Edited by A. J. C. WILSON. Pp. xxix + 883. Dordrecht: Kluwer Academic Publishers, 1992. Price Dfl 400, US\$ 244.00, £139.00. ISBN 0-7923-1638-X. Because of the special character of this work, and in lieu of a review, a detailed table of its contents is provided in *Acta Cryst.* (1993), **A49**, 371–373. Individuals may purchase this volume, for personal use, at a substantial discount. Details are given in the advertisement facing *Acta Cryst.* (1992), **A48**, 956.

International Union of Crystallography

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Executive Secretary

It is with deep regret that the death of J. N. King is announced. Jim joined the Union as the first Executive Secretary in 1969 and gave loyal

service until his untimely death on April 12. He had known about his illness for about fifteen months but had continued working with remarkable fortitude almost until the end. A full obituary will appear in *Acta Crystallographica*, Section A, in due course.