International Union of Crystallography

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Report of the Twelfth General Assembly and International Congress of Crystallography

The Report of the Twelfth General Assembly and International Congress of Crystallography, held in Ottawa, 16–25 August 1981, has been published in the May 1983 issue of *Acta Crystallographica*, Section A, pages 425–480.

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Report of the Executive Committee for 1981

The Report of the Executive Committee for 1981 has been published in the May 1983 issue of *Acta Crystallographica*, Section A, pages 481–499. It reports on the meetings and publications of the Union, the work of its Commissions, and the work of bodies not belonging to the Union on which the Union is represented.

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Current Crystallographic Books 1970 *through* 1981

The December 1982 issue of *Journal of Applied Crystallography* [*J. Appl. Cryst.* (1982), **15**, 640–676] includes a new comprehensive booklist, commissioned by the IUCr and edited by the Book-Review Editor, John H. Robertson. Dr Robertson has written the following note about the list.

Anyone with an interest in seeing the total range of currently available books on crystallography, and virtually all topics connected with crystallography, can take advantage of the new booklist. It is published not as a separate booklet, but in the *Journal of Applied Crystallography* (*JAC*). *JAC* can be found, of course, in any good library.

It is sometimes quite useful to have a document of this kind at hand, on one's desk, for reference. Copies of this new booklist *can* be obtained from the Chester office of the IUCr; however, as photocopying is nowadays so efficient and routinely available, the IUCr would prefer crystallographers who have such equipment in their institutions to *make their own copies*, if that is reasonably convenient. The Chester office will gladly supply copies to those who cannot easily make their own – in the developing, or third-world countries, particularly.

This new booklist is the successor to Helen Megaw's list (of about 1965, up-dated about 10 years ago by Michael Woolfson). This new list has about 1200 entries. It differs from previous lists in having the books classified into some 30 or so subject areas, rendering it much less tedious to consult, and in the use of various type-faces, making it rather easy for a comparatively casual user to scan up and down the pages to pick out what is interesting in his or her own speciality. The period covered is the decade 1970–1981, with a sprinkling of 1982 titles included. Incidentally, one book that's *not* in the list (because it has appeared only recently) is a reprint of the famous James classic, *Optical Principles of X-ray Diffraction*.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

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The chemistry of the metal–carbon bond. Vol. 1. Edited by F. R. HARTLEY and S. PATAI. Pp. xii + 1071. London: John Wiley, 1982. Price £125·00

This book deals with the structure, thermochemistry and characterization of organometallic compounds. It has 22 chapters, written by individual authors: 11 on synthesis, one on structure, one on thermochemistry, five on analysis and one each on IR and Raman spectroscopy, NMR and mass spectroscopy. Each chapter goes into its subject quite deeply. Unfortunately several of the structural formulae are not well drawn and give a false (or no) idea of the stereochemistry. However, the book will be a very useful addition to the exclusive series *The Chemistry of Functional Groups*, edited by Patai.

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Structure and bonding in crystals. Vols. I and II. Edited by M. O'KEEFE and A. NAVROTSKY. Pp. 327 (I) and 357 (II), Figs. 226, Tables 86. New York: Academic Press, 1981. Price £31·80, US $40.00 (I) and £33·80, US $51.00 (II).

These two volumes are a direct outcome of a conference held (in January 1980 at Castle Hot Springs, Arizona, USA) by a diverse group of scientists with a common interest in principles of structure and bonding in complex solids. Fifty years had elapsed since Professor Linus Pauling published his celebrated paper on 'The Principles Determining the Structure of Complex Ionic Crystals'. Linus Pauling also participated in this meeting and vividly recollected the early days of crystal chemistry from his personal experience. The first chapter is a verbatim record of his recollection. The conference reviewed rather thoroughly the recent developments in various aspects of crystal chemistry.

The book consists of twenty-six chapters or papers, equally divided into two volumes. Virtually all contributors

were participants of the conference. However, the two volumes are by no means conference proceedings. The contributors were encouraged to present overviews of their fields of research and their bearings on related fields. This very appropriate practice has made the book much more readable and beneficial to scientists and students of diverse disciplines.

The conference concerned itself exclusively with inorganic compounds. In addition to simple compounds, silicates and related compounds also received much attention. A few papers were devoted to alloys and intermetallic compounds. Throughout the two volumes Pauling's classical book was closely and frequently referred to. Here I should mention a statement made by the editors in the preface:

> Before this renaissance, virtually the only guide to the factors determining crystal structure was the principles set out in the early days of solid state chemistry and put in definitive form in the chemists' 'bible' – Pauling's *Nature of the Chemical Bond.* Indeed, in dealing with complex silicates, it is little exaggeration to state that there had been little progress (until recently) since the formulation of the celebrated 'Pauling's Rules' 50 years ago.

This statement may well reflect the opinion of most contributors.

The twenty-six chapters can be divided, by and large, into four groups. The first group, from chapter 2 to chapter 7, reports on work which makes rather exact calculations and predictions of the structure, stability, and properties of solids of simple types from the electronic properties of the isolated atoms. The development of atomic pseudopotentials with their successful application to atoms in crystals has been one of the remarkable advances in solid-state science. An alternative approach is to apply theoretical methods developed for molecules, such as MO theory, to crystal-chemical problems. The second group, from chapter 8 to chapter 12, belongs to this category. Each of the two approaches has merits and demerits. The present state of theoretical treatment of solid-state structures allows more exact calculations often at the expense of applicability and clarity.

The understanding of the older topics such as bond length, bond strength, ionic radii, *etc.*, has been renewed and refined. Some of these advances are very impressive and useful indeed. For instance, the valence-sum rule is a refined form of Pauling's electrostatic valence rule. In the light of the distortion theorem one can elucidate the experimental fact that with elevation of pressure Si changes from tetrahedral to octahedral coordination. Chapters 13–19 present these concepts and the last three papers discuss their applications in geosciences.

As the inorganic structures determined by X-ray diffraction nowadays become increasingly complex, the classification of solids and the systematic description of the relationships between their structures present a particularly important problem. In the remaining chapters one can see that many complex structures are made much easier to appreciate and understand when described in an ingenious way.

Most chapters cover the literature up to 1980 or even later.

The editors have done a very good job in organizing thirty-five conference participants to turn out such an up-to-date and coherent book of high quality. It is highly recommendable to structural chemists and crystallographers, solid and materials scientists, geochemists and geophysicists or to any of those who wish to keep up with recent developments in various aspects of crystal chemistry.

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Inorganic stereochemistry. By DAVID L. KEPERT. Pp. xii + 227. Heidelberg: Springer-Verlag, 1982. Price DM 154.00, US $71.70.

The importance of an adequate understanding of stereochemistry in the practice of inorganic chemistry is unquestioned. The wide variety of coordination numbers and structural types known makes any attempt at a systematic approach to structure correlation and the rationalizing of diverse structural types extremely valuable. This work, which is Volume 6 in the Springer-Verlag series entitled 'Inorganic Chemistry Concepts', attempts just such a task, as an outgrowth of a series of articles written by the same author for the well known series 'Progress in Inorganic Chemistry'. The potential reader should understand, however, that new sections, together with the more unified treatment of the book, definitely make the whole add up to more than the sum of the parts.

The author's approach to understanding and rationalizing stereochemistry is based on a systematic quantitative application of the common ideas regarding electron-pair repulsion. The first chapter sets out the elements of this simple theory, which incorporates important refinements such as individual atomic repulsion-energy coefficients, effective bond-length ratios, and normalized bite parameters for multidentate ligands. Of the many possible types of multidentate ligands, the author treats only bidentate and single-chain tridentate ligands.

The second chapter begins with a systematic treatment of the types of classic geometric polyhedra useful in a chemical context. The chapter then continues with a careful discussion of the origins and types of distortions which relate actual chemical coordination polyhedra to the idealized polyhedra. While some of these distortions (those arising from the different size of faces in the semiregular and non-uniform polyhedra for example) are consequences of the repulsive forces which create the polyhedra in the first place, others are shown to be a consequence of the constraints associated with variations in the normalized bites of chelating ligands. Since a wide variety of such chelating ligands is available, the author is careful to demonstrate how the different coordination geometries possible for a given coordination number are related to one another, as well as how they depend on the bite parameters of the chelate ring.

The remaining chapters deal with the stereochemistries associated with coordination numbers from four through twelve. For each of the coordination numbers treated, plots showing repulsion energy as a function of structural variables allow the author to deal with the relative repulsion