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Book Reviews

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Structure Correlation. Edited by Hans-Beat Bürgi and Jack D. Dunitz. pp. XXIV + 888 (2 volumes). Weinheim: VCH Verlagsgesellschaft, 1994; ISBN 3-527-29042-7; 398 DM.

As structure determination by single-crystal X-ray diffraction became prevalent crystallographers began to compile structural databases. As databases became accessible structural scientists began to use the complications to discern patterns of molecular and ionic interactions and deformations. In the mid-1970s Bürgi and Dunitz published a series of papers; showing how reaction paths, *e.g.*, for nucleophilic addition to a carbonyl group, could be deduced from crystallographic data. Those papers marked the beginning of the field that has become known as Structure Correlation. While the approach was not entirely new (*cf.* Bent's 1968 paper on donor-acceptor interactions), the new data and tools available opened up many lines of inquiry.

Bürgi and Dunitz have remained at the center of this expanding field. Their two-volume book **Structure Correlation** is intended to be an overview of modern methods for interpreting structural (*i.e.*, crystallographic) data. The book focuses on molecular substances, including inorganic complexes and biological macromolecules, but ionic materials are also discussed. Some chapters center on detailed interpretations of bond lengths and angles within classes of molecular fragments while other chapters are devoted to the interactions between molecules, *i.e.*, to the principles of molecular aggregation and crystal packing. The breadth of topics covered is impressive. Twenty-eight authors, many of whom had previously co-authored papers with Bürgi or Dunitz, contributed to the 18 chapters. The cohesion of the book was guaranteed by the vision and efforts of the editors, who also wrote three of the central chapters.

Volume 1 begins with a presentation of tools. Coordinate systems transformations, and symmetry are treated in the first two chapters; some aspects of databases are described in chapter 3; statistical and numerical methods of data analysis are outlined in chapter 4. These four chapters are dense, but are necessary because the topics are seldom covered adequately in books accessible to physical scientists. A first-time reader might be well advised to start with the excellent Preface, to continue with the first few pages of Chapter 1, and then to jump to Chapter 5. In this chapter titled "Structure Correlation; the Chemical Point of View" Bürgi and Dunitz ouline the history and assumptions of the method and describe relationships between structural data and the underlying potential-energy surfaces.

Volume 1 continues with three chapters on reaction paths (transformations of carbonyl derivatives; nucleophilic substitution reactions; ligand rearrangements and substitutions in transition-metal complexes) and one on conformational analysis. Volume 2 begins with three chapters on crystal packing (extended inorganic structures; hydrogen-bonded assemblies; van der Waals crystals). It continues with five chapters on proteins (ligand-receptor interactions; steriod receptors; patterns in secondary and tertiary protein structure; correlation of protein structure with sequence; prediction of structures of hexapeptides) and a final chapter on structural patterns in nucleic acids. Volume 2 concludes with several appendices, including a lengthy

table of standard bond lengths based on data in the Cambridge Structural Database, and an index.

Most chapters cover the literature through 1991; many include references dated 1992. Many chapters also discuss unpublished work. The average number of references per chapter is 86 and the average number of Figures, a few of which are in color, is 20. The book is nicely produced and largely free of obvious errors.

These volumes should be of wide interest. They demonstrate the richess of crystallographic data as interpreted by imaginative scientists with some background in statistics. The book provides the general reader with an excellent overview of the science made possible by the crystallographic databases and provides chemists and biochemists interested in actually using the method with plenty of examples and guidance.

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"**Molecular Magnetism**" by Oliver Kahn, VCH Publishers, Weinheim, 1993; ISBN 3–527–89566–3; 380 pages; DM 160.

A field of wide and growing interest derives great impetus from a monograph that assembles the fundamentals in a clear and accessible manner. With this marvelous book, the field of molecular magnetism now has such a monograph.

The study of molecular magnetism encompasses systems whose molecular architectures vary widely in complexity. Many practitioners focus their efforts on the magnetism of an individual center; others on discrete clusters; yet others on extended arrays of interacting centers. The unique feature of this book is that it provides a clear discussion of the entire spectrum of systems, and thus is of use to any practitioner.

After an introductory chapter that presents the fundamental equations associated with magnetic measurements, the next four chapters explain the properties of molecules containing a single (unique) paramagnetic metal ion. They describe systems of progressively greater complexity, beginning with molecules without first-order orbital contributions and progressing through systems with orbital momentum, with spin transitions, and with intermediate or admixed spin. Next come four chapters (6–9) on dinuclear centers, again beginning with the simplest case of isotropic coupling and proceeding to introduce such complexities as anisotropic and antisymmetric interactions. Chapter 10 deals with higher nuclearity clusters and ends what may be viewed as a 9-chapter section on discrete molecular entities.

Chapters 11 and 12 describe extended arrays of interacting magnetic centers. Chapter 11 discusses linear chains systems, where the magnetic interactions between chains can (largely) be ignored compared to the interactions between neighbours within a chain. Chapter 12 then treats magnetically ordered systems, the area of Prof. Kahn's most recent major contributions. Chapter 13 represents a kind of coda to this masterwork in that up to this point the interactions are associated with electrons in localized orbitals, while this chapter discusses the properties of polynuclear species in which the unpaired

electrons may be delocalized, a situation that Kahn denotes as spin-dependent delocalization, and others describe in terms of mixed-valency or double exchange. An Appendix then assembles a variety of tables useful in calculations of magnetic properties.

A main thrust of this book is to present the theory underlying magnetic phenomena at the "temperature" of the baby bear's porridge: "not too hot, and not too cold, but just right." At this, the author succeeds admirably. His aim is not too low, and it is expressly "supposed that the reader is rather familiar with the operators and matrix notations used in quantum mechanics." However, while general formulas are presented and some derivations are outlined, the emphasis is on establishing a conceptual understanding of the various models for magnetic interactions.

Although the book is, to the extent indicated, one of "theory," the theory is fully intergrated with experiment. The author makes extensive use of examples in which molecular structures are presented, along with plots of susceptibility data and a description of the interactions that give rise to the observations. Thus, both the theoretically and experimentally inclined can use this book equally well as an introduction to the area and as a foundation for further research.

In writing a book of only 353 pages, Prof. Khan had to make some choices. Thus, the emphasis is on susceptibility measurements, and epr techniques are discussed minimally. The book primarily deals with metal ion centers, rather than organic radicals, a reflection of both the authors's interests and the relative numbers of interacting systems of the two types. The discussion of individual organic radicals is cursory and appears in Chapter 12 as parenthetical remarks, not in Chapter 2 where logic would have it. However, the discussion of extended systems is even-handed in its treatment of the available organic-based materials.

In summary, this book provides a common foundation for experimentalists and theorists, for researchers interested in biological metal clusters and those interested in designing molecule-based bulk magnets. No. laboratory devoted to molecular magnetism can be considered as completely furnished without at least one copy.

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Stereochemistry of Organic Compounds, by Ernest L. Eliel and Samuel H. Wilen with a chapter on Stereoselective Synthesis by Lewis N. Mander; John Wiley & Sons, Inc., 1994; ISBN: 0-471-01670-5; xv + 1267 pages; $74.95.

"Stereochemistry of Organic Compounds," represents the first truly comprehensive book on stereochemistry to appear since the remarkable, "Stereochemistry of Carbon Compounds," by Professor Eliel was published in 1962. It is rare in science when a book remains the standard reference in a field for more than thirty years. This was true with respect to Professor Eliel's book. Any consideration of the present book by Eliel and the late Samuel Wilen invites comparison with the earlier work if only because the earlier work has remained the standard in the field. Like the earlier work, this massive,

1210 page, volume promises to have a major impact on the field of stereochemistry. Much more than a text book, more general than a treatise or monograph, this readable and comprehensive book should find a place in the private libraries of most practicing research chemists and academic chemists. This book has been written to appeal both to the specialist and the scientist who will make only occasional use of stereochemical concepts. The appended glossary, for example, will be especially useful to the non-specialist.

The greater emphasis of the book on structural rather than dynamic stereochemistry is indicated by a listing of the chapters; Introduction, Structure, Stereoisomers, Symmetry, Configuration, Properties of Stereoisomers. Stereoisomer Discrimination, Separation of Stereoisomers. Resolution. Racemization, Heterotopic Ligands and faces (Prostereoisomerism, Prochirality), Stereochemistry of Alkenes, Conformation of Acyclic Molecules, Configuration and Conformation of Cyclic Molecules, Stereoselective Synthesis, Chirootical Properties, Chirality in Molecules Devoid of Chiral Centers

This volume continues the same tradition of scholarship and attention to historical development that characterized the earlier work. The authors provide extensive citations to the original literature. They make very heavy use of reviews, chapters and monographs to cover the literature of most subjects where such secondary sources are available. But they also provide fairly comprehensive coverage of the original literature especially when dealing with the development of new ideas. The scholarly bent of the authors has led them to devote special care and attention to the inception of new ideas and experimental areas. Reading a number of brief historical accounts of the development of a concept or method will give pleasure to some readers although others may regard such concerns irrelevant.

Clearly the size of this volume reflects the breadth of material that can be considered to fall within the boundaries of the discipline of stereochemistry. However, even within such a large volume, much has been omitted. The title of the present work refers to Organic Compounds. Clearly most of the exciting developments in inorganic stereochemistry have been necessarily omitted. One might have thought that the term "Organic Compounds" in the title would include more than the term " Carbon Compounds" of the earlier volume. However, the scope is largely limited, as in the earlier volume, to the stereochemistry associated with carbon. The stereochemistry of silicon, nitrogen, sulfur and phosphorous compounds, which have seen very significant developments in recent years are neglected, as is the impact of stereochemistry on reaction mechanisms and the study of labile configurational units. While some may see these omissions as a major defect, it is clear that there was a need to limit the area of coverage. Stereoselective synthesis has been the most active and dynamic area in stereochemistry in recent years. The long chapter by Mander succeeds in covering the major concepts without becoming a mere listing of examples.

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