The current volume of the series continues the excellent tradition of its predecessors, by offering the reader comprehensive and current information on several subjects of importance to specialists in computational chemistry as well as their medicinal chemistry colleagues. Each of the six chapters and the appendix are written by well-known leaders in their respective fields who provide fascinating demonstrations of their extensive expertise. The breadth of computational topics covered makes the volume important to those wishing to gain insight outside of their core area of expertise.

The table of contents is surprising in its high level of detail. This is particularly helpful, since it reads more like an outline of the chapters. The volume provides comprehensive indices: an index of authors cited, an excellent subject index, and a list of contributors and their affiliations. There is also a complete listing of the contents and authorship of the previous 10 volumes in the series.

The book is a high-quality production, all around. It is recommended for individuals, researchers, and institutional libraries.

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From Chemical Topology to Three Dimensional Geometry. Edited by Alexandru T. Balaban. Plenum Press, New York, NY. 1997. xviii + 420 pp. 16 × 23 cm. ISBN 0-30645462. $125.00.

Graph theory, a branch of mathematics, was discovered in the 19th century; present day chemists probably are familiar with graph theory and chemical topology as representations of chemical molecules as lines and points or as a connectivity matrix. There is a burgeoning literature in this field, particularly as it relates to QSAR.

The 10 chapters of this book by Balaban and 16 coauthors span the spectrum from organic to biological to inorganic molecules and size ranging from small alkanes to Fullerenes and transmembrane proteins. With the exception of the QSAR and protein chapters, the emphasis is on research and theory.

QSAR based on graph-theoretical descriptors reflects computational efficiency. Instead of high-level quantum mechanical calculations, algebraic indices derived from connection tables of molecular graphs may be computed and correlated to biological activity of compounds. However, one commonly encountered objection is the seeming "2-dimensional" nature of graph theory descriptors. Chapters 1−3 discuss approaches to making the indices reflect the "3-D" nature of real molecules, including 3-dimensional geometry, conformations, and chirality. In the first chapter, molecular similarity attributes are ranked in order of importance for biological activity, including *disposition* of electrical charges, of polar groups, of H-bond donors and acceptors, and of lipophilic and hydrophilic regions. *Disposition is* a 3-dimensional concept.

Chapter 4 treats one of the most important problems of medicinal chemistry: the extraction of a QSAR equation from biological data. The equation can be used predictively to evaluate the therapeutic potential and toxicity of new molecules, prior to synthesis. The effective use of topological descriptors takes on an added urgency in light of the mainstream importance of combinatorial chemistry. Virtual libraries of millions of molecules can be computationally screened with an efficient predictive equation, based on quickly computed descriptors. Real examples of these QSAR equations are given in physical properties, lipophilicity, chromatographic retention time, analgesic potency, and enzyme inhibition.

In the present age of bioinformatics, the relationship between gene sequence and the primary structure of its expressed protein product is understood. However, the problem of protein folding to the tertiary structure is largely unsolved. As Chapter 5 points out, the 3-D structure of a protein is a necessary prerequisite to rational design of small molecule ligands. The sequences of over 30 000 proteins are known, but only 3000 experimental structures are known. Chapter 5 adds to the armamentarium of protein prediction with-theory and practical examples. The treatment of transmembrane proteins, of which the neurotransmitter receptors are the most important, provides a valuable insight into these molecules.

Chapter 6 concentrates on the representation and characterization of molecules, rather than similarity or structure−property relationships. The characterization discussion focuses on defining structural invariants which are mathematical properties of a structure. These are unique for a given structure, but they do not allow reconstruction of the structure. In this chapter the authors proceed from the fundamentals of graph theory through methods which characterize the 3-D nature of real molecules and finally to a consideration of chirality.

Chapters 7−9 deal with Fullerenes, which are of interest because of their unique position in molecular orbital theory. A fundamental category of chemical structures is the one where the members are composed of a single element, carbon being the most notable. Chapter 7 deals with Fullerenes in the context of the connection between geometry and electronic structure. Methods of chemical topology are applied to define a Fullerene, the number possible for a given carbon number, and their structures and properties. In Chapter 8, the possibility of toroidal Fullerenes is introduced. They are predicted to be stable, and at least by analogy, they are not less likely than the hollow spheres which are now known. The central importance of carbon and the large number of conjugated species are treated in the broad context in Chapter 9. Structural enumeration, electronic stability, and properties are interrelated with topology.

The formation of a mathematical graph by the vertices and edges of polyhedra leads to a connection to coordination chemistry and crystal packing. With a reasonable level of mathematical formality in symmetry operations and graph theory, Chapter 10 establishes the

possible isomers of a given coordination number and their orbital properties.

The stated aim of this book is "to provide the reader with an up-to-date account of how one can provide mathematically non sophisticated molecular descriptors encompassing 3-D aspects of molecules. The advantages of such descriptors are an easy intuitive grasp of their significance, the possibility to compute them for any imaginable structure, and their power to be used in QSAR studies and in molecular modeling for drug design." The book seems to go well beyond this ambitious goal. The QSAR chapters are a valuable reference for pharmaceutical and medicinal chemists; the protein prediction method is important reading for structural biochemists; the Fullerene and hydrocarbon chapters are fascinating for computational chemists; and the inorganic chapter provides a glimpse of one theoretical entry point into this area which may become more important with advances in solid-state chemical physics.

This book is addressed to graduate students and research scientists who are interested in molecular modeling, in Fullerene research, in drug design, and in modern mathematical chemistry. The subject matter is mathematical; nevertheless, the narrative can be comprehended by readers having a knowledge of basic algebra. The index, table of contents, and literature citations are good and thorough. The writing is clear and revealing, supplemented by good illustrations. It is well-worth reading, particularly with the appealing subject matter selected.

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Books of Interest

Natriuretic Peptides in Health and Disease. Edited by Willis K. Samson and Ellis R. Levin. Humana Press, Totowa, NJ. 1997. x + 337 pp. 18 x 26 cm. ISBN 0-896-03453-4. $125.00.

Methods in Molecular Biology. Volume 100. Nitric Oxide Protocols. Edited by Michael A. Titheradge. Humana Press, Totowa, NJ. 1997. xi + 324 pp. 16.5 x 23 cm. ISBN 0-896-03537-9. $59.50.

Pharmacologic Analysis of Drug−Receptor Interaction. Third Edition. By Terry Kenakin. Lippincott-Raven, Hagerstown, MD. 1997. xiii + 491 pp. 16 x 24 cm. ISBN 0-397-51815-3. $99.00.

Advances in Experimental Medicine and Biology. Volume 423. In Vitro−In Vivo Correlations. Edited by David Young, John G. Devane, and Jackie Butler. Plenum Press, New York and London. 1997. ix + 300 pp. 17 x 25.5 cm. ISBN 0-306-45600-1. $95.00.

Methods in Molecular Biology. Volume 90. Drug−DNA Interaction Protocols. Edited by Keith R. Fox. Humana Press, Totowa, NJ. 1997. x + 278 pp. 16 x 23.5 cm. ISBN 0-896-03447-X. $69.50.

Methods in Molecular Biology. Volume 79. Polyamine Protocols. Edited by David M. L. Morgan. Humana Press, Totowa, NJ. 1998. ix + 186 pp. 16 x 23.5 cm. ISBN 0-89603-448-8. $59.50.

Endothelin. Molecular Biology, Physiology, and Pathology. Edited by Robert F. Highsmith. Humana Press, Totowa, NJ. 1997. ix + 274 pp. 16 x 23.5 cm. ISBN 0-89603-436-4. $99.50.

Methods in Molecular Biology. Volume 89. Retinoid Protocols. Edited by Christopher P. F. Redfern. Humana Press, Totowa, NJ. 1998. xvi + 434 pp. 15.5 x 23.5 cm. ISBN 0-89603-438-0. $79.50.

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