

Book Review

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Supramolecular Assembly via Hydrogen Bonds II. Structure and Bonding, 111 Edited by D. M. P. Mingos (St. Edmund Hall, Oxford, UK). Springer-Verlag: Berlin, Heidelberg, New York. 2004. xii + 180 pp. \$149. ISBN 3-540-20086-X.

Bing Gong

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Carbonic Anhydrase: Its Inhibitors and Activators. CRC Enzyme Inhibitors Series, Volume 1. Edited by Claudiu T. Supuran, Andrea Scozzafava (Universita degli Studi, Firenze), and Janet Conway (Pfizer Inc., New York). CRC Press LLC: Boca Raton, FL. 2004. xii + 364 pp. \$139.95. ISBN 0-415-30673-6.

This book is a fascinating overview of the initial discoveries, current status, and future directions of the development of both inhibitors and activators of the carbonic anhydrases (CAs). Carbonic anhydrases are responsible for the reversible hydration of carbon dioxide to bicarbonate and a proton. These ubiquitous enzymes, present throughout virtually all living organisms, including animals, plants, algae, bacteria, and archaebacteria, are involved in a vast number of physiological processes. The book highlights the fact that CAs are perhaps a uniquely broad and interesting family of enzymes because the reaction they catalyze is linked to respiration, acid-base homeostasis, photosynthesis, and other biosynthetic pathways. It also emphasizes the fact that they are involved in the transport of CO₂ or bicarbonate. Therefore, CAs affect fundamental physiological phenomena in biology such as cell growth, metabolism, apoptosis, and cancer.

The contributors focus on the α -class of CA and the 14 known human CA isozymes, some cytosolic (CA I, CA II, CA III, CA VII, and CA XIII), others membrane-bound (CA IV, CA IX, CA XII, and CA XIV), one mitochondrial (CA V), one secreted (CA VI), and three acatalytic forms (CARP VIII, CARP X, and CARP XI). Each chapter is a self-contained unit exploring an important aspect of current CA research, including (1) their physiological roles and mechanisms of action, (2) a review of the chemistry of inhibitors, including both sulfonamide and nonsulfonamide inhibitors, (3) an in-depth review of QSAR studies on sulfonamide inhibitors, (4) a discussion of activators, (5) other CA research initiatives, such as the plausible links between CA and cancer, gastroenterology, nephrology, and neurology, and (6) the possible role of the acatalytic forms. The authors are investigators or teams of CA researchers who are internationally recognized experts in the CA field, and as such, their individual contributions are current and relevant to the overall theme of the book, which is to provide a state-of-the-art overview of the latest developments and challenges in CA research.

An important aspect of the book is its emphasis on the necessity of acquiring a detailed understanding of the catalytic mechanism of CA, both enzymatic and structural, in the development of inhibitors and activators. The reader will gain knowledge from past investigators (of special note is the contribution of the late Thomas Maren) in the development of CA inhibitors that are now used to treat and prevent a variety of diseases, such as glaucoma, epilepsy, congestive heart failure, mountain sickness, gastric and duodenal ulcers, neurological disorders, and osteoporosis. The reader will also be given insight into possible future directions and applications of CA inhibitor studies in the treatment of cancer and dermatological, gastroenterological, renal, and neurological diseases. This volume

represents a vast accumulation of knowledge in the CA field and is a good review of the successes thus far of therapeutic agents for the treatment of disease as well as an exploration of the potential for developing novel therapeutic agents using improved CA selectivity with reduced side effects.

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This volume of *Structure and Bonding* contains four reviews on supramolecular assemblies based on H-bonding interactions. Various aspects of molecular crystal engineering are described in three of the chapters, and work on hydrogen bond-templated assemblies is summarized in another.

The first chapter, "Hydrogen Bonding Interactions between Ions: A Powerful Tool in Molecular Crystal Engineering" by Braga, Maini, Polito, and Grepioni, deals with H-bonding interactions with charge assistance. Its contents are divided into nine sections, with attractive subtitles corresponding to different aspects of charged hydrogen bonds. The topics discussed in this review are of fundamental importance and should be of interest to readers outside the field of molecular crystal design. Unfortunately, the prolix style of writing makes reading the article very difficult.

In the second chapter, "Hydrogen-Bonded Supramolecular Chain and Sheet Formation by Coordinated Guanidine Derivatives", Hubberstey and Suksangpanya exhaustively list examples of H-bonded, metal-containing supramolecular chains and sheets based on guanidine derivatives. As pointed out by the authors, most of the studies discussed are independent, and there are no obvious trends that can be found from the known examples. Readers interested in such systems can find numerous references in this review.

Chapter 3, "Hydrogen-Bonding Templated Assemblies" by Vilar, is the only review that does not focus on H-bonded solidstate structures; rather, its topics are H-bond-templated formation of macrocycles, cages, catenanes, rotaxanes, and helicates. Dynamic combinatorial libraries, in which only a limited number of examples based on H-bonding are known, are also presented. Interesting prospects and future possibilities of the field are described, including self-replicating systems based on both natural and unnatural scaffolds. Finally, photodimerization of olefins as directed by H-bonding templates is discussed, wherein the potential of achieving chemical transformations in a highly selective, controlled fashion is demonstrated.

The last review in this volume, "Hydrogen Bonded Network Structures Constructed from Molecular Hosts" by Hardie, is a description of recent efforts to develop host-containing molecular crystals. This is a timely topic because it combines traditional studies of host-guest supramolecules with the design of solid-state structures. Designs based on hosts such as crown ethers, calixarenes, cyclotriveratrylene, cyclodextrins, and cucurbiturils are discussed. Recent progress in these systems is nicely summarized.

Overall, this book focuses mainly on H-bonded assemblies in the solid state. It will be useful to those who are interested in quickly looking up data and references in the discussed fields. **Bing Gong**, *State University of New York*

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Applications of Evolutionary Computation in Chemistry. Structure and Bonding, 110. Edited by Roy L. Johnston (University of Birmingham). Series edited by D. M. Mingos (St. Edmund Hall, Oxford, UK). Springer-Verlag: Berlin, Heidelberg, New York. 2004. x + 184 pp. \$169.00. ISBN 3-540-40258-6.

Volume 110 of *Structure and Bonding* deals with computational approaches and methods that are based upon the principles of biological evolution. The book is divided into six chapters plus a summary chapter, a list of suggested readings, and a subject index.

Chapter 1 is a basic introduction to evolutionary computational methods such as evolutionary (EA) and genetic algorithms (GA). This is a strong starting chapter, and the graphical representations make the theoretical component easy to grasp and comprehend for the nonspecialist. This introductory chapter should be useful even for those who have a sound background in predictive theory, for it lays open the field very well with regard to what has developed and what may be on the horizon.

The remaining chapters deal with applications of the concepts of EA and GA to optimization of global clusters, prediction of structures from diffraction data, prediction of crystal and protein structures, and drug design. The chapters on diffraction-based structure and crystal structure prediction were perhaps the most interesting and intriguing sections of the book. It appears that EA and GA approaches can make an impact in these areas, as evidenced by some of the data presented in these chapters. Curiously, some of the work presented in the chapter on diffraction/structure determination covered prediction of polypeptide structures, which in a sense stole the "thunder" from the chapter on protein folding. In comparison, the chapter on optimization of global clusters provided little in the way of real data and relied more upon dry discussion. Similarly, the chapters on drug discovery and protein folding/structure prediction were a bit lean with regard to the analyses of real data. These three chapters could have benefited from inclusion of more published or unpublished data or figures to emphasize the points raised. Perhaps a later volume on these topics will provide more details.

The figures, tables, and text were all printed clearly and easy to read. The brevity and concise approach of this volume make it a reference text that is not ponderous to read (184 pages) and is quick to look through when searching for a topic. Most of the citations draw upon primary references from the late 1990s through 2002, and thus many of the topics tap into recent, important, peer-reviewed developments in each field. However, it would have been helpful to potential readers if the full citation format were utilized, instead of defaulting to the abbreviated author/year/journal format and leaving out the article titles.

Overall, I recommend this volume to theoreticians and chemists who are unfamiliar with these areas but have an interest in working in this growing, challenging area. This book may also be useful as a handy, brief overview for those who are involved in EA and GA programming in the chemical sciences, or as a companion text to be used in a graduate-level theoretical/ computational course.

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