

## Book Reviews \*

**Genomics: The Science and Technology behind the Human Genome Project.** By Charles R. Cantor and Cassandra L. Smith (Boston University). John Wiley & Sons, Inc.: New York. 1999. xviii + 565 pp. \$89.95. ISBN 0-471-59908-5.

This book is comprised of 15 chapters and an appendix that encompasses descriptions of the principles, theories, and methods for analysis of DNA from a short length of DNA to a complete chromosome. Chapter 1 provides a brief overview of DNA chemistry and biology by introducing its nomenclature, chemical and structural attributes, chemical synthesis, enzymatic synthesis and manipulation, cloning, and usage as a molecular tool. The chapter concludes with a discussion of the human genome project with emphasis on the size of the genome in relationship to that of other organisms and the number of genes therein. Chapter 2 is about chromosomes, both bacterial and eukaryotic, and includes discussions on their structure, organization, number, purification, unusual characteristics, and the arrangement and distribution of genes between them. The next three chapters focus on the principles and theory behind the primary techniques utilized to analyze DNA. These include DNA hybridization, the polymerase chain reaction (PCR), and DNA electrophoresis.

Chapter 6 leads the reader into genetic analysis and describes how it is utilized to locate genes of interest. Included in this chapter is a useful glossary of genetic terms, e.g., haplotype, genotype, and phenotype, along with informative descriptions of the principal methods of genetic analysis, such as linkage mapping and supporting methods of DNA analyses. Chapter 7 describes cytogenetics and pseudogenetics, i.e., the methods by which DNA markers, sequences, or genes are physically located in the genome at the level of the chromosome. As in the previous chapter, the authors include the underlying principles and techniques of DNA analysis that are utilized to dissect the genome at this level. Chapters 8 and 9 address the methods utilized to generate physical maps of a given genomic material. These higher resolution maps define the actual (or structural) location, positioning, and order of markers or DNA fragments in a chromosome.

The next three chapters address the initial crux of the human genome project, DNA sequencing. In these chapters, the authors describe the current methods and strategies for small- and large-scale DNA sequencing and discuss future or potential methods of DNA sequencing.

In chapter 13, the authors describe how genes may be identified by one of several cloning techniques. The chapter emphasizes identification of disease-related genes and, in this respect, addresses the identification (or diagnosis) of sequence variations and alterations, e.g., point mutations and trinucleotide repeats. Chapter 14 covers analytical and preparative methods that are based upon usage of oligonucleotides to manipulate, isolate, analyze, and regulate DNA (or RNA) through Watson–Crick and non-Watson–Crick base-pair interactions. Also in this chapter is a discussion on sequence-specific cloning procedures, including subtractive cloning and coincidence cloning.

Cantor and Smith close their book with a chapter on the results and implications of the human genome project. Attention is focused on the analyses of the vast amount of sequence data generated from the project to identify all genes and their respective functions. Finally, as a bonus, the appendix provides a list of related databases and their respective URL addresses.

This book is comprehensive in the sense that the authors have provided the underlying mathematical, physical, chemical, and biological bases of DNA analysis at a level that is suitable for engagement by a broad readership. It presents the human genome project with an appropriate amount of definition, illustrative presentation, and historical perspective. The book is well indexed and as such is also useful as a reference.

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JA995725L

10.1021/ja995725L

**Advances in Supramolecular Chemistry. Volume 6.** Edited by George W. Gokel (Washington University School of Medicine). JAI Press: Stamford, CT. 2000. x + 316 pp. \$115.00. ISBN 0-7623-0557-6

This edition is part of an excellent series of books presenting reviews on current research in the general field of supramolecular chemistry. The seven chapters of this volume encompass a variety of topical subfields, ranging from molecular self-assembly to the design of functional enzyme mimics. Each chapter is extensively referenced and clearly presented and should appeal to a broad readership with interest in supramolecular chemistry.

Chapter 1, entitled “Molecular Self-Assemblies through Coordination: Macrocycles, Catenanes, Cages, and Tubes”, deals with metal ion-mediated self-assembly. Authors Fujita and Biradha provide a focused account of their own research involving the coordination of palladium and platinum with geometrically predisposed heterocyclic ligands toward the controlled generation of topologically defined organometallic complexes. The authors present an evolution of increasingly complex superstructures. The guest-directed selection of a given cage superstructure from a dynamic library of components is a fascinating highlight of this chapter.

The theme of self-assembly is continued in Chapter 2, entitled “Chiral Self-Assembled Structures from Biomolecules and Synthetic Analogues”. This is the longest chapter in this volume and addresses the relation between the chirality of molecules and their derived aggregates. Beginning with a historical perspective, Nolte and Feiters develop a detailed overview of chiral superstructures assembled from precursors drawn from the “chiral pool”. Related unnatural systems are described. The authors emphasize amphiphilic molecular precursors and the attendant use of solvophobic and H-bonding forces toward the assembly of helical fibers.

In Chapter 3, entitled “Spherical Molecular Containers: From Discovery to Design”, MacGillivray and Atwood present an account of work performed in their laboratories concerning the design of discrete molecular and supramolecular objects incorporating closed cavities. The authors describe the development of a rational design strategy for the construction of such molecular containers according to the principles of solid geometry. Platonic solids and Archimedean polyhedra are described in relation to illustrative natural and man-made examples. The authors apply their powerful design principle toward the logic-driven retrosynthesis of molecular containers yet to be prepared.

Chapter 4, written by Schneider, Eblinger, and Sirish, is entitled “Synthetic Peptide Receptors: Noncovalent Interactions Involving Peptides”. This chapter begins with a survey of covalent scaffolds for the attachment of parallel and antiparallel peptidic strands. These models provide insight into the nature of the interactions between peptide strands and set the stage for a subsequent discussion of peptide receptors that operate in organic and aqueous media.

The fifth chapter, by Riley, is entitled “Rational Design of Synthetic Enzymes and Their Potential Utility as Human Pharmaceuticals: Development of Manganese(II)-Based Superoxide Dismutase Mimics”. The author focuses on a description of research from his laboratories on the development of pentaaza macrocyclic ligand complexes of manganese(II) as functional mimics of the superoxide dismutase enzymes. Computational, organic, and inorganic chemistry are applied toward the design of a potential therapeutic agent.

In the next chapter, “Designing Active Sites of Synthetic Artificial Enzymes”, by Suh, the discussion on artificial enzymes is extended with an overview of strategies for the design of functional artificial enzymes. Catalytic elements are treated as modules for attachment to molecular, macromolecular, and supramolecular scaffolds. A fascinating variety of systems possessing variable catalytic efficiencies is derived.

This volume concludes with a review entitled “The Relevance of Supramolecular Chemistry for the Origin of Life”, by Luisi. The question of the origin of life is likely to capture the imagination of scientists from all fields. In this account, the importance of surfactant aggregates is discussed in regard to self-replication, chemical auto-poiesis, and catalysis mediated by vesicles. The author supports his views with his own experimental results.

In summary, the sixth volume of this series offers a fascinating and

\*Unsigned book reviews are by the Book Review Editor.

diverse set of accounts concerning important topics in supramolecular chemistry. This outstanding compilation would make a valuable addition to a research library or a personal collection.

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JA004727Z

10.1021/ja004727z

**Current Methods in Inorganic Chemistry. Volume 1. Theoretical Foundations of Molecular Magnetism.** By Roman Boca (Slovak Technical University). Elsevier: Amsterdam and New York. 1999. xiii + 874 pp. ISBN 0-444-50229-7

This is an interesting book that covers the basic theory of and describes in detail the magnetic behavior of molecules. It should prove very useful to the practitioner in this area because it collects many of the important equations, results, and derivations in one place. It also provides a useful summary of the field for those who want to interpret data and perform manual calculations. This book does not focus on using the machinery of modern computational chemistry to solve such problems, which, in my opinion, is an important drawback. It is written at the level of a first/second-year graduate student in physical chemistry and would be extremely difficult for most experimental inorganic chemists without a full year graduate level course in quantum mechanics. There are 11 chapters and 6 appendices. Each chapter ends with a short, useful summary.

Chapter 1 describes the basic mathematics and quantum mechanics needed to read the book. It provides a useful summary, especially as a refresher, and contains many helpful tables. The section on angular momentum is quite nice, not surprisingly, as this is at the core of much of the rest of the book. The discussion of the ways to couple angular momentum in quantum mechanics is well-done. The sections on tensor properties and molecular symmetry will not be too helpful if one has not seen these topics elsewhere.

Chapter 2 describes macroscopic magnetic properties based on statistical mechanics. I thought that the author might have introduced Heisenberg's formalism on magnetism here or at least reference the original work, but this was not done. Again, the tables are incredibly useful with some on the partition function of molecules as well as others on the definitions of magnetic susceptibilities and thermodynamics. Chapter 3 defines the magnetic properties of a single molecule. This chapter defines the gauge problem and also introduces the concepts of spin, both of electrons and nuclei, and the spin-orbit interaction.

Chapter 4 describes the relativistic approach to the solution of the Schrodinger equation and the Dirac equation in order to directly introduce spin. This is a very nice chapter describing the basic solutions for this complex equation. Again, the tables and the detailed presentation of the solutions are very useful, especially the table on relativistic Hamiltonian terms. A weakness of this chapter and throughout the book is the lack of connections to modern computational methods and software that would allow one to actually solve many of these problems on a computer. For example, there is no detailed discussion of the types of basis sets needed to provide relativistic quantum chemical atomic and molecular solutions. This could have been remedied if the referencing included more modern texts and articles on how to actually use computers to address these issues. Thus, although this book has references to many of the classic texts in the area of molecular magnetism, there are few to modern texts after 1990.

Chapter 5 describes the available methods for calculating diamagnetic and paramagnetic susceptibilities for molecules. It is a nice summary of the available methods (GIAO, IGLO, LORG, etc.), but it does not give details on how to actually do the calculations. It also does not show how closely GIAO, IGLO, and LORG are related, for example, as shown by the Handy and Kutzelnigg groups. The summaries are very useful, but with all of the computational work in this area in terms of predicting nuclear magnetic resonance shifts, it would have been helpful to have a better description of the computational aspects.

Chapter 6 describes magnetic susceptibilities in more detail and makes some of the first connections to experiment with the traditional formulas for temperature dependence. There is also a section on methods for optimization. Chapter 7 provides a description of magnetic materials including ferromagnets and ferrimagnets.

Chapter 8 describes traditional approaches to the study of a single magnetic center with a focus on transition metal centers in complexes. This chapter provides a useful detailed description of crystal field

calculations of magnetic transition metal ions that enables the reader to work easily through a variety of complex equations. The tables are again very helpful and contain many details that are often left out of most other texts on this topic.

The final three chapters present more complex magnetic spin systems, including spin crossover, dinuclear systems, and multinuclear systems. The interactions are worked out in detail, which should be of great help to those who work in this area. One modern area of molecular magnets that is missing is a discussion of organic magnets, such as those pioneered by Miller and Epstein, and the importance of three-dimensional ordering in making practical magnetic materials. This research area has some very complex spin couplings, and it would have been nice to have some discussion of this here.

I have a couple of minor points to make about the book. The presentation could have been helped by numbering the equations. The subject index is weak, and I found it hard to find topics that I knew were in the book. Finally, while there are very few typos in the main body of the text, there are quite a few in the references, especially in the spelling of author's names.

Overall, this a useful, highly specialized text in the area of molecular magnetism. It will be very useful to practitioners as well as to physically inclined inorganic chemists. It should also benefit those interested in the fundamental theory in this area.

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JA995800S

10.1021/ja995800s

**In Our Own Image: Personal Symmetry in Discovery.** By István Hargittai (Budapest Technical University, Eötvös Loránd University and Hungarian Academy) and Magdolna Hargittai (Eötvös Loránd University and Hungarian Academy). Kluwer Academic/Plenum Publishers: New York. 2000. x + 236 pp. \$49.95. ISBN 0-306-46091-2.

This is an interesting book that examines the role of symmetry in scientific discovery and inquiry. Apart from an introductory chapter and a general one on Perception and Symmetry, this book centers around six areas of symmetry as represented by six personalities: Johannes Kepler for modeling, R. Buckminster Fuller for molecules, Linus Pauling for helices, Aleksandr I. Kitaigorodskii for packing, J. Desmond Bernal for quasicrystals, and Pierre Curie for dissymmetry. As the authors state, their intent was not to focus on the personalities by themselves, but to use them as "icons" or jumping-off points for a discussion of scientific creativity based on that particular form of symmetry. This is a book about patterns, how they have inspired and shaped scientific discoveries throughout history, and how they may continue to influence scientific advances today. It is written for chemists and other related professionals, but also for the layperson who recognizes the design of everyday things and has an open mind.

JA004766A

10.1021/ja004766a

**Molecular Modeling and Prediction of Bioactivity.** Edited by Klaus Gundertofte (H. Lundbeck A/S) and Flemming Steen Jorgensen (Royal Danish School of Pharmacy). Kluwer Academic/Plenum Publishers: New York. 2000. xvi + 502 pp. \$110. ISBN 0-306-46217-6.

This book features the contributions from the 12th European Symposium on Quantitative Structure-Activity Relationships held in August 1998. New developments in the field of QSAR and other drug candidate screening technologies are covered in this volume. The 29 full papers and over 100 poster presentations are organized into the following sections: New Developments and Applications of Multivariate QSAR; The Future of 3D-QSAR; Prediction of Ligand-Protein Binding; Computational Aspects of Molecular Diversity and Combinatorial Libraries; Affinity and Efficacy Models of G-Protein Coupled Receptors; New Methods in Drug Discovery; and Modeling of Membrane Penetration.

JA004752S

10.1021/ja004752s