Additions and Corrections

A New Class of Fluorinated Polymers by a Mild, Selective, and Quantitative Fluorination [*J. Am. Chem. Soc.* **1998**, *120*, 6830−6831]. YU REN, TIMOTHY P. LODGE, AND MARC A. HILLMYER*

The first reported example of difluorocarbene addition to a polydiene was by R. E. Cais and S. Siddiqui using $PhHgCF_3$ as the difluorocarbene source and polybutadiene as the substrate (See: *Macromolecules* **1986**, *19*, 595). In addition, difluorocarbene and difluorovinylidene (generated by irradiation of the corresponding chlorofluorocarbons) have been used to modify the surface of polybutadiene by M. W. Thomsen and co-workers (See: *Macromolecules* **1989**, *22*, 481; *Macromolecules* **1991**, *24*, 6343). These references were unfortunately not included in our publication.

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Book Reviews

Reviews in Computational Chemistry. Volume 11. Edited by Kenny B. Lipkowitz and Donald B. Boyd (Indiana University-Purdue University at Indianapolis). Wiley/VCH: New York. 1997. xxiv + 431 pp. $120.00. ISBN 0-471-19248-1.

This book is an excellent entree into the world of biological and pharmacological modeling programs and techniques. The book covers three categories: computer-aided ligand design, 3D quantitative structure−activity models, and two specialty areas (lipophilicity calculation and treatment of counterions in DNA modeling). The first five chapters deal with areas closely linked to drug design and have discussions on three different levels: an introductory level suitable for someone barely familiar with the field, a classification and description of techniques suitable for a worker in a related field or an interested graduate student, and a description of cases and programs suitable for a worker already in the field. The sixth chapter, on treatment of counterions in DNA modeling, is more suitable for the novice. Overall, this book does an excellent job of providing background in a clear, verbal, nonmathematical way, and then summarizing current applications with plenty of recent primary literature references. For those new to the field of computational chemistry (or those outside the field with a need to understand these models), there is an appendix giving an overview of Internet resources in computational chemistry.

The first two chapters cover computer-aided ligand design, or de novo design. The area of de novo design is focused on inventing novel compounds which will bind effectively to known protein active sites. Chapter 1, Recent Advances in Ligand Design Methods by Mark A. Murcko, is an overview of methods, with excellent verbal descriptions of the contrasts between different techniques of creating an appropriate ligand, such as fragment location, sequential buildup, and whole molecule matching. A section on evaluating the differences and advantages among methods is well-written, and there is a long section (which can be skipped) on the details of currently available programs and their methods.

Chapter 2, Current Issues in De Novo Molecular Design by David E. Clark, Christopher W. Murray, and Jin Li, details a step-by-step path through a de novo design project, including description of the active site, ligand structure generation, and structure evaluation. The sections are conveniently titled as questions (sort of an FAQ of de novo design). The most interesting section covers successful case studies in the literature. This section makes clear the notion that de novo design is effectively creating ligands which bind the desired active site.

Chapters 3 and 4 are very similar in topic, but are different enough to warrant inclusion of both. The respective chapters are Theoretical and Practical Aspects of Three-Dimensional Quantitative Structure−Activity Relationships by Tudor I. Oprea and Chris L. Waller and Approaches to Three-Dimensional Quantitative Structure−Activity Relationships by Giovanni Greco, Ettore Novellino, and Yvonne Connolly Martin. There is an overview of classical QSAR in Chapter 3 for the novice to standard quantitative structure−activity relationships (QSAR). In standard QSAR, the effect of a structural change on a parent molecule (such as changing substituents) is correlated with a particular property, such as acidity. Both chapters overview 3D-QSAR, with a bit more math in Chapter 3. The definition in Chapter 4 of 3D-QSAR is given as "quantitative models that relate the biological activity of small molecules with their properties calculated in 3D space".

The differences between the two chapters is that Chapter 3 discusses the theoretical underpinnings, accuracy, predictive power, and explanatory power of 3D-QSAR, while Chapter 4 is more of a path through a 3D-QSAR project. Chapter 4 includes descriptions of different techniques, which is to say, different available programs.

Chapter 5 is Computational Approaches to Lipophilicity: Methods and Applications by Pierre-Alain Carrupt, Bernard Testa, and Patrick Gaillard. Lipophilicity is considered the most important property in QSAR studies of potential drugs; hence, its explicit treatment in this volume is appropriate. The chapter takes the same approach as the first four. The initial section lays a nice introductory foundation for the newcomer. Following that, an overview of theories and calculational methods is given in a verbal (rather than overly mathematical) description. There is a detailed section on current programs including authors, parameters used, and differentiation of applicability of methods. There is also a very useful section with examples of applications in drug design.

Chapter 6 veers from the rest of the book in that it does not deal with drug design techniques. This chapter is Treatment of Counterions in Computer Simulations of DNA by Ganesan Ravishanker, Pascal Auffinger, David R. Langley, Bhyravabhotla Jayaram, Matthew A. Young, and David L. Beveridge. The chapter details methods of treating the mobile counterions needed to neutralize a DNA simulation. A well-written background section is followed by an overview of issues dealt with in a simulation, which is followed by a literature survey. This chapter has the fewest recent references; the other chapters have 10−20 references from 1996 and 1997, but this chapter has only 2 such references.

This book is an excellent addition to a highly regarded series. This particular volume should be of interest to a very wide range of readers, even to those who are only tangentially working with computer-aided ligand design (or drug design). The verbal descriptions of techniques

and methods and the cataloging of the advantages and accuracies of various programs make this an extremely valuable book for those unfamiliar with computational methods.

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Foundations of Modern Biochemistry. Volume 3. Further Milestones in Biochemistry. Edited by Margery G. Ord and Lloyd A. Stocken (Oxford University). Jai Press: Greenwich and London. 1997. x + 346 pp. $109.50. ISBN 0-7623-0078-7.

This third volume in the series Foundations of Modern Biochemistry continues its focus on "quantum leaps" or milestones in the development of important topics in biochemistry. The first volume attempted to explain to younger scientists the remarkable achievements of early biochemists working in the 19th century and first half of the 20th century without modern equipment and easily purchasable supplies including radiolabeled substrates. In the second volume of the series, the review of progress in biochemistry was continued into modern times by inviting distinguished scientists to write articles based on advances in their fields with emphasis on information storage and transfer from DNA. The current volume continues the presentation of different topics in biochemistry, again with distinguished scientists summarizing the background and approaches in the elucidation of complicated biological problems. Three broad general areas are covered in this volume. The first area involves bioenergetics including articles on chemiosmosis, photosynthesis, muscle contraction, and bacterial motility. The second area involves different aspects of biological regulation including articles on membrane receptors, protein phosphorylation, and the regulation of gene expression in bacteria. The final article contains a detailed description of antibody specificity and diversity as proteins.

As with any collection of articles written by different authors, considerable unevenness in the presentations has resulted in terms of overall length of the article, completeness of references sited, and the depth to which the subject is probed. Despite the different approaches to these important topics, this reader was constantly impressed with the descriptions of the scientific reasoning processes that occurred as a field developed. In every article, the earliest observations are presented with the original scientist's explanations and hypotheses, sometimes incorrect, followed by a description of proposed experimental approaches to unravel the problem. As described in one article, most scientists spend their lives working on small aspects of a larger problem, adding observations to the field by making important and relevant experimental findings; however, when a truly creative "giant" emerges and examines the accumulated data, completely new insights into a subject are produced. Consequently, a "quantum leap" in the field is achieved. One striking example of a major breakthrough in a field was described in the chapter on bacterial motility. Until the 1960s, studies of bacterial motility were purely descriptive with minimal understanding of the tactic responses and major controversies about the energy sources for the process. Some progress had been made in understanding the structure of bacterial flagella that moved bacteria forward by propagating waves. At this time, a major breakthrough in our understanding of both bacterial motility and environmental sensing was advanced by Julius Adler, who developed techniques for studying chemotaxis and isolating nonchemotactant and nonmotile mutants.

Scientists and students will enjoy reading many of the articles in this book depending on their interests and backgrounds. For a more senior scientist who has worked for many years in certain fields or followed the literature closely in that field, reading these articles resembles looking through a photoalbum of one's past professional life. For example, reading the history of chemiosmosis made it possible for me to recall arguments among prominent scientists at scientific meetings as to the plausibility of Mitchell's seemingly radical hypothesis. In addition, the chapter on protein phosphorylation reads like a history of ideas developed to understand signal transduction in its various manifestations via different kinases and second messengers. By contrast, reading the chapters on subjects with which the reader has not been closely involved presents a wonderful overview of the field based on an excellent logical historical perspective. Hopefully, graduate students and junior faculty who have not shared in the year-to-year development of these fields will also share in the historical presentation of the excitement of discovery as new data are obtained. Everyone can appreciate the logic by which these experiments were conceived. In general, the chapters are easy to read with the information presented in reasonable depth without burdening the reader with understanding the jargon of the field. Overall, this book was enjoyable to read as well as informative. The major gain for the reader from this book is rekindled admiration for the many scientists who preceded us and gratitude for their wisdom and persistence in tackling these difficult problems.

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Hydrogen Bonding: A Theoretical Perspective. By Steve Scheiner (Southern Illinois University). Oxford University Press: New York. 1997. xix + 375 pp. $85.00. ISBN 0-19-509011-X.

This is an excellent and masterful book, remarkable for the breadth, depth, and insight of its coverage. References are current up to 1995, with a few from 1996. The presentation is often historical, proceeding from simpler to higher-level calculations, but many of the earliest studies have been omitted in order to concentrate on the more reliable recent results.

The viewpoint is that calculations have reached the stage where they are reliable, even for hydrogen bonds, which are a severe test for calculations because the interactions are weak and the potential-energy surface is quite flat. Moreover, calculations offer the freedom from the complications of solvent that often perturb the experimental observations, and calculations can provide a dissection of the interaction energy into physically meaningful components. Scheiner offers an operational definition of the hydrogen bond in terms of a set of observable consequences—geometry, energy, electronic redistribution, and spectral features.

The book begins by introducing the quantum mechanical framework. The methodology is restricted to ab initio calculations, without any consideration of semiempirical methods and little attention to density-functional theory calculations, which have only recently become feasible. There is a description of basis sets and an explanation of the acronyms used to describe them. The significance of electron correlation and the methods for treating this are explained. I would have preferred equations to make some of these descriptions more precise, but the words are usually sufficiently clear and less intimidating for the general reader. There is a good explanation of how the thermodynamic quantities ΔE, ΔH, and ΔS can be calculated, and a careful distinction is drawn between the thermodynamic ΔE, which includes electronic, vibrational, translational, and rotational contributions, and ΔE_{elec}, the electronic contribution to the energy, which is often all that is reported. Sources of error, especially basis-set superposition error, are recognized, along with methods for overcoming them.

The results of calculations are presented in order of increasing distance from the most stable geometry. The first long chapter is on the geometry and energetics of a wide range of hydrogen-bonded systems. These range from those between hydrogen halides and simple bases to those involving water, amines, imines, nitriles, carbonyl compounds, carboxylic acid, and amides, and up to the interesting cases of the nucleic-acid base pairs and the relative stabilities of their hydrogen bonds. The intriguing question of the relative stability of H-bonds and D-bonds is also discussed.

The next two chapters are on broader regions of the potential-energy surface. The first of these covers vibrational spectroscopy of hydrogen-bonded complexes, including both vibrational frequencies and intensities. The second considers the interconversion pathways between minima on the surface. Among the systems discussed in detail are the modes for reversal of donor and acceptor atoms in HX dimers and the much more complicated cases of water and ammonia dimers.

One chapter discusses cooperative phenomena associated with the fact that formation of one hydrogen bond increases the donor and acceptor powers of the constituents. Among the structures considered are linear aggregates of HCN, cyclic HX polymers, various water aggregates, and some mixed systems.

The long final chapter, on a selection of disparate topics, is the most stimulating. Scheiner discusses the questionable cases of the weak H-bond acceptors X_2, CO, CO_2, N_2O, SO_2, and CCl_2, as well as the

case of hydrogen bonding by a C−H bond, which is a weak H-bond donor. My own interests are addressed in an extensive treatment of hydrogen bonds between ions and neutral species. These are unusually strong and show the possibility of being centrosymmetric, a question that can authoritatively be addressed by high-level computations. The relation between H-bond strength and the basicity of the atoms involved is discussed. Another topic is the relative basicity and H-bond ability of the syn and anti lone pairs in carboxylate ions. Finally, Scheiner considers the energetics of hydrogen transfer, which converts AH···B into the gas-phase ion pair $A^-\cdots HB^+$, as well as the extent to which this latter may be stabilized in a polar solvent, as modeled by a dielectric continuum.

One aspect that I much appreciate is that there are frequent references to experimental values, permitting comparisons between the calculated and experimental results. Also, Scheiner displays a healthy skepticism and a recognition of the limitations of the methods. I found a couple of minor misstatements (pp 54 and 61), but as far as I could tell the book is otherwise quite faithful to the topic.

The book is logically organized, with a good table of contents, a list of abbreviations, a subject index, and an index to H-bonded complexes, but there is no author index to the ca. 1100 references. A large number of tables throughout the book provide concise comparisons of the data, such as listings of the geometry of the water dimer at various levels of theory and of the change of vibrational frequencies of HF upon dimerization. Each chapter concludes with a useful summary.

In summary, this book offers an authoritative guide to the current status of a wide range of high-level calculations on diverse aspects of hydrogen bonds. It will provide much information for anyone doing research in hydrogen bonding.

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Industrial Enzymes and Their Applications. By Helmut Uhlig. Wiley: New York. 1998. xii + 454 pp. $94.95. ISBN 0-471-19660-6.

The objective of this book is to examine in detail a wide range of enzymes that have proven industrially valuable by virtue of their efficiency in catalyzing specific commercial processes. This book achieves its objective and provides an excellent overview of the field of industrially important enzymes. Consisting of eight chapters and two appendices, this book is extensively referenced and does include recent citations. The material in each chapter is presented in a logical and understandable manner, and each chapter is well-illustrated with relevant figures and tables.

The initial chapter provides a general overview of the historical aspects of enzymes plus indicates newly developed biotechnological applications for enzymes. Basic principles of enzymology are explained in simplified terms in the second chapter. In addition to outlining enzyme kinetics and nomenclature, this chapter defines specific types of enzyme units, which proves helpful in understanding the material covered in later chapters. In the third chapter, detailed descriptions of enzymes relevant to the hydrolysis of carbohydrates, proteins, or lipids and of commercially important oxidoreductases are provided. The nature of the reactions catalyzed by these industrial enzymes and their respective properties are examined in this chapter. In addition, the manufacturers of technical enzyme preparations are indicated throughout this chapter. The techniques employed in the immobilization of enzymes are described concisely in the fourth chapter. Despite the potential of such techniques, the limited commercial use of only two types of immobilized enzymes, namely, glucose isomerase and penicillin amidase, is clearly explained from an economic perspective. Speculation on the future outlook of using other immobilized enzyme systems in industrial processes is also noted in Chapter 4. The specific applications of commercially available technical enzyme preparations are described in Chapter 5, which is the longest chapter in the book. This chapter indicates which technical enzyme preparations can be used to enhance the wet milling of grains, the brewing of grains, the production of alcohol, the processing of baking and milk products, the production of juices and wines, the hydrolysis of animal and plant proteins, the processing of leather, the sizing of textiles, the cleansing action of detergents, the modification or hydrolysis of fats and oils, the nutritional availability of animal feeds, and the lysis of microbial cells. This chapter concludes with a discussion of the commercial utilization of glucose oxidase alone or in conjunction with catalase to stabilize various food and beverage products by reducing their glucose or oxygen content. The legal considerations of using technical enzyme preparations in foods are explored in Chapter 6 by outlining the regulatory requirements set by agencies of various countries as well as by indicating the enzymes approved for food use in selected countries. In addition, the technical information regarding an enzyme preparation that should be documented prior to submitting an enzyme approval application is presented in Chapter 6. In Chapter 7, the economic importance of developing processes that have increased product yields, improved product quality, or enhanced raw material utilization is emphasized. This chapter explains how the utilization of industrial enzymes can lessen the energy consumption costs of commercial processes as well as can lower the filter clarification and sterilization costs of processes involving beverages or fermentation broths. An examination of what determines the current costs of technical enzymes is also made in this chapter. The eighth and final chapter of the book estimates the worldwide market for technical enzyme preparations used in food and nonfood processes. A minor concern regards the length of some of the chapters in the book. For example, Chapter 5 encompasses 181 pages while Chapters 7 and 8 are only 6 and 2 pages long, respectively. It might have improved the presentation quality of the book if some chapters were subdivided and others were combined.

Overall, I would recommend this well-written book as an excellent reference source. Its comprehensive approach to the understanding and use of industrial enzymes should make this book valuable to chemists interested in enzyme research and development.

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Progress in Inorganic Chemistry, Volume 45. Edited by Kenneth D. Karlin (Johns Hopkins University). Wiley and Sons: New York. 1996. vii + 510 pp. $125.00. ISBN 0-471-16357-0.

This is the 45th volume of the series. It is comprised of six well-written and highly authoritative reviews. Selective Recognition of Organic Molecules by Metallohosts (Canary and Gibb) reviews host−guest chemistry involving metal ions functioning in various ways. Both first and second coordination sphere effects are discussed. Metallacrowns: A new Class of Molecular Recognition Agents (Pecoraro et al.) discusses the synthesis and properties of a wide variety of metallacrown complexes. Much of the work that is reviewed was carried out in Pecoraro's laboratories. The Interpretation of Ligand Field Parameters (Bridgeman and Gerloch) is not intended to be a comprehensive review of ligand field studies. Rather, it is more a tutorial focusing on the principles of interpretation of ligand field parameters and on the ligand fields themselves. Chemistry of Transition Metal Cyanide Compounds: Modern Perspectives (Dunbar and Heintz) for the most part reviews work of the last twenty years. There is particular emphasis on the supramolecular motifs that have been reported such as those based on the Hofmann clathrates and on the prussian blues. Assembling Sugars and Metals: Novel Architectures and Reactivities in Transition Metal Chemistry (Piarulli and Floriani) describes studies directed at the systematic preparation of metal−sugar complexes. Oxygen Activation Mechanism at the Binuclear Site of Heme-Copper Oxidase Superfamily as Revealed by Time-Resolved Resonance Raman Spectroscopy (Kitagawa and Ogura) reviews work on the subject, much of which was carried out by the authors and their associates.

The 45th volume of *Progress in Inorganic Chemistry* is an essential component of any research library.

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