Additions and Corrections

Solvent-Accelerated Decarboxylation of *N*-Carboxy-2-imidazolidinone. Implications for Stability of Intermediates in Biotin-Dependent Carboxylations [*J. Am. Chem. Soc.* **1996**, *118*, 12495−12498]. JUBRAIL RAHIL, SHAOCHUM YOU, AND RONALD KLUGER*

Page 12497: The activation parameters for the reaction in water, based on the data in Table 2, are the following: $\Delta H^{\ddagger} =$ 21 kcal/mol and $\Delta S^{\ddagger} = -8.0$ eu, pH 10.2; $\Delta H^{\ddagger} = 19$ kcal/mol and $\Delta S^{\ddagger} = -5.7$ eu, pH 6.1.

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Book Reviews

Reviews in Computational Chemistry, Vol. 9. Edited by Kenny B. Lipkowitz and Donald B. Boyd (Indiana University-Purdue University at Indianapolis). Wiley/VCH: New York. 1996. xxxiii + 282 pp. $120.00. ISBN 1-56081-930-8.

This is the ninth volume in this on-going series and continues the excellent efforts by these editors to bring together applications of state-of-the-art computational chemistry methods. This volume contains five chapters that address computational problems of specific chemical types and includes peptides, oligosaccharides, and organic molecules, as well as the calculation of free energies and molecular shape descriptors.

Chapter one, Peptide Mimetic Design with the Aid of Computational Chemistry, by James Damewood, Jr., presents 31 case studies, encapsulated in 80 well-documented pages. These examples are a good resource for didactic lessons of successful applications of peptiomimetic design. A prerequisite to the success of these studies was availability of X-ray crystal structures for the target proteins upon which the modeling studies were performed. In most cases, standard applications of a variety of computational programs were carried out.

Chapter two, Free Energy by Molecular Simulation, by R. P. Straatsma, reviews the advantages and disadvantages in the use of thermodynamic perturbation and thermodynamic integration methods in the calculation of relative free energy differences. In many cases, the choice is predicated on the availability of computational resources which engenders a choice between adequate methods and the practicality of the calculations. The review provides numerous examples of the pitfalls these methods entail.

Chapter three, The Application of Molecular Modeling Techniques to the Determination of Oligosaccharide Solution Conformations, by Robert J. Woods, focuses on the choice of parameters for the description of oligosaccharides as their variable degree of flexibility dictates whether a statistically accurate ensemble of conformations or a single conformer is appropriate. Because counterions for oligosaccharides are important, explicit treatment of solvent is crucial.

Chapter four, Molecular Mechanics Calculated Conformational Energies of Organic Molecules: A Comparison of Force Fields, by Ingrid Pettersson and Tommy Liljefors, reviews the relative merits and limitations of various molecular mechanics force fields. Each of the components of the force field is defined, and a comparison is made with each of several typically available force field programs with their reliability to describe specific functional molecular features. On the basis of these data, those force fields which are derived for MMFF93, MM2, and MM3 have the best overall results.

Chapter five, Molecular Shape Analysis, by Gustavo A. Arteca, provides an overview of shape parameters and a guide to their key applications, along with criteria for choosing the appropriate shape parameters. A large part of the chapter deals with scaling and dimensionality of the descriptors. These methods can be powerful tools for the description of several independent geometrical or topological properties.

This book will serve those looking for new perspectives in the field and is a recommended addition to every structural biology and computer modeling laboratory library.

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Phytochemical Diversity: A Source of New Industrial Products. Edited by Stephen Wrigley, Martin Hayes, Robert Thomas, and Ewan Chrystal. The Royal Society of Chemistry: Cambridge. 1997. $135.00. xi + 254 pp. ISBN 0-85404-717-4.

This book presents the proceedings of a symposium held at the University of Sussex, Brighton, U.K., in April 1996. The purpose of the symposium was to present the potential utility of phytochemicals to the pharmaceutical and agricultural industries from both academic and industrial perspectives, to include recent technological advances, and to address industrial exploitation of phytochemical diversity. This book fulfills its objectives very well and should be interesting reading for phytochemical researchers. It provides a good overview of phytochemical research with an emphasis on potential medicinal/agricultural utility and commercialization. It also underscores the need to provide compensation for source countries and indigenous peoples who have often been exploited in the past.

Most of the chapters deal with medicinal aspects of natural products. The opening chapter is a well-presented and informative presentation by G. M. Cragg and co-workers from the NCI and describes the NCI experience in collection, screening for cytotoxicity, and anti-HIV activity, and includes recent examples. This chapter complements chapters in the ACS Symposium Series 534, Human Medicinal Agents from Plants, edited by Kinghorn and Balandrin. The presentation by Cragg et al. also reflects the sensitivity of the NCI to the intellectual property rights of indigenous peoples and source countries. The questions of intellectual property rights and compensation are also addressed in presentations by K. Beese and by M. F. Cantley.

There are presentations which provide illustrative examples of plant selection, extraction, and bioactivity-directed isolation. Besides the chapter by Cragg et al., a presentation by M. I. Choudhary and Atta-ur-Rahman includes isolation and characterization of several bioactive compounds. This particular chapter suffers from unnecessarily excessive crystallographic details while providing insufficient information on the various bioassay techniques employed. Several chapters are devoted to the utilization of ethnopharmacological guidance. Thus, a chapter by A. I. Gray and co-workers deals with an attempt to survey the ethnobotany of Colombia, provides some examples, and also points out the frustration of botanical taxonomy. R. Cooper and co-workers from Shaman Pharmaceuticals present a chapter which describes the operational philosophy of their company (ethnopharmacologically-based plant selection) and compare their track record with "random screening"

approaches. Various antimalarial agents from Thai medicinal plants are discussed in a chapter by C. Mahidol, H. Prawat, and S. Ruchirawat.

A number of presentations in the book deal with particular biochemical targets as opposed to whole cell screening techniques. R. J. Nash and co-workers have screened British plants for alkaloids which inhibit glycosidase. P. M. Shoolingin-Jordan and co-workers have looked for phytochemicals which selectively inhibit enzymes involved in tetrapyrrole biosynthesis. C.-j. Chang et al. have utilized protein tyrosine kinase inhibition as a biochemical screen and briefly mention other biochemical screens in their repertoire. M. I. Chicarelli-Robinson et al. from Xenova Ltd. discuss utilization of both plants and microbes as sources of their active natural products, $GABA_A$ receptor agonists and compounds which reverse P-glycoprotein-mediated drug efflux to overcome multidrug resistance of tumors.

There are chapters which present "alternative" methods for obtaining bioactive natural products. A. M. Stafford and C. J. Pazoles of Phytera Ltd. discuss the advantages of using plant tissue culture techniques over traditional native plant phytochemistry. Two different chapters by J. T. Sime of Zylepsis Ltd. and J. R. Hanson, University of Sussex, show how microbial biotransformation of readily available or inactive phytochemical starting materials can lead to more useful materials. Similarly, partial syntheses or semisyntheses are presented by J. H. P. Tyman for conversion of cheap, readily available phytochemicals to materials such as vitamins, hormones, and antibiotics.

Several chapters are devoted to potential commercialization of plant biochemicals. X. Q. Zhu and co-workers discuss the cultivation and extraction of *Ginko*. There is a discussion of temporal variation of components in *Ginko* extracts, but without a statistical analysis, the results are not meaningful. K. Beese provides an overview of the cost of commercialization of natural products as opposed to synthetic materials. B. Gilbert's chapter dealing with the potential commercialization of Amazonian natural products is very similar to the one in the ACS Symposium Series 588 (Chemistry of the Amazon, Edited by Seidl, Gottlieb, and Kaplan).

A major problem in phytochemical research is keeping abreast of all the material. A chapter by J. Buckingham and S. Thompson of Chapman-Hall compares and contrasts the various information sources available. The presentation suffers, however, in omitting illustrative examples of searches.

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Dana's New Mineralogy. By Richard V. Gaines, H. Catherine W. Skinner, Eugene E. Foord, Brian Mason, and Abraham Rosenzweig. Wiley/VCH: New York. 1997. xlv + 1819 pp. $250.00. ISBN 0-471-19310-0.

This eighth edition attempts to describe, catalog, and classify all known and recognized minerals reported in the literature up to December 31, 1995. It presents the results of nature's own experiments in chemical synthesis. Some anthropogenic minerals are included as well as some data from synthetic equivalents of minerals. This edition is presented against a background of changing ideas of the nature, properties, relationships, genesis, and uses of mineral species. It appears at a time when mineralogy has close affiliation with solid-state physics, materials science, and inorganic chemistry, biology, and other more wide ranging fields of science and technology. There is an Appendix of New Minerals for 1996. Indexes include the List of Mineral Names in Numerical Order, List of Mineral Names in Alphabetical Order, and a General Index.

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Molecular Mechanics Across Chemistry. By Anthony K. Rappé (Colorado State University) and Carla J. Casewit (Calleo Scientific). University Science Books: Sausalito. 1997. xii + 444 pp. $56.60. ISBN 0-935702-77-6.

Computer-assisted model building and visualization of molecular and polymer structures has become an everyday tool in chemical and biochemical research and education. The popular software for this is now so easy to use that the fundamental molecular mechanics science behind it hardly ever draws the attention of nonspecialist users and occupies little space in their manuals. Now there is a book that introduces the basic theory of molecular mechanics and shows how it can contribute to chemistry. Rappé and Casewit's broad survey of molecular mechanics theory and practice is structured as an advanced undergraduate text. Nearly 100 homework exercises, with solutions at the back, are included; the ones that require modeling software can be worked with just about any of the popular desktop computer modeling packages. After an introductory overview, applications to organics, proteins, drug design, DNA, synthetic polymers, and inorganics are described with appropriate examples. A brief concluding chapter explains the provenance of molecular mechanics parameters and suggests ways to augment parameter sets when needed. While written in case study form with a classroom environment in mind, this book will do just as well for independent study. Copious references to the literature are included; while most of them are from the 1980s and early 1990s, the structure and flavor of molecular mechanics as presented here still represent very well what the countless modeling programs being introduced each year offer to chemistry students and researchers. This book is warmly recommended.

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Handbook of Liquid Crystal Research. Edited by Peter J. Collings (Swarthmore College) and Jay S. Patel (Pennsylvania State University). Oxford University Press: Oxford and New York. 1997. xv + 600 pp. $195.00. ISBN 0-19-508442-X.

This book is a timely and extremely useful resource describing the science and technology of liquid crystal (LC) materials. The book's 15 chapters are divided equally into those with scientific and technological focus in addition to a brief introductory chapter. As the editors point out in the preface, the field of liquid crystals has grown so much in the last 25 years that it is no longer possible to be aware of the entire field, and so the focus has been on recent work in limited areas. The editors have done an excellent job of identifying topics of current relevance and in getting the participation of many of the most active researchers in the LC field. While similar in title to the *Handbook of Liquid Crystals* published some years ago, this is not an update to that book, but something equally useful and quite distinct. In fact, an up-to-date reference work on liquid crystals has been lacking for some years now, and this volume will help to fill that void.

Topics range from the synthesis of new liquid crystals to the physics and engineering of LC displays. Both the materials and device design of these displays are described over several chapters. While the unstated focus is on liquid crystals for display, optical switching, and nonlinear optics applications, other chapters cover to a lesser extent nondisplay LC materials including polymer liquid crystals and lyotropic surfactants. Those areas needed to understand LC switching are very well covered and include the electric field effects of liquid crystals, LC interfaces, and thin films as well as phase structure. Also discussed are polymer-dispersed LC displays and the engineering of both active and passive matrix displays. Twisted nematics and surface-stabilized ferroelectric LC devices are also covered along with the background information needed to understand them.

A good portion of the book describes contemporary developments in the fundamental study of liquid crystals. The recently discovered defect phases and new ferroelectric low molar mass and polymer LCs are also described in great detail. There is a significant effort made in all but the display physics chapters to broadly cover many of these classes of LC materials. The display physics chapters concentrate instead on the behavior of low molar mass LCs of interest primarily to the display community as well as aspects of electronic design. Since the book is intended to be useful to members of both the LC chemistry and physics communities, one of the major achievements of the editors is the very readable nature of all chapters, regardless of discipline. The individual chapters are richly illustrated with many figures and drawings; however, no color plates were used for any of the LC textures. Many of these figures will be superb for classroom use.

Despite the overall excellence of the volume there are some aspects

that detract from the work. A review of all the references indicate that many of the chapters must have been largely prepared in or around 1993. While the delay in going to print does not diminish the overall quality of the work, it means that some new advances are undoubtedly missing from the chapters. The chapters dealing with the synthesis and chemistry of liquid crystals adequately cover the major classes of liquid crystals, but those dealing with technology focus only on displays and optics and largely ignore the important developments in the field of thermotropic and lyotropic polymers, for example. These new polymers are becoming increasingly important for the microelectronics industry due to their precision molding capabilities (thermotropic), and of course, the high modulus properties of lyotropic polymers are well-known. The area of surfactants which is driving the recent fascinating work on templated growth of silicates and metal nanostructures is not covered here. The broad scope of the book has meant that the editors have had to necessarily focus their topical coverage, but the lack of much discussion of these newer aspects may limit the appeal of this book for these developing communities.

The individual chapters largely focus on work covering a 10−15 year period. While each chapter is quite detailed, it is written in an easy to read way. As an illustration, the chapter on chiral and achiral liquid crystals covers LC structure and function thoroughly without any historical review. Newly synthesized LC molecules are well described, but older compounds are not. A stated goal of the editors was not to be overly comprehensive; thus, to study the earlier work on liquid crystals, even that 20 years old, requires the reader to go to previous references. As another example, the chapter on theory deals largely with the scientifically popular blue phase, computer simulation of liquid crystals, and other developments of recent interest but does not provide much of the more basic theoretical aspects of liquid crystals. To read about Maier-Saupe theory, for example, other sources such as the books by de Gennes and Prost or de Jeu will be required. One last point to note is the tendency of some of the authors to overly focus on their own work. Nevertheless, the editors maintain a generally balanced volume.

As a truly useful reference work for the more advanced reader, both the cited literature and the index must be well executed. In this book the editors have been careful to require detailed citations and even provide a journals abbreviation list. The index appears to be equally thorough although it is surprisingly brief for a work of 600 pages.

In summary, anyone with an interest in the field of LC research and many of the developments in it over the last 10−15 years will want a copy of this excellent volume. However, it should not be the reader's only reference on liquid crystals, nor the reader's first book on liquid crystals, since the handbook is obviously intended for the more advanced reader.

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Advances in Supramolecular Chemistry, Vol. 4. Edited by George W. Gokel (Washington University School of Medicine). JAI Press: Greenwich. 1997. xi + 338 pp. $109.50. ISBN 1-55938-794-7.

This book is the fourth in an excellent series presenting review articles on recent research in supramolecular chemistry. The volume is comprised of 7 diverse chapters by 24 contributing authors, with each chapter dedicated to a specific area in the field. While such a volume cannot cover all important subject areas in supramolecular chemistry, the editor has succeeded in assembling a series of contributions that reveal the breadth of the field. Each chapter contains references that are carefully selected, relevant, and recent (numerous references are from 1996). For the most part, this book is clear and concise, and will appeal to a wide range of scientists interested in supramolecular chemistry.

In the first chapter entitled Supramolecular Photoionic Devices, de Silva et al. provide a comprehensive account of molecular systems that operate via the interconversion of ionic and photonic signals. A well-crafted introduction sets the stage for a logical exploration of the field. Each of the subsequent subsections examines numerous supramolecular systems that are comprised of lumophores and receptors (typically ion receptors). Emphasis is placed on systems with switchable luminescent output and the potential emulation of electronic devices by these systems.

The second chapter by Inoue and Wada focuses on the thermodynamics of molecular recognition in both synthetic and biological systems. A theoretical analysis, based on the compensatory enthalpy−entropy relationship, is shown to apply to a variety of host−guest systems. The authors' theory allows for a quantitative determination of the degree of conformational changes and the extent of desolvation upon molecular association.

The third and seventh chapters deal with synthetic anion receptors. The third chapter by Sessler et al. primarily focuses on research from their laboratory on anion binding by sapphyrins. This interesting chapter demonstrates the range and power that protonated sapphyrins possess as anion binding agents, and offers very extensive references of anion binding in general. The seventh chapter by Holman et al. provides more of a general review of anion receptors and the challenges faced in their design. The chapter emphasizes host systems that exhibit a high degree of affinity or selectivity in anion binding, and provides a fascinating account of the variety of systems that have been investigated recently.

The fourth chapter by Anzai and Osa describes protein-based multilayered systems that are assembled using avidin−biotin complexation. The authors provide an account of their research that illustrates the successful use of their multilayered assemblies as high-performance biosensors. The next chapter by Kobuke discusses progress that has been made in the design of artificial ion channels. Although one of the figures in this chapter is upside-down, the chapter effectively covers a variety of systems that successfully mimic the function of natural ion channels. In addition, Kobuke provides an excellent account of the various methodologies in this area.

The sixth chapter by Odashima et al., which is the longest chapter in the book, details the development of sensing membranes that are based on biomimetic and biological receptors. These authors, in primarily discussing their own research, illustrate the ability to prepare a multitude of sensing membranes by incorporation of synthetic or natural receptors in the membrane material. The chapter demonstrates how functions such as transmembrane signaling, coupled active transport, and ternary complex formation are used for the sensing of target molecules in an amplified manner.

In summary, the fourth volume of this series continues to offer well-written, interesting, and up-to-date accounts of important topics in supramolecular chemistry. It is highly recommended for research libraries and personal collections.

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