Additions and Corrections

Carbohydrates: United Atom AMBER* Parameterization of Pyranoses and Simulations Yielding Anomeric Free Energies [*J. Am. Chem. Soc.* **1996**, *118*, 2078−2086]. HANOCH SENDEROWITZ, CAROL PARISH, AND W. CLARK STILL*

Page 2082: Some of the data given in Table 4 are incorrect. The correct data for Table 4 follow:

Table 4. Relative Energies (kcal/mol) of 2-Methoxytetrahydropyran (**2**) Conformations Calculated by *ab initio* Methods and the New Force Field[a]

	HF/6-311++G**//HF/6-31G* [b]	AMBER*
axial		
trans	(3.68)[c]	(4.95)[c]
gauche$^-$	(10.11)[c]	8.73
gauche$^+$	0.00	0.00
equatorial		
trans	(5.48)[c]	(6.07)[c]
gauche$^-$	0.94	0.95
gauche$^+$	3.93	4.11

[a] See footnotes of Table 3. [b] From ref 24. [c] Not an energy minimum, O5−C1−O1−C constrained to geometry indicated.

JA9654185

S0002-7863(96)05418-2

The Cyclohexadienyl Radical in the Thermal Syn−Anti Isomerization of Two Crossed Pentaenes of the Type of Bis-Homofulvalene [*J. Am. Chem. Soc.* **1996**, *118*, 6660−6665]. W. VON E. DOERING,* LUDMILA BIRLADEANU, KESHAB SARMA, AND LIMING SHAO

Page 6660: The last author's name is Liming Shao, not Li-Sming Shao as appeared in the journal.

JA965419X

S0002-7863(96)05419-4

Insight into the Fluid-Phase Miscibility of Ester and Ether Phospholipids through Analysis of Nearest-Neighbor Recognition [*J. Am. Chem. Soc.* **1996**, *118*, 7069−7074]. TAKEHISA DEWA AND STEVEN L. REGEN*

The percentage of cholesterol that is referred to in this paper, and also in previous papers in this series, is expressed as the percentage of cholesterol present with respect to the total number of moles of phospholipid monomers.[1−4] In terms of true mole percentages, values given as 10, 20, 30, and 40 mol % are, in fact, 9, 17, 23, and 29 mol %, respectively.

(1) Dewa, T.; Vigmond, S. J.; Regen, S. L. *J. Am. Chem. Soc.* **1996**, *118*, 3435−3440.
(2) Vigmond, S. J.; Dewa, T.; Regen, S. L. *J. Am. Chem. Soc.* **1995**, *117*, 7838−7839.
(3) Davidson, S. M. K.; Liu, Y.; Regen, S. L. *J. Am. Chem. Soc.* **1993**, *115*, 10104−10110.
(4) Krisovitch, S. M.; Regen, S. L. *J. Am. Chem. Soc.* **1993**, *115*, 1198−1199.

JA965420W

S0002-7863(96)05420-0

*Book Reviews**

Steroid Receptors and Antihormones. Edited by David Henderson, Daniel Philibert, Arun K. Roy, and Georges Teutsch. Annals of the New York Academy of Sciences. New York Academy of Sciences: New York. 1995. 416 pp. ISBN 0-89766-938-X.

The proceedings of the New York Academy of Sciences conference on Steroid Receptors and Antihormones contain an up-to-date review of the field by noted experts representing the leading laboratories of the world. Professor Elwood Jensen served as the Honorary Chairman of this conference. Dr. Jensen and his associates initially observed, in the late 1950s, the concept that steroid hormones alter cell function through hormone-specific receptor proteins. Since then the field of steroid hormone action has undergone a remarkable transformation with the ultimate documentation of steroid receptors as ligand-activated transcription factors. Molecular cloning and structural studies have revealed that steroid hormone receptors belong to a superfamily of structurally similar transcription factors that include vitamin D receptor, thyroid hormone receptors, retinoic acid receptors, and a number of "orphan receptors" whose activating ligands are yet to be identified. Such an enormous conceptual advancement has opened up many possibilities for potential applications of steroid analogs for the benefit of human health.

JA965542O

S0002-7863(96)05542-4

Compendium of Organic Synthetic Methods, Volume 8. By Michael B. Smith (University of Connecticut—Storrs). Wiley-Interscience: NewYork. 1995. xxii + 631 pp. $64.95. ISBN 0-471-57319-1.

This volume offers a highly focused and selective look at several thousand functional group transformations. This desktop resource provides quick access to the recipes of the newest, most useful reactions and transformations. It also affords an opportunity to browse the vast body of recent literature for new reactions and transformations that may be of interest. Volume 8 features 1200 more entries than Volume 7. It covers functional group transformations and carbon−carbon bond forming reactions appearing in the literature from 1990 to 1992. It presents approximately 1400 examples of published reactions for the preparation of monofunctional compounds and approximately 1640 examples of reactions that prepare difunctional compounds with various functional groups. Chemical transformations are classified first by the reacting functional group of the starting material and then by the functional group formed. The transformation, major reagents that effect the transformation, yield percentage, and stereochemistry are all clearly shown. There are also indices for both monofunctional and difunctional compounds.

JA965634D

S0002-7863(96)05634-X

Ullmann's Encyclopedia of Industrial Chemistry, Fifth, Completely Revised Edition, Volume A24: Polysaccharides: Silicon Compounds, Inorganic to Stains, Microscopic. Edited by Barbara Elvers, Steven Hawkins, William E. Russey, and Gail Schulz. VCH: NewYork. 1994. xv + 580 pp. $325.00. ISBN 3-527-20124-6.

The fifth, completely revised edition of *Ullmann's Encyclopedia of Industrial Chemistry* is two encyclopedias in one. Divided into 36 volumes, the encyclopedia consists of an Alphabetically Ordered Series of 28 volumes containing all articles on industrial chemicals, product groups, and production processes covering all aspects of the chemical and allied industries, together with the Basic Knowledge Series of 8 B volumes describing principles of chemical engineering, new and proven analytical methods, and the essentials of environmental protection technology. In addition an updated Cumulative Index to both the A and B volumes is distributed annually. Printed in an easy-to-read double column format, this encyclopedia is designed to provide the reader with a clear sense of orientation and rapid access to a wealth of information. Each article features consistent organization, an introductory table of contents, an extensive set of headings, and well-designed illustrations, formulas, and tables.

JA945073V

S0002-7863(94)05073-0

Kirk-Othmer Encyclopedia of Chemical Technology, Volume 14: Imaging Technology to Lanthanides.. Edited by Jacqueline I. Kroschwitz and Mary Howe-Grant. Wiley: New York. 1995. xxviii + 1116 pp. $295.00. ISBN 0-471-52683-5.

This is the 14th volume of a 25-volume encyclopedia set, 4 volumes being published each year. The Fourth Edition is similar in format to the earlier editions with updates to the entries as necessary and the addition of several new subjects. This volume contains 39 entries ranging from Imaging Technology to Lanthanides. This volume does not contain an index; however, paperback indexes are published every four volumes, and the supplement and index volumes are scheduled for publication in 1998.

JA955227M

S0002-7863(95)05227-9

Vibrational Spectra and Structure: Vol. 21: Optical Spectra and Lattice Dynamics of Molecular Crystals. Edited by G. N. Zhizhin and E. I. Mukhtarov (Russian Academy of Sciences). Elsevier: Amsterdam. 1995. xvii + 447 pp. $281.25. ISBN 0-444-82295-X.

The current volume is a single-topic volume on the optical spectra and lattice dynamics of molecular crystals. The book is divided into two parts. Part I covers both the theoretical and experimental investigations of organic crystals. Part II deals with the investigation of the structure, phase transitions, and reorientational motion of molecules in organic crystals. In addition, appendices are given which provide the parameters for the calculation of the lattice dynamics of molecular crystals, procedures for the calculation of frequency eigenvectors of utilizing computers, and the frequencies and eigenvectors of lattice modes for several organic crystals. A large amount of Russian literature is cited, some of which has not previously been available to scientists in the West.

JA955394M

S0002-7863(95)05394-7

The Internet: A Guide for Chemists. Edited by Steven M. Bachrach (Northern Illinois University). ACS: Washington, DC. 1996. xv + 344 pp. $23.95. ISBN 0-8412-3224-5.

The use of the Internet is changing so rapidly that it is virtually impossible to have an up-to-date book on the subject, but this group of authors has done an outstanding job. There is an extensive use of on-line references. As a result, the reader will find information that has been updated since the publication of this book, effectively updating the book.

The first eight chapters of the book deal with the Internet in general. These chapters are highly recommended for nonchemists as well as chemists. The topics covered in these chapters include a brief history of the Internet, the use of electronic mail, gopher, the World Wide Web, Internet accessible databases, and electronic conferencing. The e-mail chapters include information on using electronic mailing lists.

The final five chapters address issues more specific to use of the Internet for the exchange of chemical information. The topics in these chapters include information about chemistry-related mailing lists, gopher sites of particular interest to chemists, chemistry specific applications of the World Wide Web, and the impact of the Internet on the chemical industry.

*Unsigned book reviews are by the Book Review Editor.

Probably the most noticeable feature of this book is that the authors consistently treat both sides of the information provision issue. They discuss how to access information on the Internet, and they also supply detailed information about becoming an information provider. They give references and specific information about setting up mailing lists, conferences, and servers. They also provide very useful guidelines on setting up the services in such a way as to keep them manageable.

The only possible weakness in the coverage is the assumption that most chemists will be using some form of UNIX e-mail. While this may be a valid assumption for our more computer-oriented colleagues, it is likely that a POP mail client like Eudora is more commonly used by many chemists. Thus, a chapter addressing this type of e-mail usage would have been highly desirable.

Overall, the authors of this book have done an excellent job of covering a rapidly moving target, and it is highly recommended for nonchemists as well as chemists.

Gary D. Anderson, *Marshall University*

JA965578G

S0002-7863(96)05578-3

Science of Fullerenes and Carbon Nanotubes. By M. S. Dresselhaus (MIT), G. Dresselhaus (MIT), and P. C. Eklund (University of Kentucky). Academic Press: San Diego. 1996, xviii + 965 pp. ISBN 0-12-221820-5.

Here is a thoroughly edited and proofread volume which is a delight to read and which should prove to be an enduring source of reliable information for many years. The book contains an extensive presentation of the fullerene story, from ancient references to the truncated icosahedron, through the post-gram-scale explosion of fundamental research, to the most recent speculation on possible applications.

The authors begin with a historical discussion of carbon clusters, and thereafter spend an entire chapter on the various forms of carbon and carbonaceous materials. The next two chapters present the structure of C_{60} and some higher fullerenes, and symmetry considerations. Syntheses of fullerenes via laser ablation of carbon electrodes, combustion, resistive heating of carbon rods, and plasma discharge between electrodes are discussed in Chapter 5, along with the chromatography and extraction techniques necessary for the production of clean samples.

The issue of fullerene growth models is covered in the next chapter. A good discussion of the special stability of the 60- and 70-carbon molecules is given. Crystal structure information on C_{60} and what is known in this area about the higher fullerenes come next. Because the electrical properties of doped fullerenes have generated so much attention in the research community, the authors have written a 50-page 171-reference chapter on endohedrally, exohedrally, and substitutionally doped fullerenes.

Work on the various methods of growing ordered arrays of fullerenes is presented in Chapter 9. Cyclic voltammetry and its relationship to the alkenoid organic chemical reactivity of C_{60} are then discussed. Chapters on IR and Raman spectroscopy, molecular orbital theory and electron energy levels, UV−VIS−NIR behavior, and thermal and electrical properties are followed by an informative chapter on superconductivity. Other subjects covered include NMR, ESR, surface techniques, magnetic properties, and tubes. The chapter on tubules is more than 100 pages long.

Perhaps the chapter that most readers will turn to first is the last: the applications chapter. From the viewpoint of chemists, materials scientists, business people, and futurists, the possibilities are without limit. Both devices which have been made and possible uses which have yet to be demonstrated are discussed. The subject matter includes batteries, microchip fabrication, self-assembled monolayers, quantum wires, catalysts, lubricants, etc.

This volume contains 20 chapters, most of which have in excess of 100 references. The 900+ pages of text and 46-page index make for a book which is indispensable. It is a publication of use both to groups on the cutting edge of fullerene/tube science and applications and to novices wishing to obtain a basic knowledge of buckminsterfullerene.

Robert V. Honeychuck, *George Mason University*

JA965593L

S0002-7863(96)05593-X

Neural Networks for Chemical Engineers. Edited by A. B. Bulsari (Lappeenranta University of Technology, Finland). Elsevier: Amsterdam. 1995. ix + 680 pp. $285.25. ISBN 0-444-820970-3.

With the plethora of books on neural networks one can find in a bookstore, this is one book that most engineers, in addition to chemical engineers, may find worth keeping handy as a personal reference in spite of its price tag. The book comprises 2 sections and 27 chapters.

The first section, Chapters 1−6, presents a comprehensive overview of various neural network models. Chapter 1 reviews 7 main types of neural network models, namely, the multilayered perceptron (MLP, detailed in Chapter 3), learning vector quantization network (LVQ), group method of data handling network, Hopfield network, Elman and Jordon network, Kohonen network (detailed in Chapter 2), and adaptive resonance theory (ART) network. Although it is arguable that the 7 are the main representations of all neural networks, e.g., the LVQ net derivable from the Kohonen net, and Elman and Jordon nets from MLP, the introduction quickly leads readers into the realm of neural networks. Additional neural network models, such as the neocognitron, Boltzmann perceptron, ART2, and radial basis function (RBF) network, though not mentioned in Chapter 1, can be found in later chapters throughout the book. Chapter 4 offers an insight into a problem to which most engineers seek answer in using neural networks: What is the maximal number of nodes required in an MLP hidden layer? The fifth chapter is a good summary of neural networks and compares its utility with classical propositional logic—connectionism vs symbolism, the two main camps of artificial intelligence.

In spite of its place in Section 1, Chapter 6, along with Chapters 7−27, presents 22 application case studies of neural networks. The applications include vision (Chapters 6 and 21), nonlinear process control (Chapters 7, 15, 19, and 25), data prediction, rectification, and filtering (Chapters 8, 9, 13, 16, and 24), process dynamics analysis, system identification, and state variable and disturbance estimation (Chapters 10, 14, 19, and 23), fault detection (Chapters 11 and 14), data pattern recognition/classification (Chapter 17), and process modeling (Chapters 18 and 20).

Chapter 12 discusses local modeling as a tool for semiempirical and semimechanistic process modeling. Though a solid chapter, the reviewer fails to find its connection with neural networks—the subject matter of the book. It is worth mentioning that several non-chemical-engineering subjects are discussed in this book, making the book appealing to a general engineering audience. Examples of such subjects include genetic algorithm application to neural networks (Chapter 1), visualization of speech signals using a self-organizing map (Chapter 14), multiresolution (wavelet) representation of neural networks (Chapter 20), implementation of fuzzy rule-based systems through neural networks (Chapter 21), and implementation of multivariate statistics using neural networks (Chapters 26 and 27).

It is also worth noting that the contributors to this book come from all around the world, from the U.S.A., U.K., Finland, South Africa, Japan, Spain, Switzerland, Portugal, Slovenia, Mexico, and Norway. The editor has done an admirable job in integrating the work from around the globe on the subject of neural networks.

Yee-Wei Huang, *Kansas State University*

JA955254C

S0002-7863(95)05254-1

Inclusion Chemistry with Zeolites: Nanoscale Materials by Design: Topics in Inclusion Science, No. 6. Edited by Norman Herron and David R. Corbin (DuPont Co.). Kluwer Academic: Dordrecht, The Netherlands. 1995. xv + 340 pp. $199.00. ISBN 0-7923-3606-2.

Zeolites are crystalline microporous materials that possess relatively large cages interconnected by molecular-sized channels. The zeolites, therefore, play host to a variety of guest molecules. The nature and the type of the occluded molecules and the interaction between the guest and the host molecules determine the properties of such zeolitic materials. The editors of this volume set out to bring together a collection of review papers emphasizing recent developments in various aspects of guest−host interactions or inclusion chemistry with zeolites. They have succeeded admirably in doing so.

The book has 11 chapters each written by active researchers in the field. The first chapter discusses the probing of intrazeolite space by adsorption of probe molecules of varying size and geometry. The second chapter reviews the concept of structure direction in the synthesis

of clathrasils and high-silica molecular sieves. The role played by the size, geometry, and chemical nature of the structure-directing agent on the crystalline structure and the dimensionality of the pore structure is discussed thoroughly. The next two chapters deal with the use of structural techniques such as powder X-ray diffraction and NMR spectroscopy to study the guest−host interactions. The third chapter discusses in detail the studies on desorption of Xe from zeolite rho and the location of adsorbed stilbene in ZSM-5 by X-ray diffraction. The fourth chapter details the use of probe molecules such as xenon and aromatics adsorbed in X and Y zeolites with NMR spectroscopy to determine the guest−host interactions. The fifth chapter reviews the computational tools such as molecular dynamics and Monte Carlo simulations available for modeling the behavior of adsorbed molecules in zeolites. The discussion is illustrated with specific examples of microdynamics of benzene in X and Y zeolites. The next three chapters discuss encapsulation of different molecules in zeolites. The sixth chapter discusses various encapsulation techniques such as metal cluster, template and zeolite synthesis methods, and the characterization methods to determine the location of the metal complex in the zeolite cavity. The next chapter reviews the methods of encapsulating the transition metal ion complexes in zeolite Y. The eighth chapter discusses the role played by the structure-directing agent in the assembly process of zeolites. The reactivities of zeolites with encaged organometallic complexes of Mn^{3+}, Co^{2+}, and Ru^{2+} have been determined using a variety of reactants. The use of zeolites with encaged guest molecules to carry out photochemical reaction has been discussed in the next chapter. It is demonstrated that the cation embedded in the zeolite matrix can be used to control the photophysical and photochemical properties of the guest molecules encapsulated in zeolites. The final two chapters deal with the optical and electronic properties of zeolites encapsulated with metals, semiconductors, polymer particles, and alkali-metal clusters.

Even though most of the reviews are quite up-to-date, there are exceptions. The first chapter, for example, is more like an introduction to the subject matter that sets the stage for the remaining chapters in the book rather than an independent and thorough review of "recent developments". A great majority of the references cited therein are from the 1970s and the 1980s, and a very few are from the 1990s. Overall, however, this is an excellent book. It represents a compilation of reviews in different aspects of zeolite-inclusion chemistry. The various methods of synthesizing entrapped molecules in zeolites, the methods of characterization, and properties of such zeolitic materials are delineated by the experts in the field and compiled in a single source. The book deserves to be on the shelf of research scientists working in the area of zeolite synthesis and characterization. However, the prohibitively expensive purchase price of the book will be a detriment to many who would want to do so.

Dhananjai B. Shah, *Cleveland State University*

JA965582S

S0002-7863(96)05582-5

Mineral Scale Formation and Inhibition. Edited by Zahid Amjad (The B.F. Goodrich Co.). Plenum: New York. 1995. 350 pp. $110.00. ISBN 0-306-45195-6.

This book documents the proceedings of the symposium Mineral Scale Formation and Inhibition, held at the American Chemical Society Annual Meeting, August 21−26, 1994, in Washington, DC. The symposium was sponsored by the Division of Colloid and Surface Chemistry. This book provides an introduction to the type and severity of scaling problems in both industrial and biological systems. A total of 30 papers were presented. This volume also contains papers that were not presented but were in the symposium program.

JA965541W

S0002-7863(96)05541-2

Electronic Properties of Solids Using Cluster Methods: Fundamental Materials Research. Edited by T. A. Kaplan and S. D. Mahanti (Michigan State University). Plenum: New York. 1995. 200 pp. $89.50. ISBN 0-306-45010-0.

This volume is a part of a series of books, which will appear at the rate of about one per year, addressing fundamental problems in materials science. The topics will cover a broad range of topics from small clusters of atoms to engineering materials. The topics will involve chemistry, physics, and engineering, with length scales ranging from angstroms up to millimeters. The emphasis will be on basic science rather than on applications. Each book will focus on a single area of current interest and will bring together experts to give an up-to-date discussion of their work and the work of others. Each article contains enough references that the interested reader can access the relevant literature. This volume records invited lectures given at the workshop on Electronic Properties of Solids Using Cluster Methods, held at Michigan State University, July 17−19, 1994.

JA965547L

S0002-7863(96)05547-3

Encyclopedia of Common Natural Ingredients Used in Food, Drugs, and Cosmetics, Second Edition. By Albert Y. Leung (Consultant, Natural Products) and Steven Foster (Consultant, Medicinal and Aromatic Plants). Wiley: New York. 1996. 650 pp. $150.00. ISBN 0-471-50826-8.

This expanded and revised edition is the only single-source reference devoted to the approximately 500 naturally derived ingredients currently included in a wide range of cosmetics, food items, and drugs. This volume is twice the size of the first edition and updates all the original entries of the first edition. A new category, Health Foods/Herbal Teas, is included. This book also contains an alphabetical presentation of the entries according to common names, and cross-referenced to scientific names in the index. This book includes a glossary of the most commonly encountered terms used in the botanical industry, an in-depth coverage of each ingredient, including general description, chemical composition, uses and commercial preparations, and synonyms, as well as regulatory status and references, and a general reference list. The inclusion of a new classification on Chinese medicinal herbs offers information that appears for the first time in English. This classification presents both classical and modern Chinese medicine.

JA9655496

S0002-7863(96)05549-7

Kirk-Othmer Encyclopedia of Chemical Technology, Volume 17: Nickel and Nickel Alloys to Paint. Edited by Jacqueline I. Kroschwitz and Mary Howe-Grant. Wiley: New York. 1995. xxviii + 1082 pp. $295.00. ISBN 0-471-52686-X.

This is the 17th volume of a 25-volume encyclopedia set, 4 volumes being published each year. The Fourth Edition is similar in format to the earlier editions with updates to the entries as necessary and the addition of several new subjects. This volume contains 33 entries ranging from Nickel and Nickel Alloys to Paint. This volume does not contain an index; however, paperback indexes are published every four volumes, and the supplement and index volumes are scheduled for publication in 1998.

JA9656107

S0002-7863(96)05610-7

Biology of α_2-Macroglobulin, Its Receptor, and Related Proteins. Edited by Wolfgang Borth (Mount Sinai Medical Center), Richard D. Feinman (State University of New York Health Sciences Center in Brooklyn), Steven L. Gonias (University of Virginia in Charlottesville), James P. Quigley (State University of New York at Stony Brook), and Dudley L. Strickland (American Red Cross). Annals of the New York Academy of Sciences. New York Academy of Sciences: New York. 1994. 521 pp. $140.00. ISBN 0-89766-886-3.

This book reviews the biological importance of α_2-macroglobulin (α_2M) and the α_2M receptor/low-density lipoprotein receptor related protein (LRP). The mechanism of the α_2M proteinase reaction and the function of α_2M as a carrier of growth factors, cytokines, and toxins are discussed, with emphasis on the structure and function of LRP and its relation to cancer and atherogenesis.

JA965623K

S0002-7863(96)05623-5