Book Reviews *

Neural Networks for Chemists. By Jure Zupan (National Institute of Chemistry, Slovenia) and Johann Gasteiger (Technische Universitat Munchen) VCH: New York. 1993. xx + 306 pp. £28.00. ISBN 1-56081-793-3.

This book affords a careful introduction to the use of neural networks in processing data from chemical experiments. The late 1980s and early 1990s witnessed an explosion in publications on neural networks. As the authors point out, by 1992 there were more than 500 references covering applications of neural networks related to chemistry alone. This situation can be daunting to the beginner. By focusing on a carefully selected set of networks and applications, the authors have provided a useful reference for students and for professional chemists wishing to learn about the use of neural networks in data analysis.

The background section covers the essential basics: linear discrimiration, the introduction of nonlinear elements into the discrimination paradigm, and several types of networks. The treatment of networks includes chapters on the Hopfield network, the adaptive bidirectional associative network, the Kohonen network, and counter-propagation and back-propagation of errors. The book provides explicit presentations of the algorithms for each of the networks considered.

The authors have covered a wide range of applications; the chapter titles include The Clustering of Multicomponent Analytical Data for Olive Oils, The Reactivity of Chemical Bonds, HPLC Optimization of Wine Analysis, Quantitative Structure—Activity Relationships, The Electrophilic Aromatic Substitution Reaction, Modeling and Optimizing a Recipe for Paint Coating, Fault Detection and Process Control, The Secondary Structure of Proteins, Infrared Spectrum—Structure Correlation, and Nonlinear Projection of Molecular Electrostatic Potentials. Although there is no historical section, the references at the end of the introductory chapters point out the basic references necessary for the reader to gain an appreciation for the history of the subject. Hecht-Nielson (Hecht-Nielson, R. Neurocomputing; Addison Wesley Publishing Co.: Reading, MA, 1990) gives a lively, if somewhat partisan, account of developments in the field until 1990. The references to papers on applications are current to 1992.

One of the most useful aspects of the book is a walk-through of the whole process for each application: experimental design, choice and organization of the data, selection of network architecture and parameters, and analysis of the results. It should not be forgotten that any artificial neural net is only a tool of the neural net the researcher was provided at birth. Matching the natural structure of the data to the architecture of the network is essential to successful applications of artificial neural networks. The authors have made comparisons between competing neural network approaches in each application and have provided a balanced assessment of the strengths and weakness of each approach. The authors have also indicated where further research is necessary to improve the performance of artificial neural networks. The careful approach embodied in this book is an antidote to the hype which has attended neural networks in recent years.

Albert F. Lawrence, Syracuse University

JA934742M

Principles of Bioinorganic Chemistry. By Stephen J. Lippard (Massachusetts Institute of Technology) and Jeremy M. Berg (Johns Hopkins University School of Medicine). University Science Books: Mill Valley, CA. 1994. xvii + 411 pp. \$30.00. ISBN 0-935702-73-3.

This handsome text contains 13 chapters on seminal topics in bioinorganic chemistry. The authors begin with an overview of metals in nature, why metals were selected for particular functions, and how metals are used and regulated in biological systems. The book follows with characteristics of biological molecules, physical methods used to characterize such molecules, and specific examples from enzyme and protein chemistry. An especially detailed chapter on Atom and Group Transfer contains more than 56 bibliographic references, 52 of which

are dated from 1980 or later. While other bioinorganic texts published recently are either at the extremes of complexity, Lippard and Berg's treatment of bioinorganic chemistry is well-balanced and at an appropriate level for undergraduates as well as graduate students in chemistry, biology, or medicine.

Besides its technical accuracy and near error-free text, one of the strongest features of this book is in the manner in which graphics and schemes are presented. The illustrations in the text not only convey the intended messages, but they improve understanding of the basic concepts portrayed in the graphics. For example, the mechanistic schemes provided for the reaction cycle of cytochrome P-450_{camphor} are visually stimulating and are much easier to comprehend than the myriad of such cycles present in the literature. The study problems at the end of each chapter are creative and thought-provoking and provide ample opportunities for both qualitative and quantitative practice. Of some 280 bibliographic references cited in the text, 101 are up-to-date (from the 1990s), 133 are dated from the 1980s, and 46 are important references from 1970 or earlier. This reflects the still relatively young age of the field of bioinorganic chemistry.

This text is highly recommended for those interested in understanding the field from a chemical, biological, or medical approach. It can be used by students, professors, and physicians and even at the advanced placement level for high school chemistry students. It is certainly a comprehensive and important addition to the small number of bioinorganic texts available today.

Maureen Kendrick Murphy, Russellville High School, AL

JA945138U

Conformational Behavior of Six-Membered Rings. Analysis, Dynamics and Stereoelectronic Effects. Edited by Eusebio Juaristi (Politécnica Nacional Mexico). VCH: New York, Weinheim, and Cambridge. 1995. xiii + 306 pp. \$100.00. ISBN 1-56081-683-X.

Eliel (University of North Carolina) provides a concise (24 page, 138 ref) review hitting the highlights of conformational analysis, over half of which concerns six-membered ring compounds. Bushweller (University of Vermont) gives a 34-page (124 ref) discussion of A values for over 100 substituents, their thermodynamic parameters where studied, and activation parameters for ring reversal in monosubstituted cyclohexanes. Cremer and Szabo (Univ. Göteborg) cover ab initio calculations in 77 pages (136 refs), thoroughly discussing the "conformational globe" energy surface for cyclohexane (although unfortunately not clearly defining the angles involved with diagrams), as well as discussing substituted cyclohexanes, unsaturated ones, cyclohexyne, and cyclohexane radical cation. Osawa (Toyohashi Univ. Tech.) and Varnali (Bogazici Univ.) discuss molecular mechanics calculations (22 pages, 72 refs) including fused-ring systems, bicyclohexyl derivatives, 1,4-dihydrobenzene derivatives, and their polymers and 4 pages on carbohydrates. Franck (Hunter Coll./CUNY) gives a thoughtful 42page (96 ref, a few from 1994) discussion on stereoelectronic effects, including facial attack preferences at substituted cyclohexanones, cyclohexyl radicals, and unsaturated systems and 14 pages on both the thermodynamics and kinetic consequences of anomeric effects. Kleinpeter (Univ. Potsdam) provides extensive coverage of the conformational analysis compounds having ring CH₂ groups replaced by S, S⁺R, SO, SNR, Se, and their combinations in 43 pages (306 refs, through 8/93). Bentrude (University of Utah) comprehensively discusses steric and stereoelectronic effects in 1,3,2-dioxaphosphorinanes, including 6 pages on pentacovalent phosphorus compounds (49 pages, 223 refs through 10/93). Explicit coverage of the largest classes of sixmembered ring heterocycles, those containing oxygen and nitrogen,

^{*}Unsigned book reviews are by the Book Review Editor.

will have to be sought elsewhere, but coverage of the topics included seems both reasonably up-to-date and usefully thorough.

Stephen F. Nelsen, University of Wisconsin, Madison

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Magnetic Resonance in Food Science. Edited by P. S. Belton (AFRC Institute for Food Research, Norwich, U.K.), I. Delgadillo and A. M. Gil (University of Aveiro, Portugal), and G. A. Webb (University of Surrey, Guildford, U.K.). Royal Society of Chemistry: Cambridge, U.K. 1995. ix + 292 pp. £55.00. ISBN 0-85404-725-5.

This book is the proceedings of the Second International Conference on Applications of Magnetic Resonance in Food Science held in September of 1994. It covers the application of both EPR and NMR methodologies to food science. The book is organized into four parts: Applications of magnetic resonance, Analysis and authentication, Magnetic resonance and nutrition, and Magnetic Resonance in the study of biopolymers and complex systems. Seventy-five poster presentations were also made at the conference. Unfortunately neither their abstracts nor titles appear in the book. The conference was oriented toward illustrating how magnetic resonance can be useful to food scientists. Accordingly, the book is something of a mixture of articles on basic principles of magnetic resonance and on applications to food science. Two groups of individuals will be interested in the book. Magnetic resonance specialists will be interested in how their techniques have been applied to food science. They will find that a remarkable range of approaches have been used including high-resolution studies, methods relying on relaxation, imaging, and dynamic analysis. Specialists in food science who seek to keep current on how new technologies are being brought to bear on their field have an obvious interest in the book. Unless they already have a good grasp on magnetic resonance techniques, they will find it difficult to understand the basis of the experiments which are described. However, they will get a good overview of the kinds of things that have been learned using magnetic resonance approaches. The book is a useful addition to a research library collection. It is effective in making the case that magnetic resonance is an important technique in food science and illustrates a wide range of applications.

Edwin H. Abbott, Montana State University

JA955253K

Advances in Strain on Organic Chemistry. Volume 4. Edited by Brian Halton (Victoria University of Wellington). JAI Press: Greenwich, CT. xi + 350 pp. \$97.50. ISBN 1-55938-832-3.

This monograph is collection of five chapters written by noted experts on topics of current interest to chemists whose interest is strained organic molecules. The topics and authors include Matrix-Isolation of Strained Three-Membered Ring Systems (Wolfram Sander and Andreas Kirshfield, pp 1–80), Synthetic Utility of Cyclobutenones (Harold W. Moore and Benjamamin R. Yerxa, pp 81–162), Electrophilic Additions to Bicyclo[1.1.0]Butanes (Manfred Christl, pp 163–224), From Spiropentanes to Linear and Angular Oligo- and Polytriangulanes (Armin de Meijere and Sergei Kozhushkov, pp 225–282) and [n]Staffanes (Piotr Kaszynski and Josef Michl, pp 283–331). The diversity of topics and depth of coverage successfully convey the current level of vigorous activity in the area. An author/subject index is included.

The first chapter on matrix isolation (chapters, unfortunately, are not numbered) discusses examples of highly reactive three-membered rings classified by the elements contained in the structure. Sections on strained rings, often in locally challenging environments, contain the following elements: carbon, silicon, nitrogen, oxygen, sulfur, and two or more different heteroatoms. The chapter contains numerous references to some of the esoteric arts learned from experience such as matrix distillation and different product distribution as a function of the matrix or glass (Ar, Xe, EPA) that is used in the technique. The authors provide a critical and informative description of the current state of matrix isolation techniques. In the following chapter the synthetic versatility of cyclobutenones and derivatives from squaric acid is described as synthons for a large variety of aromatic products, often phenolic. Major advantages of the method are that bimolecular

reactions of the substituted ketenes, generated from cyclobutenones, are conducted at moderate temperature, typically < 140 °C, highly regiospecific, and in good yield. Mechanisms of these multistep transformations are suggested.

In the third chapter, mechanisms for cationic rearrangements derived from the bicyclobutane ring system are given a relatively fresh perspective. The role of substituents, geometry of the intermediate, and computational predictions are brought to bear on the matter of equilibrating classical cyclopropylcarbinyl cations and the bicyclobutonium ions. In the following chapter, a relatively new term, polytriangulanes, is coined to describe the family of hydrocarbons that consist exclusively of spiro-attached three-membered rings. Coverage of topic is comprehensive and includes synthetic strategies, spectral data, thermochemical properties, and chemical behavior. Some of the conceptual difficulties intrinsic to numerical estimates of strain (pp 257–262) are elegantly described for the progression from cyclopropane, spiropentane, and to higher triangulanes.

The topic of the concluding chapter on [n]staffanes, oligomeric hydrocarbons containing n bicyclo[1.1.1]pentane cages connected at the bridgehead positions, is also a new term in the chemical lexicon. Methods of synthesis of these highly strained hydrocarbons, their remarkable thermal stability, and other physicochemical properties of these rodlike substances as well as their tendency to form supramolecular assemblies are described.

The collection of reviews gathered by the editor might be described as strained molecules from the matrix, to melting points, and to monolayers. It records well the range of advances. Some of the chapters contain an excessive number of typos although most are minor and do not significantly impede the flow of the ideas. A larger concern is the incorrect figures 267–269 (pp 137) and the absence of figures for structures 53a and 53b (pp 173). A 40% academic/professional discount for this and previous volumes is available from the publisher.

Robert T. Conlin, University of North Texas

JA9552095

Dictionary of Cytokines. By Horst Ibegaufts (University of Munich, Germany). VCH: New York. 1994. xxi + 778 pp. \$110.00. ISBN 3-527-30042-2.

The book entitled Dictionary of Cytokines written by Dr. Horst Ibelgaufts of Munich, Germany, gives a broad and an appreciable detailed definition of cytokines and other factors as well as agents which influence the biologic and clinical functions of cytokines. According to the author, this dictionary is his attempt to map through the jungles, morasses, and deserts of cytokine-land. To that extent, I think the authors did a very great job for the reasons stated below.

In addition to extensively reading the book, I also loaned the book to a couple of my colleagues and to three of my graduate students, whose research is on cytokines. Each of the students had the book for at least one and half weeks, during which time they made extensive references to it. Generally, all the students as well as the faculty members who read the book concluded that the book has a very strong attribute in that it provides a substantiative knowledge about all the cytokines known to date. I rated it very good to excellent. The author did a wonderful job in describing the biochemical nature (basic chemical and biological characteristics), the sources, the target cells, and the biological as well as clinical importance of each cytokine. Given that Interleukin-15 (IL-15) has just recently been described, it was even more impressive to note that the author had included information on this cytokines in the addendum. With regard to the literature citations, overall, I felt that they were within current status in that, in some instances, the author provided citations up to 1994 and some cases up to 1992/93. I consider this to be very reasonable and acceptable. In addition to cytokines, the author also provided information about other agents which either influence the biologic effects of cytokines or which have been used in conjunction with cytokines in a number of studies. It is well written and edited. Therefore, the book will be very good for established scientists in the field of cytokines. Furthermore, it would be very suitable for graduate students and medical students as well physicians in training and in practice, who can use it as a desk top reference book. Considering the rate at which the cytokine literature has been growing in the last decade, a dictionary of cytokines was long overdue. The book by Ibelgaufts fulfills its objectives and provides