Additions and Corrections

Pericyclic Arrays in the Solid State. Azooxide and Azodioxide Donor−Acceptor Complexes with Tetracyanoethylene [*J. Am. Chem. Soc.* **1995**, *117*, 6617−6618]. SILAS C. BLACKSTOCK,* KATHY POEHLING, AND MELINDA L. GREER

The reported formation constants (K_f) for complexation of DBO-oxide and DBO-dioxide with tetracyanoethylene (TCNE) are in error. K_f for DBO-oxide/TCNE should be 0.78 M^{-1} and for DBO-dioxide/TCNE should be 2.34 M^{-1}.

JA9654591

S0002-7963(96)05459-5

Book Reviews *

Understanding Chemical Reactivity, Volume 16. The Reaction Path in Chemistry: Current Approaches and Perspectives. Edited by Dietmar Heidrich (Universität Leipzig). Kluwer Academic: Dordrecht, The Netherlands. 1995. x + 297 pp. $145.00. ISBN 0-7923-3589-9.

The notion of a reaction path (RP) is shared by most chemists and introduced in qualitative terms already at the first-year undergraduate level. This multi-author volume provides an up-to-date description of the RP concept as it is used in electronic structure theory and molecular dynamics.

The first part of the book deals in four chapters with the definition of an RP as the line connecting the transition state with reactant(s) and product(s). The discussion here goes from a loose definition of reaction paths (X. Chapuisat) over an introduction to the minimum energy path (MEP) (A. Tachibana and T. Iwsai) and its invariance properties (W. Quapp).

The first chapter in this section (P. G. Mezey) provides a more abstract discussion of the reaction path concept. The discussion in the first section is very informative for the novice as well as the specialist. The mathematical and abstract discussions are illustrated with many concrete examples that covers the different types of RP's one might encounter. Essentially all aspects of the reaction path concept are covered, and there is a minimum of overlap from chapter to chapter.

The second part of the book covers various methods used in generating potential energy surfaces and locating RP's. Helgaker, Ruud, and Taylor afford a comprehensive discussion of the powerful second-order methods used to locate stationary points on the potential energy surfaces and trace minimum energy paths. Quapp, Imig, and Heidrich deal with the topology of reaction paths and the various ways in which they can be obtained.

The last two chapters in this section focus on the actual calculation of potential energy surfaces by quantum mechanical methods. Seifert and Krfger manage to give an almost comprehensive coverage of the promising density function method whereas A. J. Soboolewski and W. Domcke cover the establishment of potential energy surfaces by ab initio methods illustrated by specific applications. All four chapters underline the power of theoretical methods in generating potential energy surfaces and the sophistication by which we can search out the chemically significant regions.

The third section essentially describes how one makes use of reaction paths to calculate reaction rates by employing statistical methods. This section merges reaction dynamics and quantum chemistry, traditionally two distinct areas of research. A. D. Isaacson brings us beyond ordinary transition state theory by introducing canonical variational transition state theory (CVT) and its relation to the reaction path. The discussion is illustrated by many useful examples from the literature and covers also the introduction of tunneling effects. Truhlar illustrates the use of his CTV method by combining different levels of electronic structure theory in a direct dynamics approach along the reaction path. C. Meier and V. Engel review in a final chapter experimental efforts to obtain information about RP's by time-resolved femtosecond spectroscopy.

This book will be of use to any chemist with a desire to know about how chemical reactions are described in detail. It is especially useful for the computationally minded researcher who wants to go beyond the standard description of chemical reactions in terms of structures of reactant(s), transition state, and product(s). It could be used as a textbook in an advanced graduate course. I recommend it highly for personal purchase and consider it a must for any library.

Tom Ziegler, *University of Calgary*

JA965587P

S0002-7863(96)05587-4

High-Speed Countercurrent Chromatography. Edited by Yoichiro Ito (National Institutes of Health) and Walter D. Conway (SUNY−Buffalo). Wiley: New York. 1996. xxiii + 454 pp. $79.95. ISBN 0-471-63749-1.

High-Speed Countercurrent Chromatography is volume 132 in the John Wiley Chemical Analysis series. The book is divided into three main sections titled Instrumentation, Special Techniques, and Applications. The book's fourteen chapters are written by leading authorities in the field.

Chapters 1 and 2 discuss the basic analytical and preparative instrumentation, general methodology, operating parameters, and fundamental principles governing two-phase distribution and solute partitioning in a rotating coil and under centrifugal force fields. Terms associated with high-speed countercurrent chromatography (HSCCC) are also defined. Special techniques of combined HSCCC−mass spectrometry, dual countercurrent chromatography, foam countercurrent chromatography, and pH-peak-focusing and pH-zone-refining countercurrent chromatography are described in Chapters 3−6, respectively. Examples are included in each chapter to illustrate the method's applicability for chemical separations and quantitative analysis. The final eight chapters are devoted to practical separations and/or isolations involving natural products, medicinal herbs, marine natural products, antibiotics, thyroid hormone derivative *N*-(bromoacetyl)-3,3′,5-triiodo-L-thyronine and *N*-(bromoacetyl)-L-thyroxine, synthetic dyes, proteins and rare earth elements. Numerous examples of important practical separations, which were taken from the recent (mid-1980s to 1992) chemical and pharmaceutical literature, are reviewed. For many of the separations the authors give specific solvent systems and operating conditions used in the HSCCC method. Alternative separation methods are also briefly mentioned in the case of marine natural products.

I highly recommend *High-Speed Countercurrent Chromatography* to analytical and pharmaceutical chemists involved in the design of separation methods. There is a heavy emphasis on the separation of pharmaceutically important compounds in the book. Instructors of chemical separation courses will also find the book to be an extremely valuable reference source.

William E. Acree, Jr., *University of North Texas*

JA9655294

S0002-7863(96)05529-1

*Unsigned book reviews are by the Book Review Editor.

Polymers and Other Advanced Materials: Emerging Technologies and Business Opportunities. Edited by Paras N. Prasad (State University of New York—Buffalo), James E. Mark (University of Cincinnati), and Ting Joo Fai (Standard and Industrial Research). Plenum Press: New York. 1995. xxiii + 791 pp. $159.50. ISBN 0-306-45210-3.

This book continues the tradition of providing the scientific community with information on some of the most important advances reported at a series of conferences on Frontiers of Polymers and Advanced Materials. The meeting covered in this proceedings volume was held in Kuala Lumpur, Malaysia, January 16−20, 1995. It follows earlier proceedings, a conference in New Delhi in 1991, and another in Jakarta in 1993. All of these conferences focused on the most recent and important advances in a wide range of carefully chosen subject areas dealing with advanced materials and new technologies. The conference covered by these proceedings emphasized composites and blends, high-performance materials, sol−gel and processed materials, advanced materials from natural products, and multifunctional and smart materials. There was also a separate symposium on business opportunities.

JA965680D

S0002-7863(96)05680-6

Reviews in Computational Chemistry, Volume 8. By Kenny B. Lipkowitz and Donald B. Boyd (Indiana Univeristy-Purdue University at Indianapolis). VCH: New York. 1996. xxi + 324 pp. $110.00. ISBN 1-56081-929-4.

This volume, the latest in a continuing and valuable series, contains five reviews. Four of the chapters describe useful new computational methodologies, and the fifth describes the application of computational techniques to the newest form of carbon, the discovery of which recently was rewarded with the Nobel Prize.

Chapter 1, Computations in Treating Fullerenes and Carbon Aggregates, by Z. Slanina, S.-L. Lee, and C. Yu (National Chung-Cheng and National Tsing Hua Universities, Taiwan) [44 pp, 399 references, but none after 1994, and only a very few from that year] begins with a good discussion of computational methodologies, particularly the semiempirical, which would be useful in more general contexts than just fullerenes. It also provides an interesting discussion of topological approaches to enumerating fullerenes and considered why C60 so predominates among carbon cages. Discussion of substituted fullerenes or shrink-wraps is minimal.

Chapter 2, Pseudopotential Calculations of Transition Metal Compounds: Scope and Limitations, by G. Frenking, I. Antes, M. Böhme, S. Dapprich, A. W. Ehlers, V. Jonas, A. Neuhaus, M. Otto, R. Stegmann, A. Veldkamp, and S. F. Vyboishchikov (University of Marburg) [67 pages, 224 references, a handful from 1995] begins with the useful warning that knowing how to run a program is not the same as knowing what to calculate and understanding the results. It includes a good definition of the problem of dealing with heavy atoms, and a helpful set of rules, based on comparison of theory and experiment, for what kinds of calculations give best results for low-spin complexes. Then follow very detailed comparisons of calculated and experimental geometries and bond dissociation energies for carbonyl complexes, carbonyl ions, methyl and phenyl compounds of late transition metals, carbene and carbyne complexes, oxo and nitrido complexes, alkyne and vinylidene complexes, and chelates involving titanium. The authors conclude that accuracy comparable to that achievable for molecules of the lighter elements can be obtained through the proper choice of pseudopotential and level of electron correlation.

Chapter 3, Effective Core Potential Approaches to the Chemistry of the Heavier Elements, is written by T. R. Cundari, M. T. Benson, M. L. Lutz, and S. O. Sommerer (University of Memphis). [47 pages, 111 references, mostly 1993 and earlier, a few from 1994]. It begins with a good discussion of the specific problems raised by electron correlation for heavy atoms; treatment of relativistic effects is minimal, presumably because of the following chapter devoted to that subject. An excellent point made is that good choice of effective core potential (ecp) allows one to devote more computational resources to correlation. There is a useful description of how ecps are derived, and how optimized basis sets are generated for the noncored electrons. Then follow sections on the use of ecps with main group elements, transition metals, and lanthanides. Again, the conclusion is that the use of ecps can lead to results comparable to all-electron calculations.

Chapter 4, Relativistic Effects in Chemistry, by J. Almlöf and O. Gropen (University of Tromsø and University of Minnesota) [37 pages, 109 references, a handful from 1994] starts with a five-page review of nonrelativistic quantum mechanics, which probably is unnecessary. The subsequent discussion of relativistic qm is very difficult for a nonmathematician to follow; although the subject surely requires a mathematical presentation, the authors might recognize that statements like "Equation [44] is clearly not Lorentz invariant" imply a degree of knowledge that not all readers might possess. The chapter concludes with a brief discussion of available programs for relativistic computations and a comparison of some computational results with experiment, chiefly for the hydrides of heavy metals.

The final chapter, Chapter 5, The Ab Initio Computation of Nuclear Magnetic Resonance Chemical Shielding, by D. B. Chesnut (Duke University), [47 pages, 113 references, including several from 1995] is easily the best in the book. Because the field already is reviewed annually, the author attempts to provide a pedagogical introduction, illustrated with selected examples, rather than a comprehensive, up-to-date review. The key difficulties in producing useful results are identified as rovibrational and solvent effects, and the author notes that the tendency of calculation to produce greater shifts than observed is in accord with the expected direction of rovibrational effects. There follows a quantitative treatment of the theory, leading eventually to a general description of three relatively widely used methods, those of Ditchfield, Kutzelnigg and Schindler, and Hansen and Bouman. An excellent device is the working through of a sample calculation, from the selection of the basis set to interpretation of the results, which is done here for cyclopropene. Finally, four sets of shielding calculations are reviewed with emphasis on the physical and chemical understanding derived from the comparison of theory and experiment.

Good author and subject indices to the whole volume have been supplied by the editors. The series continues to be one of the most useful information sources for computational chemists.

Raymond C. Fort, Jr., *University of Maine*

JA965725A

S0002-7863(96)05725-3

Loss Prevention and Safety Promotion in the Process Industries, 2 volumes. Edited by J. J. Mewis (Katholieke Universiteit Leuven), H. J. Passman (TNO Defence Research, Delft), and E. E. De Rademaeker (Prevention Management International, Antwerp). Elsevier: Amsterdam. 1995. 1504 pp. $338.25. ISBN 0-444-82136-8.

Proceedings of the 8th International Symposia, Antwerp, June 6−9, 1995. The present proceedings reflect both the status of and increased research in loss prevention. Loss prevention is becoming more science-based and professional. The scientific results are also being systematically integrated in industrial practice, with respect to both the technical aspects (e.g., design) and management. Regulation, together with the responsible care approach now followed by industry, provides additional stimuli for the further development of loss prevention. The many developments, however, make it more difficult to stay abreast of progress in the whole field. These proceedings will be of use to both researchers and practitioners in industry. The following themes are presented in both volumes: Safety, Management Systems; Human Reliability; Hazards Research; Methods for Safe Design, Prevention and Protection; Risk Assessment, Including Consequence Models.

JA965677U

S0002-7863(96)05677-6

The Chemistry of Heterocycles. By Theophil Eicher (University of The Saarland) and Siegfried Hauptmann (University of Leipzig). Georg Thieme: Stuttgart, Germany. 1996. x + 504 pp. DM84. ISBN 3-13-100511-4.

The book is designed for the advanced student and research worker, and also for the industrial chemist looking for a survey of well-tried fundamental chemistry concepts as well as for information on new developments in heterocyclic chemistry. The contents of this book can serve as a basis for the design of courses in heterocyclic chemistry. The authors demonstrate that general chemical principles of structure, reactivity, and synthesis can be elucidated by using examples from heterocyclic chemistry. Of the 12.5 million chemical compounds currently registered, about half contain heterocyclic systems. Heterocycles are important, not only because of their abundance but also because of their chemical, biological, and technical significance. Heterocycles count among their number many natural products such

as vitamins, hormones, antibiotics, and alkaloids, as well as pharmaceuticals, herbicides, dyes, and other products of technical importance (corrosion inhibitors, antiaging drugs, sensitizers, stabilizing agents, etc.). This book presents the structure and physical and spectroscopic features of each heterocycle; important chemical properties, reactions, and syntheses are also discussed. Synthesis is normally approached as a retrosynthetic problem, and is followed by selected derivatives, natural products, pharmaceuticals, and other biologically active compounds that contain the basic heterocycle structure. Information is given on the use of heterocycles in synthesis and in selected synthetic transformations. Emphasis is placed on preparative and synthetic aspects of heterocyclic chemistry, supported by references to recent primary literature, reviews, and books on experimental chemistry.

JA965693R

S0002-7863(96)05693-4

Organic Thin Films and Surfaces: Directions for the Nineties, Volume 20. Edited by Abraham Ulman (Polytechnic University, Brooklyn). Academic Press: San Diego. 1995. 100 pp. $84.95. ISBN 0-12-523485-6.

The Physics of Thin Films, consisting of 19 volumes since 1963, if one of the longest running continuing series in thin film science. The thin film field has become the basis for a number of major industries, such as semiconductors, hard coatings, optoelectronics, and magnetic storage. With the development of inorganic thin films, a special field of organic thin films has emerged, is developing rapidly, and is also becoming one of increasing importance in materials science research and applications (e.g., polymer science and biomaterials). This series will move beyond the basic physics of thin films. It will address the most important issues of both inorganic and organic thin films, in their theoretical as well as their technological aspects.

JA965617O

S0002-7863(96)05617-X

Drug Prototypes and Their Exploitation. By Walter Sneader (University of Strathclyde). John Wiley: Chichester, U.K. 1996. xii + 788 pp. ISBN 0-471-94847-0.

This book provides an analysis of 1200 pharmaceuticals, identifying the key prototype drugs from which all the medicinal compounds currently in general use are derived. It charts the history and development of major therapeutic drug classes, showing how fundamental scientific discoveries have been clinically exploited. Attention is focused on how the inadequacies of many drug prototypes as therapeutic agents have been overcome by the development of chemically-related analogues. The 240 drug prototypes described in this book are assigned to six major groups on the basis of their origins: mineral and inorganic sources, plants, animals or the human body, microorganisms, screening of synthetic chemicals, and serendipitous discoveries. Within these groups more specific categories are defined in order to elucidate further how prototypes have been discovered. The information relating to the subsequent exploitation of these compounds is presented using the practical approach of a chemical "family tree". This helps to indicate where the probabilities for future development may lie, as well as expose those areas which appear to have been neglected.

JA9657418

S0002-7863(96)05741-1

Handbook of Thermodynamic Tables, Second Edited and Revised Edition. By Kuzman Raznjevic. Begell House, Inc.: New York. 1996. vi + 247 pp. $77.50. ISBN 1-56700-046-0.

This volume is an important compilation of the thermal properties of selected solids, liquids, vapors, and gases. It covers foods, metals, alloys, building materials, industrial gases, refrigerants, and more. Included are hard-to-find data on thermal conductivities, specific heat capacities, dynamic viscosity, and properties of compounds.

JA965738O

S0002-7863(96)05738-1

Enzyme Engineering XII. Edited by Marie-Dominique Legoy and Daniel Thomas. Annals of the New York Academy of Sciences. New York Academy of Sciences: New York. 1995. xiii + 506 pp. ISBN 0-89766-928-2.

This volume contains the proceedings of the Twelfth International Enzyme Engineering Conference, sponsored by the Engineering Foundation, New York, and held in Deauville, France, September 19−24, 1993. The conference focused on scientific as well as engineering aspects of enzyme technology, including recent advances in protein and metabolic engineering, supramolecular biochemistry, and new biocatalysts such as ribozymes and absymes. This conference was able to integrate all of the new tools and concepts of molecular biology without reductionism and enabled a cross-fertilization between microscopic (chemistry and molecular biology) and macroscopic (bioreactors, biosensors, and supramolecular complexes) levels.

JA965627P

S0002-7863(96)05627-2

Symmetry Through the Eyes of a Chemist, Second Edition. By Istvan Hargittai (Budapest Technical University and Hungarian Academy of Sciences) and Magdolna Hargittai (Hungarian Academy of Sciences). Plenum Press: New York. 1995. xii + 469 pp. $85.00. ISBN 0-306-44851-3.

This book surveys chemistry from the point of view of symmetry. Examples from chemistry and other fields are presented. The author notes that "despite its breadth, our book was not intended to be comprehensive or to be a specialized treatise in any specific area". The book is set up as follows: After the introduction (Chapter 1), the simplest symmetries are presented using chemical and nonchemical examples (Chapter 2). Molecular geometry is then discussed in qualitative terms (Chapter 3). Group-theoretical methods (Chapter 4) are applied in an introductory manner to the symmetries of molecular vibrations (Chapter 5), electronic structure (Chapter 6), and chemical reactions (Chapter 7). These chapters are followed by a descriptive discussion of space-group symmetries (Chapter 8), including the symmetry of crystals (Chapter 9).

JA965616W

S0002-7863(96)05616-8

A Multilingual Glossary of Biotechnological Terms (IUPAC Recommendations). Edited by Hans G. W. Leuenberger (F. Hoffmann-La Roche, AG), Bertrand Nagel (Seipelweg), and Heinz Kolbl (Bayer AG). VCH: Weinheim, Germany. 1995. 251 pp. $78.00. ISBN 3-906390-13-6.

This volume contains IUPAC-approved definitions of over 230 terms most frequently used in the multidisciplinary field of biotechnology, together with their translation into six further languages, namely, French, German, Japanese, Portuguese, Russian, and Spanish. The terms are presented in dictionary format for easy look-up. The aim has been to facilitate communication among chemists, chemical engineers, biologists, and bioengineers, and to render biotechnology more accessible to the chemical profession. The scope of this work includes the fields of microbiology, genetic engineering, biochemistry, molecular biology, biochemical engineering, and bioprocessing and general concepts of biotechnology, which makes this compilation an indispensable reference.

JA965618G

S0002-7863(96)05618-1

Topics in Molecular Organization and Engineering: Strategies and Applications in Quantum Chemistry. From Molecular Astrophysics to Molecular Engineering. Edited by Y. Ellinger (Ecole Normale Supereure & Observatoire de Paris) and M. Defranceschi (Commissarat a l'Energie Atomique). Kluwer Academic: Dordrecht, The Netherlands. 1996. xiv + 461 pp. $207.00. ISBN 0-7923-3837-5.

This book was initiated by the symposium Molecules in Physics, Chemistry, and Biology, which was held in Paris in 1986. Appropriately dedicated to Professor Raymond Daudel, the symposium was both broad in its scope and penetrating in its detail. The sections of the symposium were (1) The Concept of a Molecule; (2) Statics and Dynamics of Isolated Molecules; (3) Molecular Interactions, Aggregates and Materials; (4) Molecules in the Biological Sciences; and (5) Molecules in Neurobiology and Sociobiology. These proceedings have been arranged into eighteen chapters which make up the first four volumes of this series: (Volume 1) General Introduction to Molecular Sciences, (Volume II) Physical Aspects of Molecular Systems, (Volume III) Electronic Structure and Chemical Reactivity, and (Volume IV) Molecular Phenomena in Biological Sciences.

JA965739G

S0002-7863(96)05739-3