Additions and Corrections

The First Structurally Characterized Homofullerene (Fulleroid) [*J. Am. Chem. Soc.* **1999**, *121*, 7971−7972]. ANDREW F. KIELY, ROBERT C. HADDON,* MARK S. MEIER,* JOHN P. SELEGUE, CAROLYN PRATT BROCK,* BRIAN O. PATRICK, GUAN-WU WANG, AND YONGSHENG CHEN

Professor François Diederich has pointed out that in some higher adducts of C_{70} there are examples of C7−C8 adducts in which the C7−C8 bond is opened. This work is reported in Herrmann et al. [Herrmann, A.; Rüttimann, M. W.; Gibtner, T.; Thilgen, C.; Diederich, F.; Mordasini, T.; Thiel, W. *Helv. Chim. Acta* **1999**, 261−289] and should have been cited in our manuscript. We regret the oversight.

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Book Reviews *

Reviews in Computational Chemistry. Volume 13. Edited by Kenny B. Lipkowitz and Donald B. Boyd (Indiana University−Purdue University at Indianapolis). Wiley-VCH: New York. 1999. xxxiii + 426 pp. $135.00. ISBN 0-471-33135-X.

As we all know, when one begins to work in a new area it is a good thing to have a chat with someone who is already an expert in that field. But it is better to do some background reading first, so that intelligent questions may be asked. If the new field happens to be in the broad purview of "computational chemistry", one cannot generally do better than to try to find an appropriate article in the highly successful *Reviews in Computational Chemistry* series. The basic philosophy of the editors (Kenny B. Lipkowitz and Donald B. Boyd) seems to be to help the authors produce chapters that are complete, accurate, clear, and accessible to experimentalists (in particular) and other nonspecialists (in general). As a contributor to Volume 10 of the series, I can attest to the careful attention the editors give to helping authors achieve these goals. I especially recommend this particular volume to computational and theoretical graduate students and postdocs who are beginning new computational projects, as well as experimentalists using molecular modeling software (such as GAUSSIAN, SPARTAN, AMBER, etc.).

Volume 13 covers a typically wide spectrum of topics. The tone is set in the Preface, wherein the editors describe the contributions of such luminaries as Norman L. Allinger and Michael J. S. Dewar in a highly entertaining and interesting narrative. The Preface also presents citation statistics that highlight the increasingly important role of computational chemistry in the literature. The chapters themselves are of typically high caliber. The title of Chapter 1 (by Thomas Bally and Weston Thatcher Borden) is, revealingly, "Calculations on Open-Shell Molecules: A Beginner's Guide". I cannot stress enough how useful and unique such a guide is. The authors, who are experimental physical organic chemists, stress simple, physical explanations for spin contamination, symmetry breaking, and Jahn−Teller effects in this context, and discuss how these effects can impact the predictions made. It is highly readable, even entertaining (!).

Chapter 2 (by Neil R. Kestner and Jamie E. Combariza) focuses on "Basis Set Superposition Errors: Theory and Practice". If every person who contemplated publishing an article containing ab initio calculations were to consult this chapter first, many errors in the literature would be avoided. This chapter should be required reading for anyone who attempts to assess the energetics of chemical reactions using quantum-mechanical methods. Chapter 3 (by James B. Anderson), titled "Quantum Monte Carlo: Atoms, Liquids Clusters, Liquids and Solids", provides a timely and extremely well-written tour of quantum Monte Carlo methods and their broadest range of applications. As someone who uses Monte Carlo methods extensively in my own work, I am happy to have this article to show to any student who is about to start working in this area.

Those who are using molecular dynamics and Monte Carlo methods to simulate aqueous systems cannot do better than to consult Chapter 4 (by Anders Wallqvist and Raymond D. Mountain), which provides an extensive review of "Molecular Models of Water: Derivation and Description". In this chapter the authors do an excellent job of explaining how the various models are obtained. Chapter 5 (by James M. Briggs and Jan Antosiewicz) addresses the "Simulation of pH-Dependent Properties of Proteins Using Mesoscopic Models", nicely explaining the physics behind the various approaches in the process. This article, which champions the finite difference Poisson−Boltzmann method for pK_a calculations, is sure to stir interesting discussions in the literature of this field. Finally, as if to demonstrate that computational chemistry is a many-headed Hydra, Chapter 6 (by Harold E. Helson) focuses on "Structure Diagram Generation". This technology underlies all chemical drawing software as well as databases that use drawings as a tool for organizing chemical structure data. This chapter left me with a better appreciation for just how much still remains to be done in this field, and for the complexity of some of the interesting problems that remain in this important subfield of molecular graphics.

Robert Q. Topper, *The Cooper Union for the Advancement of Science and Art*

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Quantum State Diffusion. By Ian Percival (Queen Mary and Westfield College, London). Cambridge University Press: New York. 1998. 169 pp. $49.95. ISBN 0-521-62007-4.

The theory and applications of quantum state diffusion (QSD) are clearly presented by Ian Percival. QSD is an alternative computational and theoretical approach to rationalize recent experiments in quantum physics and to understand future technologies in quantum cryptography and quantum computation.

The book's focus is divided into describing the physics of open quantum systems and addressing fundamental issues in quantum mechanics. Percival starts by introducing classical one-dimensional Brownian motion and fundamental properties of stochastic processes. Basic quantum theory and notation are introduced. Entanglement is used to motivate the discussion, since it is central to the quantum theory for open systems. From the introductory material, general QSD theory and localization are developed. The latter is a property of QSD that links classical and quantum mechanics and provides the dynamics for the process of quantum measurement. The QSD equation is derived

*Unsigned book reviews are by the Book Review Editor.

from the Lindblad master equation, and alternative forms of the equations and the connection with quantum jumps are discussed. Graphic illustrations for simple solutions are presented, and a description of the numerical methods for the QSD equations are provided. An introduction to using standard QSD software available on the Internet is presented. The book gives experimental and theoretical reasons for the current interest in alternative quantum theories. An appeal is made to fundamental physics, where primary state diffusion is derived independently from two different sets of principles. The book concludes with the classical dynamical theory of quantum localization, the semiclassical limit of QSD, and the theory of localized systems with linear dynamics.

This is a well-written book that is specialized in understanding quantum state diffusion. It is suitable for readers who have a solid understanding of quantum theory, especially for physicists and physical chemists in the applied fields of quantum optics, quantum statistics, and theoretical molecular biology. The strengths of this book are in its organization and clarity. Equally exciting is how fundamental theory is used to understand modern experimental problems in quantum physics. In short, Percival's book serves to convey the fundamental ideas behind QSD and revive an interest in alternative quantum theories.

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Understanding Humic Substances. Advanced Methods, Properties and Applications. Edited by Elham A. Ghabbour (Northeastern University) and Geoffrey Davies (Northeastern University). Royal Society of Chemistry: Cambridge. 1999. xvi + 286 pp. $125.00. ISBN 0-85404-799-9.

This book was developed from the proceedings of the third Humic Substances Seminar held at Northeastern University on March 22−23, 1999. Chapter 1 introduces the multidisciplinary nature of humic acid research by addressing the question, "What is humic acid?", and its ever-modified answers throughout the past 40 years. New research on the biology, chemistry, physics, and physiology of humic substances using a variety of state-of-the-art techniques is covered in the remainder of the book.

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Progress in Colloid and Polymer Science. Volume 114. Physical Chemistry and Industrial Application of Gellan Gum. Edited by K. Nishinari (Osaka City University). Springer: Berlin, Heidelberg, New York. 1999. xvii + 131 pp. $89.95. ISBN 3-540-66389-4.

This book is comprised of 19 papers that cover the study of the mechanism of sol−gel transition of gellan gum from a variety of disciplines, e.g., NMR, rheology, differential scanning calorimetry, light scattering, osmotic pressure, small-angle X-ray scattering, and scanning tunneling microscopy to name a few. The papers are derived from presentations at the 4th International Conference on Hydrocolloids in Osaka in October 1998.

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Pauling's Legacy: Modern Modelling of the Chemical Bond. Theoretical & Computational Chemistry. Volume 6. Edited by Z. B. Maksic (Rudjer Boskovic Institute, Zagreb) and W. J. Orville-Thomas (Aberystwyth, Wales). Elsevier: Amsterdam. 1999. 782 pp. $360.50. ISBN 0-444-82508-8.

This book contains 28 photoready chapters devoted to the legacy of Linus Pauling. In the preface, the editors state that the goal of the volume is to put the beautiful and enormously successful simple models of chemical bonding advocated by Pauling "into the language of modern quantum chemistry, thus providing a deeper justification for many of (his) concepts". The chapters succeed in doing that as well as much more. Virtually the whole range of Pauling's interests is covered in the volume. In particular, the valence bond (VB) theory championed by Pauling is dealt with extensively. While VB theory has obvious conceptual advantages relative to the molecular orbital theory that is more familiar to most students of chemistry, its use in quantitative calculations was relatively slow to develop. However, the generalized VB theory of Goddard (which is regrettably not reviewed here) and other modern approaches, such as the spin-coupled treatment of the late Joe Gerratt and his collaborators (reviewed in Chapter 18), have become valuable quantum chemical tools, especially for problems in which qualitative interpretations are sought.

Beginning with a thorough and masterful discussion of VB theory and its relationship to other quantum chemical approaches by Roy McWeeny (Chapter 13), there are eight consecutive chapters devoted to VB methods and their application. The latter include treatments of diatomic cations (Chapter 15), aromatic and other π electron systems (Chapters 13, 17, 18, and 19), and hypervalent and electron-deficient compounds (Chapters 16 and 20). Other topics of interest to Pauling at various points in his long career are also addressed in the book. These include his early interests in polarizabilities and magnetic susceptibilities (Chapters 5 and 6) as well as electronegativity (Chapter 7); midcareer forays into the structure of proteins and amides (Chapters 11, 24, 25, and 26) and hydrogen bonding (Chapter 22); and the subject of solid-state structure that occupied him late in life (Chapters 4 and 28).

The book closes with a delightful epilogue by Dudley Herschbach that touches on both scientific and personal aspects of Pauling. The latter are not to be found elsewhere in the book and provide both interesting and entertaining reading. I heartily recommend this book to anyone with an interest in seeing how the early "slide-rule days" ideas of Pauling have evolved into highly sophisticated computational and interpretive tools that are an integral part of modern chemical science.

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Lecture Notes on Fullerene Chemistry: A Handbook for Chemists. By Roger Taylor (University of Sussex). Imperial College Press: London. 1999. xiv + 268 pp. $48.00. ISBN 1-86094-104-4.

It was only in 1990 that a third allotrope of carbon was isolated and became available for study. It is certain that few developments in chemistry have generated so many papers in the literature in such a short time. While this explosive growth of fullerene chemistry makes comprehensive documentation difficult, a broad pattern of fullerene reactivity is emerging. In his *Lecture Notes on Fullerene Chemistry: A Handbook for Chemists*, Roger Taylor, a leading researcher in the area, reveals this pattern.

The book begins with a brief account of the events leading up to the isolation of the first fullerenes and the Nobel Prize for Smalley, Curl, and Kroto. There is a nice treatment of fullerene structure and nomenclature using Schlegel diagrams which are also used to make fullerene substitution patterns quite clear.

The remainder of the book is a survey of the different aspects of fullerene reactivity. There are chapters on hydrogenation, reduction, nucleophilic addition, and radical addition and a lengthy chapter on cycloaddition reactions. Professor Taylor follows with chapters on fullerene oxidations, inorganic and organometallic derivatives, and fullerene polymers and a brief treatment of endohedral fullerenes.

This volume includes references to major papers through 1997 and even some from 1998. Although the lack of an index is a drawback, this book will provide a useful introduction to people seeking to learn more about the rapidly growing field of experimental fullerene chemistry. Since much of this chemistry has not gone beyond the survey stage, the book poses almost as many questions as answers and will certainly open many new research areas to imaginative chemists.

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