Additions and Corrections

Sodium Hypochlorite: A Convenient Oxygen Source for Olefin Epoxidation Catalyzed by (Porphyrinato)manganese Complexes [*J. Am. Chem. Soc.* **1984**, *106*, 6668−6676]. Bernard Meunier,* Elisabeth Guilmet, Maria-Eliza De Carvalho, and René Poilblanc

Our initial paper reported that the catalytic epoxidation of *p*-methoxystyrene by the Mn(TPP)Cl/LiOCl system in a biphasic medium $CH_2Cl_2/H_2{}^{18}O$ produced the expected epoxide with less than 5% of ^{18}O incorporation. More recently we described the partial incorporation of oxygen atom from labeled water within olefins or alkanes when using a water-soluble manganese prophyrin catalyst and $KHSO_5$ as oxidant via an oxo−hydroxo tautomerism (Bernadou, J.; Meunier, B. *Chem. Commun.*, **1998**, 2167−2173). Since these data on oxygen atom of high-valent metal−oxo species are of particular importance in molecular oxygen formation with the PSII manganese cluster (Limburg, J.; Vrettos, J. S.; Liable-Sands, L. M.; Rheingold, A. L.; Crabtree, R. H.; Brudvig, G. W. *Science* **1999**, *283*, 1524−1527), we decided to reinvestigate the oxygen atom origin in epoxidations with the Mn(TPP)Cl/LiOCl system in a biphasic medium $CH_2Cl_2/H_2{}^{18}O$ in the experimental conditions used in our article of 1984. We found that after 4 min of reaction, the olefin conversion reached 98% and the epoxide yield was 91%. *GC-MS analysis of the molecular peak of epoxide indicated a 88−92% of* ^{18}O *content, corresponding to 93 ± 2% of incorporation of* ^{18}O *from labeled water*. Analyses of aliquots after 8 min or 13 min of reaction time confirmed this result (Robert, A.; Meunier, B. data to be submitted for publication). The present data must be considered as more valid that the absence of label incorporation from ^{18}O-water published in our article of 1984. This fast incorporation of labeled oxygen from water within the epoxide is probably due to a rapid exchange of the oxygen atom of hypochlorite with water rather than an exchange of a high-valent manganese(V)−oxo with bulk water which is relatively slow in aqueous medium according to studies with $KHSO_5$ (Groves, J. T.; Lee, J.; Marla, S. S. *J. Am. Chem. Soc.* **1997**, *119*, 6269−6273). Consequently, potassium monopersulfate, which does not exchange quickly its peroxidic oxygen atom with bulk water, is recommended for generating high-valent metal−oxo species in labeled water and oxygen-atom exchange studies (Song, R.; Sorokin, A.; Bernadou, J.; Meunier, B. *J. Org. Chem.* **1997**, *62*, 673−678. Sorokin, A.; Meunier, B. *Eur. J. Inorg. Chem.* **1998**, 1269−1281).

We apologize for any confusion this may have caused and we thank John T. Groves and Robert H. Crabtree for fruitful discussions.

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Book Reviews *

Combined Quantum Mechanical and Molecular Mechanical Methods. ACS Symposium Series 712. Edited by Jiali Gao (State University of New York at Buffalo) and Mark A. Thompson (WRQ Inc.). Oxford University Press: New York. 1998. x + 310 pp. $110.00. ISBN 0-8412-3590-2.

This book was developed from the symposium on Hybrid Quantum Mechanical and Molecular Mechanical Methods presented at the 214th National Meeting of the American Chemical Society in 1997. The 19 papers in it are grouped in the following sections: Model Development; Ab Initio Dynamics; Solvation; and Biochemical Applications.

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The Chemistry of Fragrances. Compiled by David H. Pybus and Charles S. Sell (Quest International, UK). Royal Society of Chemistry: Cambridge, UK. 1999. xvi + 278 pp. £16.95. ISBN 0-85404-528-7.

This is one of a series of 11 inexpensive paperbacks declared suitable for teachers and students and designed to give a clear and readable introduction of the topic which should appeal to the general chemist. However, this book is more than a general introduction into the chemistry of fragrance. It a thorough, general text suitable for chemists in the fragrance industry. The text is best understood by someone having an appreciation of advanced organic chemical synthesis. There are interesting discussions of the importance of economic considerations in the development of the fragrance industry. The book has an interesting but short chapter on modern electronic aroma-sensing systems. As with most texts authored and published in Great Britain, *The Chemistry of Fragrances* is very well written and effectively illustrated with chemical structures and organic synthetic reactions. However, it is published as a paperback with small, single-spaced print that makes it a real effort for the reader to appreciate all of the interesting chemistry, examples, and illustrations that have been blended into this book.

James D. Stuart, *University of Connecticut*

JA995720O

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Essential Trends in Inorganic Chemistry. By D. M. P. Mingos (Imperial College, London, UK). Oxford University Press: Oxford, New York, and Tokyo. 1998. iv + 392. $29.95. ISBN 0-19-850108-0.

A major issue in any inorganic chemistry class is the sheer mass of information that must be handled by the students. The Periodic Table can be used to help systematize this material; however, as the author points outs in the Introduction, "The knowledge of the structure of the Periodic Table does not lead to a direct interpretation of chemical phenomena." In this book, the author explores in detail the relationship between the position of an atom in the Periodic Table and the properties of the atoms and compounds containing these atoms.

This book is organized to emphasize periodicity. The first chapter gives a brief presentation of the quantum mechanical basis of the Periodic Table. The next three chapters, on vertical trends, horizontal trends, and isoelectronic and isostoichiometric relationships, discuss various aspects of periodicity among main group elements. The final chapter deals with transition metals, lanthanides, and actinides.

The wealth of information on periodic properties of main group elements in Chapters 2, 3, and 4 makes this book an excellent reference for anyone teaching inorganic chemistry. Physical properties that are covered include ionization energies, electronegativities, electron attachment enthalpies, atomic radii, melting points, dipole moments, densities, and hardness, while chemical properties include allotropes, standard reduction potentials, acid−base properties, and chemical reactivities of oxides and hydrides. A very useful and detailed

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*Unsigned book reviews are by the Book Review Editor.

comparison of the properties of nonmetal elements is included at the end of Chapter 2. One limitation of the information that is presented is that no references for the data are given. In addition, splitting periodicity into vertical and horizontal trends is somewhat confusing because the same data are often discussed in both Chapters 2 and 3.

Because of the emphasis on periodicity, fundamental concepts in Chapters 2−4 are included in the discussion of a related periodic property. As an example, the discussion of covalent bonding is fragmented over three chapters (octet rule in section 2.4, three-center two-electron bonding in section 3.7, VSEPR theory in section 4.2, valence bond theory in section 4.5, and molecular orbital theory in section 4.6). This is a major weakness in any book that is used in a lower level (junior) undergraduate inorganic chemistry course where the students will be encountering many of these concepts for the first time. It also results in a rather disjointed discussion of topics such as hypervalency. The valence bond approach to hypervalency is discussed in great detail in section 4.5 and the molecular orbital theory approach in section 4.6. Unfortunately, little attempt is made to compare the two approaches and give the reader any appreciation of their relative advantages and disadvantages.

The final chapter in the book describes the chemistry of transition metals, lanthanides, and actinides. The approach in this chapter is more traditional, with a general discussion of bonding in coordination complexes being given before their period properties are discussed. The discussion of transition metal complexes is limited by a very elementary discussion of their electronic spectra and by a total absence of any discussion of the function of such complexes in homogeneous catalysis and bioinorganic chemistry. The periodicity discussion is somewhat confusing because infinite solids and simple salts are mixed with coordination complexes. In addition, a section on vertical trends for transition elements (5.7), which comes after the discussion of coordination chemistry, seems out of place.

In summary, this book will be a valuable reference to any chemist interested in periodicity and will also be an important reference for students in advanced main group chemistry courses. However, the manner in which fundamental concepts in structure and bonding are presented will limit its use in introductory (junior level) inorganic chemistry courses.

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Analytical Solid-Phase Extraction. By James S. Fritz (Iowa State University). John Wiley & Sons (Wiley-VCH): New York. 1999. xiii + 209 pp. $64.95. ISBN 0-471-24667-0.

This is a timely monograph on solid-phase extractions (SPE) from one of the experts in the field. This analytical technique has been widely used for a number of years in a wide variety of applications, including environmental as well as biological samples. The nine chapters in this book are logically divided into the areas of (1) Introduction and Principles, (2) SPE in the 1970s: Extraction of Organic Pollutants from Water, (3) Solid Particles for Solid Phase Extraction of Organic Compounds from Water, (4) Practical Considerations: Equipment and Techniques, (5) Ion-Exchange Sorbents, (6) Resin-Loaded Membranes, (7) Preconcentration of Metal-Ions, (8) Microscale and Semimicroscale Techniques, and (9) Applications. This represents a logical division and presentation of the topic. While the introduction and principles may seem somewhat simplistic, it represents a good starting point for the novice in the field. Others, more knowledgeable in the field, may skip this section and start directly with Chapter 2 or 3 without loss of continuity within the text. As a reviewer, I found the last few chapters on past adsorbents and applications to be most informative since these sections provide a good general overview of the capabilities of the technique.

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Monte Carlo Methods in Chemical Physics. Advances in Chemical Physics Vol. 105. Edited by David M. Ferguson, J. Ilja Siepmann, and Donald G. Truhlar (University of Minnesota). Series edited by I. Prigogine and Stuart A. Rice. John Wiley and Sons, Inc.: New York, NY. 1999. xii +517 pp. $195. ISBN 0-417-19630-4.

This book is a compilation of articles describing the application of Monte Carlo methods to a diverse set of problems in physical chemistry. The first chapter, which is a short introduction to this computer simulation method, develops the concept of importance sampling and its application to the numerical evaluation of multidimensional integrals. These ideas are discussed primarily in the context of calculating ensemble averages in the canonical ensemble; the extension to other ensembles is also briefly discussed. The introductory chapter provides a clear presentation of the concepts that are central to the Monte Carlo method, and at a level that is sufficient for the casual reader to use as a stepping stone to understanding the more advanced material found in the rest of the volume. For the interested reader, this first chapter is complemented by a set of references that point to more in-depth discussions of this powerful simulation technique.

The remainder of the volume is divided into 14 chapters that detail many of the important application areas of Monte Carlo methods in chemical physics. The evaluation of thermodynamic ensemble averages is an integral part of several of the chapters, and thus provides a clear connection to the material covered in the introduction. When the molecular species under investigation possess a large number of internal degrees of freedom, special sampling techniques are necessary to ensure the appropriate sampling of configuration space. These techniques are the subject of several of the articles, and specific issues are explored in the simulations of polymeric systems and globular proteins. The evaluation of ensemble averages is not, however, the only application of the Monte Carlo algorithm. Indeed, the calculation of multidimensional integrals is a central part of many other problems in physical chemistry. Two chapters explore applications of this nature. One article describes the calculation of absolute free energies of molecular species using adaptive path−integral methods, and another the evaluation of quantum expectation values using variational Monte Carlo techniques. Overall, the volume presents a very diverse set of topics; the subjects covered range from the study of phase equilibria to the simulation polymer systems, and from the development of quantum Monte Carlo methods to techniques for sampling initial conditions in classical trajectory simulations. Each chapter in the volume is well written and complemented with an up-to-date reference list, making this a valuable reference source for both students and advanced scientists.

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