Book Reviews *

Theory and Applications of Quantum Molecular Dynamics. By John. Z. H. Zhang (New York University). World Scientific: Singapore, New Jersey, London, and Hong Kong. 1999. xiv + 366 pp. $58.00. ISBN 981-02-3388-4.

John Z. H. Zhang, an accomplished theorist who has made many important contributions to the field of quantum molecular dynamics, has written an excellent and practical book that I anticipate will be used by many scientists who apply quantum mechanics to study chemical reactions. Because newer developments in the field are not adequately covered in existing books, there is a great need for a book of this kind. The book clearly explains the tools and methods required to calculate state-to-state reaction probabilities, cumulative reaction probabilities, resonance lifetimes and energies, etc. Moreover, the book is written in a clear expository style that facilitates understanding.

The book begins by explaining how electronic and nuclear degrees of freedom can be separated using the Born−Oppenheimer approximation. In the second chapter the author very briefly explains ab initio methods used to solve the electronic problem. The rest of the book is devoted to the solution of the nuclear problem. The subject of Chapter 3 is the calculation of the (bound) ro-vibrational states of molecules. Chapters 4−8 treat reactions between molecules. Scattering theory applied to molecular problems is presented from both the time-independent and the time-dependent viewpoints. Detailed equations are given. Chapter 9 contains a description of methods applied to study photodissociation and predissociation. Chapter 10 concerns dissociative adsorption at surfaces, and the final chapter is a summary of various semiclassical methods that could, at least in principle, be applied to the subjects of Chapters 3−10. Chapter 3 and Chapters 5−11 present modern methods of quantum dynamics: the discrete variable representation, the multi-arrangement approach to the atom−diatom reactive problem, time-dependent approaches, the reactant product decoupling method, "direct but correct" methods for computing rate constants, the initial value representation, etc. Many chapters conclude with examples taken from the author's published work.

I feel that three slight deficiencies are worth mentioning. First, the diabatic representation is incorrectly defined and explained in the first chapter. The representation Zhang identifies as diabatic is more commonly called the crude adiabatic representation. Second, Zhang tends to contrast time-dependent methods whose cost scales as N^2 with time-independent methods whose cost scales as N^3. It is, however, well known that the cost of time-independent iterative methods also scales as N^2. Third, the book is a useful summary of the theory and equations that underly the author's research, but because many of the equations in the book can be explained and understood in several ways, I feel that it would be more useful if more references to other texts were included.

In conclusion, this is an excellent book and would be a good addition to the library of anyone working in the field of quantum dynamics.

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Electroanalytical Chemistry. Vol. 21. Edited by Allen J. Bard (University of Texas) and Israel Rubinstein (Weizmann Institute). Marcel Dekker: New York and Basel. 1999. xiv + 349 pp. $175.00. ISBN 0-8247-7399-3.

The three contributed chapters in the most recent volume of this series illustrate the emergence of nanoscale chemistry in the field of electrochemistry. D. T. Mitchell and C. R. Martin (Colorado State University) present a descriptive overview of the *template synthesis* of nanoscale electrode materials. Template synthesis entails the controlled deposition of a desired electrode material within the pores of a porous membrane or other solid material. Due to the nanoscale dimensions of the deposit, these materials often exhibit unique properties that make them attractive as electrochemically controllable permselective membranes, as high-energy density intercalation materials for batteries, and as electrodes for electroanalysis.

In the second chapter, J. L. Stickney (University of Georgia) describes the expitaxial deposition of atomic layers by controlling the electrochemical potential of the substrate, so that exactly one atomic layer is formed in each step by surface-limited underpotential deposition. This technique, which has been named *electrochemical atomic layer expitaxy* (ECALE), is being investigated as a method to synthesize thin films of electronic grade compound semiconductors (e.g., CdTe and ZnS). The author provides a seminal description of the fundamental chemistry involved in ECALE and the current state and progress in this field.

In the final chapter, T. P. Moffat (National Institute of Standards and Technology) describes the operation of the scanning tunneling microscope for probing the dynamics and structure of metal electrode surfaces. The author does an excellent job in presenting a theoretical description of the STM imaging mechanism and nuances unique to investigations in an electrochemical environment. This chapter also provides a badly needed up-to-date description of progress in the field, along with in-depth analysis of fundamental STM and electrochemical phenomena. This chapter is highly recommended for anyone beginning STM investigations of the electrochemical interface.

All three chapters in Vol. 21 of *Electroanalytical Chemistry* are very clearly written, with current references to the literature.

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Applications of Hydrogen Peroxide and Derivatives. By C. W. Jones (formerly of Solvay Interox R&D, Widnes, UK). Royal Society of Chemistry: Cambridge. 1999. X + 264 pp. £59.50. ISBN 0-85404-536-8.

This monograph, published as part of the Royal Society's Clean Technology Series, is an well-organized and enjoyable overview of the chemical applications of hydrogen peroxide and related oxidants. Chapter 1 is a primer covering hydrogen peroxide (manufacture, physical properties, considerations for safe use, and toxicology). Chapter 2 describes activation by inorganic and organic species, beginning with a nice overview of reactivity patterns and continuing with a discussion of peracids, metal oxenes, transition metal complexes, percarbonate, perborate, Fenton chemistry, peroxymonosulfate, hydroperoxides, dioxiranes, and peroxyimidic acids. Chapter 3 reviews the synthetic applications of peroxygen reagents in epoxidations, hydroxylations, Baeyer−Villiger oxidations, alkene cleavages, oxidations of amines and sulfides, halogenations, and benzylic oxidations. Chapter 4 focuses on epoxidation, hydroxylation, and alkene cleavage mediated by TS-1 and other heterogeneous catalysts. Chapter 5 covers environmental applications related to destruction of organic compounds in water and soil, and Chapter 6 describes useful applications for chemical purification, pulp and paper bleaching, and metal finishing. A useful index allows searching by subject, company/process names, and, in some cases, authors.

Although readers will be initially drawn toward their own research interests and experience, the layout encourages exploration of other areas of peroxygen chemistry. In this spirit, the book could benefit from better cross-referencing of common topics. Literature citations, including patents, follow each chapter and are current through 1996−7; several recent advances (improved chiral dixoiranes, HOF chemistry, synthesis of specifically ^{18}O-labeled peroxides) are missing. Several of the chapters could benefit from more careful referencing of individual transformations or processes. There are a number of minor errors, a few of which could confuse inexperienced readers. Overall, this useful book is strongly recommended to anyone interested in oxidation or

*Unsigned book reviews are by the Book Review Editor.

peroxygen chemistry and is suitable for an advanced undergraduate or graduate level course.

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Molecular Structure Description. The Electrotopological State. By Lemont B. Kier (Virginia Commonwealth University) and Lowell H. Hall (Eastern Nazarene College). Academic Press: San Diego. 1999. xx + 245 pp. $99.95. ISBN 0-12-406555-4.

Monty Kier and Lowell Hall are very well known to the QSAR and QSPR communities for their pioneering and tireless efforts to relate essentially all types of biological and physicochemical properties to graph-theoretic descriptions of molecular structure. Their first book, *Molecular Connectivity in Chemistry and Drug Research*, published in 1976, summarized their early work and introduced many researchers to the utility of the class of *molecular* descriptors known as "connectivity indices" or "topological indices". In contrast, their latest book presents the definition and numerous applications of a relatively new class of *atomic* descriptors that they call "electrotopological state indices", abbreviated "E-state indices".

Briefly, the E-state of a given atom *i* is defined as

$$S_i = I_i + \sum_j (I_i - I_j)/r_{ij}$$

where I_i is the "intrinsic state" of atom *i* and r_{ij} is the topological distance between atoms *i* and *j*. The intrinsic state reflects the valence state electronegativity of atom *i*, which is very roughly approximated in terms of the number of non-σ-bonded electrons and the principal quantum number of the given atom. The interested reader should consult the book for further details of these indices.

The book starts with basic concepts of molecular topological indices, then quickly presents the concept of E-state atomic indices, and finally illustrates and extends that concept with numerous examples selected from the literature. Since the concept of the electrotopological state has been discussed by the authors and others for almost a decade, the authors were faced with the very significant challenge of distilling a rather large volume of literature into a relatively concise overview. As a result, although the methodology is presented very clearly, some examples are, necessarily, discussed somewhat superficially. This must have been a painful choice for the authors, who clearly are very eager to help the reader learn how to benefit from the application of their methodology. The book is written in a somewhat pedagogical fashion with recommended exercises provided near the end of most chapters. The final section of each chapter is entitled "a look ahead" and is rather effective in tempting the reader to continue through the book at a rapid pace.

To further enhance the reader's understanding and enjoyment, the book comes with a CD containing E-Calc. E-Calc is a simple program that provides a very nice way to get a feel for how E-state indices depend on structure but, unlike the authors' full-featured Molconn-Z program, does not enable the user to actually use any of the indices it calculates.

With increasing interest in high-throughput synthesis and screening, pharmaceutical and agrochemical industries are becoming increasingly interested in QSAR and QSPR methodologies. The E-state indices developed by the authors certainly merit attention in this regard, and the authors' book provides an excellent and timely introduction to the application of these indices.

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The Effects of UV Radiation in the Marine Environment. Cambridge Environmental Chemistry Series 10. Edited by Stephen de Mora (IAEA Marine Environment Laboratory, Monaco), Serge Demers (ISMER, Rimouski, Québec), and Maria Vernet (University of California, Davis). Cambridge University Press: Cambridge. 2000. x + 324 pp. $80.00. ISBN 0-521-63218-8.

The 11 chapters in this book offer a multidisciplinary review of the effects of UV radiation in the marine environment. In developing this volume, the editors tried "to follow the pathway and fate of a UV photon". Consequently, the contributions are organized in a comprehensive and logical sequence that starts with an overview of the title topic and a discussion of UV physics and optics, and then turns to subjects such as the attenuation of UV radiation in the atmosphere and in sea water, the photochemical reactions involved, the harmful effects of UV radiation on marine organisms, and the strategies these organisms have adopted to minimize the damage. References from as recently as 1998 are cited. This book should appeal to researchers and students in photobiology, photochemistry, and environmental science.

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Extraction Methods in Organic Analysis. Edited by Alan J. Handley (LGC, Runcorn). Sheffield Academic Press: Sheffield, England and CRC Press: Boca Raton, FL. 1999. xii +308 pp. $125.00. ISBN 0-8493-974005.

Although the title suggests that this might be a general text on extraction, it is not. After a very brief discussion of basic solvent extraction, the focus is on recent technologies, such as membrane extraction, solid-phase microextraction, supercritical fluid extraction, pressurized and microwave-assisted extractions, and applications (e.g., pharmaceuticals, polymers, and environmental samples) using those new technologies. It is an excellent text for those interested in applying these new technologies to sample extraction. Until the past decade, extraction technology development was substantially behind development in separations technology. As one can surmise from this text, the development and commercial introduction of accelerated and improved extraction systems has brought the level of technological development in extraction much closer to that of chromatography.

After a brief introductory chapter, the second chapter provides an excellent discussion on basic extraction procedures, followed by information on the use of membranes for extraction. A modest amount of math is included, which is useful for evaluating extraction efficacy. This chapter is followed, quite logically, by solid-phase extraction (SPE). There are numerous SPE systems available that work well. The sorbent options, as well as the appropriate SPE strategies for method development, are discussed. The next chapter is on Supleco's solid-phase microextraction system, which is a very useful, inexpensive technique for the analysis of volatiles, given the absence of a static headspace or purge-and-trap system. It also works quite well for solutions.

Supercritical fluid extraction is one of several methods that provide an excellent substitute to the rather slow, cumbersome, and solvent-intensive Soxhlet extraction. The extraction equipment involved, including analyte collection, is discussed. There are several pages on method development, including sample characteristics, selection of the appropriate supercritical fluid and conditions (temperature, pressure, flow rate, etc.), and extract collection. This is followed by several examples of food (particularly the nonpolar and slightly polar analytes) and polymer extractions. The focus of the next chapter is a logical extension of SFE, pressurized solvent extraction. Like SFE, this technique can result in a significant reduction in the solvent used and/or the extraction time required. The last technique discussed in detail is microwave-assisted solvent extraction. The emphasis in this chapter is on example applications, and a wealth of conditions and example extractions have been provided.

The last third of the text focuses on applications: biological and pharmaceutical, polymer, and environmental. All three of these chapters provide important information for scientists interested in these particular sample types.

In summary, the book is a must-have reference text for the analytical chemist. It provides a concise summary of much of the most important developmental work done in the past 10−20 years on extraction technology, in addition to a large number of published procedures. There is also very good information on how to develop new procedures for samples not discussed in the literature.

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