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BOOK REVIEWS

**Advances in Chemical Physics, Volume 140.** Edited by Stuart A. Rice (The University of Chicago, IL). John Wiley & Sons, Inc.: Hoboken, NJ. 2008. x + 290 pp. $175. ISBN 978-0-470-22688-9.

This volume presents a collection of chapters written by world-leading scientists on five seemingly distinct, yet inherently interrelated, topics. These chapters represent a symbiosis of knowledge accumulated by physical chemists over the past two decades in which new theories addressing problems at the forefront of contemporary chemical physics research are described.

The book opens with the chapter by Attard entitled "The Second Law of Nonequilibrium Thermodynamics: How Fast Time Flies". Written to be accessible to the nonexpert, this chapter provides an elegant description of nonlinear thermodynamics and nonequilibrium statistical mechanics based on the introduction of the second entropy, which is defined as "the number of molecular configurations associated with a transition between macrostates in a specified time." Transitions between macrostates can be described in terms of a flux or the rate of change. This concept allows the author to introduce the Second Law of nonequilibrium thermodynamics as the Second Law of equilibrium thermodynamics with the entropy replaced by the second entropy and the structure of the system replaced by the dynamical structure or the flux. Unlike the Second Law of equilibrium thermodynamics, the Second Law of nonequilibrium thermodynamics therefore focuses attention on time or the rate of change. According to the equilibrium Second Law, the entropy becomes maximal when the system reaches the equilibrium state. The nonequilibrium Second Law postulates that the second entropy is at a maximum when the transition flux stabilizes and the system reaches the steady state. The presentation of the formal theory is followed by a specific example of a heat flow problem, i.e., a system sandwiched between a hot reservoir and a cold reservoir. The author argues that his definition of the Second Law of nonequilibrium thermodynamics establishes a correspondence that can be used to find a nonequilibrium version of all known principles, theorems, and relationships of equilibrium thermodynamics. The natural world is dominated by nonequilibrium processes, and this presentation of thermodynamics will certainly be of great interest to physical chemists working on dynamics of macroscopic systems and philosophers of science alike.

Although thermodynamics provides an accurate description of the macroscopic states of matter, the dynamical behavior of microscopic systems is generally well described by molecular dynamics simulations. The computational difficulty of molecular dynamics simulations increases with the number of particles and the time scale of the modeled process. Many biologically and chemically interesting processes involve complex systems on the mesoscopic scale. Mescoscopic systems are too small to be well described by macroscopic state theories and too large to allow for the conventional molecular dynamics simulations. The modeling of such systems therefore represents a great challenge for theory in molecular dynamics research. In Chapter 2,"Multiparticle Collision Dynamics: Simulation of Complex Systems on Mesoscales", Kapral describes a method for accurate numerical simulations of mesoscopic molecular ensembles. The approach is based on the assumption that collisions of individual molecules are not important on coarse-grain distance and time scales and that the dynamics of mesoscopic systems can be described as the net effect of many collisions. This chapter provides a simple, yet comprehensive, description of multiparticle collision dynamics, including the discussion of the collision operators and the evolution equations. The power of the method is illustrated by a number of examples ranging from the analysis of diffusion in complex systems, to phase separation in colloidal suspensions, to the dynamics of polymers. As this is clearly an efficient and highly promising method of simulating mesoscopic systems, I would recommend this chapter as an introductory text for all beginning graduate students in chemical physics and physical chemistry.

Chapter 3 by Seideman and Gordon, entitled "Two-Pathway Excitation as a Coherence Spectroscopy", is a description of a novel spectroscopic technique that exploits the phase properties of laser light and matter and quantum interference effects to obtain information on atomic and molecular systems not readily available from conventional spectroscopies. Recent technological advances allow for the creation of laser systems with unprecedented control over the phase of light as the laser field propagates through a medium, and experimentalists may now probe the phase of the continuum wave function in measurements of photodissociation and photoionization. The authors describe how these measurements yield rich information on the structure and dynamics of atomic and molecular systems as well as the role of dissipative environments. The method is based on the same principles as coherent control of molecular processes, and the presentation should be easily accessible to readers with some basic knowledge of quantum mechanics and scattering theory. As the authors point out, coherent control is now a mature field, but coherence spectroscopy is still largely in its youth, if not infancy. This chapter may therefore serve as an excellent introduction to what may become a hot research topic in the near future.

Transition state theory is arguably the most important theory of chemistry. Its main concept—the existence of an activation complex that bridges the transition from reactants to products—has recently found applications in many other research fields, such as solid-state physics, astronomy, and cosmology. In its bare formulation, the transition state theory may, however, be quite inaccurate. Bartsch et al. describe recent advanced modifications of the theory in Chapter 4, "Time-Dependent Transition State Theory". In particular they discuss the geometric approach to multidimensional transition state theory, which allows one to construct a dividing surface—a surface that all reactive trajectories must cross—free of recrossings. Although the exposition of this chapter is rather technical, it provides an in-depth analysis of contemporary transition state theory and rewards the reader with an appreciation of the grace and beauty of this method of calculating reaction rates.

Several researchers of molecular physics and spectroscopy have recently developed experiments that could answer questions

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reaching far beyond the scope of traditional molecular science. These relatively simple experiments test some of the fundamental symmetries in nature, such as the time-reversal symmetry (T) and parity (P). Particularly interesting are the experiments that search for the permanent electric dipole moment (EDM) of the electron. A nonzero value of the electron's EDM would imply the simultaneous breaking of both T and P symmetries and the discovery of physics beyond the standard model. In the final chapter of this book, "Electronic Structure Reference Calculations for Designing and Interpreting P and T Violation Experiments", Nayak and Chaudhuri describe the computational procedure for calculating electric fields inside diatomic molecules. The chapter begins with a succinct review of the EDM measurement experiments and provides all the necessary details for *ab initio* calculations of P,T-odd effects. As this is a topic that bridges quantum chemistry, molecular physics, and high-energy physics, it will likely be of interest to a broad range of readers in both chemistry and physics. Time reversibility plays a fundamental role for all the theories described in this volume so it is quite ironic for the book to close with an overview of the work questioning the validity of the time-reversal symmetry in nature.

I have enjoyed reading this book. I have no doubt that every erudite graduate student and expert researcher in physical chemistry, chemical physics, and atomic, molecular, and optical physics will find the chapters of this volume educational and gratifying to read.

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**Raman and SERS Investigations of Pharmaceuticals.** By Monica Baia, Simion Astilean, and Traian Iliescu, (Babes-Bolyai University, Cluj-Napoca, Romania). Springer: Berlin, Heidelberg. 2008. xiv + 214 pp. $159. ISBN 978-3-540-78282-7.

This book is written from the point of view of applications of inelastic scattering spectroscopy. In recent decades, it has become clear to many researchers that interdisciplinary research is vital to success in most areas of science. Such work is demonstrated in this book. In it, spectroscopists analyze compounds synthesized by chemists to understand better the physical and chemical properties of drugs intended for clinical use. The book comprises an introductory section on the fundamentals of infrared, Raman, and surface-enhanced Raman spectroscopy (SERS), followed by eight additional chapters. Theoretical methods that are used to predict vibrational modes are initially summarized, and the SERS experiments described in the ensuing chapters are directed toward different kinds of drugs: anti-inflammatory drugs, vitamins, tranquilizers and sedatives, and drugs with antibacterial actions.

The SERS spectral analyses of the molecules studied provide data on the structure of the adsorbed species and their orientation compared to the metal surface. The influence of pH on the adsorption behavior of the investigated molecules is described. Changes observed in the SERS spectra at different pH values arise from a reorientation of the adsorbed molecule relative to the silver surface. For example, the SERS spectra collected in acidic and neutral environments indicated the chemisorption of the DCF molecule on the silver surface via the lone pair oxygen electrons of the carboxylate group, which has a perpendicular or slightly skewed orientation with reference to the silver surface. The changes in the SERS spectra recorded at different pH values demonstrate that different isomeric forms of the guest−host complex are preferentially adsorbed on the silver surface as a function of the pH values, but the adsorption of the guest molecule is maintained through the nonbonding electrons of the oxygen atom. Highly effective and convenient SERS-active substrates would increase the pharmaceutical use of Raman spectroscopy. A small number of recently created substrates that could enhance understanding of the adsorption performance of different molecules of pharmaceutical interest are thus presented.

The applications of SERS to pharmaceutical compounds constitute the strongest part of the book. The authors spend little time on mathematical modeling of the interactions involved in enhanced inelastic scattering, so readers interested in such a level of theoretical detail should look to other sources. This book focuses on an interdisciplinary approach to pharmaceutical problems and does it well.

**Robert A. Lodder,** *University of Kentucky*

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**Spectroelectrochemistry.** Edited by Wolfgang Kaim (University of Stuttgart, Germany) and Axel Klein (University of Cologne, Germany). Royal Society of Chemistry: Cambridge. 2008. x + 236 pp. $169.00. ISBN 978-0-85404-550-1.

This book covers a wide assortment of spectroelectrochemical techniques to establish spectroelectrochemistry as a widely applicable, inexpensive, and powerful method of research. The examples in the text provide the reader with illustrations of the broad application of these methods by practicing chemists and biologists, and the focus highlights the interdisciplinary nature of research in this field. *Spectroelectrochemistry*, which contains contributions written by world leaders in their respective areas, should be beneficial to most readers with even an elementary background in electrochemical methods.

Spectroelectrochemistry is generally defined as the application of spectroscopic methods to assay changes as a result of redox changes in a system. Such changes are initiated by the application of a potential by an electrochemical system. The spectroscopic methods that are included in this book consist of electronic absorption spectroscopy in the ultraviolet, visible, and near-infrared; infrared spectroscopy; resonance Raman spectroscopy; and EPR spectroscopy. The systems studied are also widely varied and provide a nice flavor of the breadth of this field. Each of the chapters includes an introduction to the methods that are covered as well as key experimental considerations.

The emphasis in this book is on metal-containing systems, but the redox changes are often organic ligand based. Most chapters focus on the types of systems that can be probed by spectroelectrochemical methods and include iron-containing proteins, mixed-valence metal complexes, metalloporphyrins, and carbon-rich organometallic complexes. There are also chapters on the methods used, and they include illustrative examples of the power of the techniques.

The coverage of *Spectroelectrochemistry* is intended to illustrate the breadth of the field but is not comprehensive, and there is some overlap of basic information on electrochemical and spectroscopic techniques. This may be useful to the novice in these fields, however, and the depth of coverage does not suffer from these independent introductions. The references are extensive and include key historical works as well as more recent examples.

Overall, *Spectroelectrochemistry* is a quality offering that will introduce the reader to the wide applicability of spectroelectrochemical methods. The broad coverage and interdisciplinary nature of the topics, the mixture of introductory and more advanced material, and the illustrative examples of spectroscopic and tabular data should make this book useful to both novices and experienced researchers in this field.

**Karen J. Brewer,** *Virginia Polytechnic Institute and State University*

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**Targets in Heterocyclic Systems: Chemistry and Properties, Volume 11 (2007).** From the series: Reviews and Accounts on Heterocyclic Chemistry. Edited by Orazio A. Attanasi (University of Urbino, Italy) and Domenico Spinelli (University of Bologna, Italy). Italian Society of Chemistry: Rome. 2008. x + 448 pp. $159.00. ISBN 978-88-86208-52-9.

This book covers the “synthesis, reactivity, activity (including medicinal) and mass spectrometry of different heterorings” in 15 chapters. A sampling of a few of them include “Synthesis and properties of covalent cofacial bisporphyrins” by Pognon et al.; “Pyrazolopyrimidines: old molecules, new targets” by Schenone et al.; and “Generation of nitroso species and their use as dienophiles in the hetero Diels Alder reaction” by Adamo and Bruschi. There is no index.

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**Mössbauer Spectroscopy in Materials Science 2008: Proceedings of the International Conference MSMS ’08, Hlohovec u Břeclavi, Czech Republic 16−20 June 2008.** Edited by Miroslav Mashlan and Radek Zbořil (Palacky University, Olomouc, Czech Republic) AIP Conference Proceedings, 1070. American Institute of Physics: Melville, NY. 2008. viii +186 pp. $119.00. ISBN 978-0-7354-0601-8.

There are 21 chapters in this book recording the proceedings of the conference “Mössbauer Spectroscopy in Materials Sciences” held in the Czech Republic in June 2008. The areas covered include “Nanoscale Systems, Conversion Electron Mössbauer Spectroscopy, Magnetism, Nanocrystalline Alloys and New Developments”, to quote from the Preface. An author index completes the book.

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**Reaction Mechanisms in Organic Synthesis.** By Rakesh Kumar Parashar (University of Delhi, India). John Wiley and Sons, Ltd.: Chichester. 2009. xx + 372 pp. $162.00. ISBN 978-1-4051-5072-9.

To paraphrase the author’s own words in the Preface, this book covers “all aspects of organic reaction mechanisms”, expanding upon the fundamentals of organic chemistry in order to understand the mechanisms and plan the syntheses. There are eight chapters, which are titled as follows: Synthetic Strategies; Reactive Intermediates; Stabilized Carbanions, Enamines and Ylides; Carbon−Carbon Double Bond Forming Reactions; Transition Metal-Mediated Carbon−Carbon Bond Forming Reactions; Reduction; Oxidation; and Pericyclic Reactions. Parashar has taken care to provide some of the latest procedural modifications to the various methods covered and to include some examples of recently published work. Each chapter is well referenced, and a subject index is provided.

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**Modified Nucleosides in Biochemistry, Biotechnology and Medicine.** Edited by Piet Herdewijn (Katholieke Universiteit, Leuven, Belgium). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim. 2008. xxvi + pp. $440. ISBN 978-3-527-31820-9.

Modified nucleosides have been well studied by bioorganic and medicinal chemists over the past five decades. Nucleosides, nucleotides, and nucleic acids have many critical roles in biological systems, ranging from storage of information to metabolic regulation and can also serve as therapeutic agents. Despite many years of research, much still remains to be learned about the roles of natural modified nucleosides and their derivatives, and many novel applications in biotechnology and medicine remain to be discovered. This book covers a variety of topics in an extremely broad field, ranging from synthetic preparations to biological and clinical applications. Although its contents could be used as an introduction to the field of modified nucleosides, some of the chapters are written at a level that might be more accessible to experts in the field. Perhaps having a more extensive introduction that put the entire set of chapters into perspective and gave a novice researcher more direction would have strengthened the book.

The book is divided into four sections: “Biochemistry and Biophysics” (Chapters 1−9), “Biotechnology” (Chapters 10−11), “Medicinal Chemistry” (Chapters 12−22), and “Antitumorals and Antivirals” (Chapters 23−25). It is more of a collection of independent review articles than a set of logically connected chapters, and the length and quality of the chapters and sections are somewhat uneven. Some topics on nucleic acids include DNA oxidation and UV-induced damage products, locked nucleic acids, and universal base analogues. Biological roles for regulatory nucleosides, such as AdoMet and *c*-di-GMP, as well as a wide range of compounds with medicinal applications, e.g., antiviral activity and inhibition of siderophore biosynthesis, are also discussed. Major emphasis is on the synthetic preparation of nucleosides.

The chapters on biochemistry and medicinal chemistry make up the majority of the book, whereas the section on biotechnology is the shortest (two chapters) and surprisingly the least informative with respect to applications. There is significant conceptual overlap between the third and fourth sections, as well a strong emphasis on certain topics in the medicinal chemistry section, leading to overlap between some chapters (including repeated figures). On the other hand, several chapters in the book have nicely balanced the background of the field with current knowledge, while providing sufficient detail for a complete understanding of the important issues. For example, Chapter 3 by Kool on the use of modified DNA bases to probe base-pair recognition by polymerases is related to existing reviews but offers a new perspective on the topic that is exciting to read. Morris and Kamath offer a detailed analysis of purine nucleoside phosphorylase inhibitors in Chapter 18 and nicely describe the structural basis for their biological activities. Although a broad and diverse set of topics is covered in this book, a reader hoping to understand certain aspects of modified nucleosides might be disappointed. There is very little coverage of the modified nucleosides in RNA and insufficient detail on some of the biological pathways of modified nucleosides presented. In fact, the first chapter, which covers only a few aspects of modified protein and RNA structure, seems out of place.

Despite some of the criticisms mentioned above, the overall quality of the book is high and it will be an important resource to the modified nucleoside community. The book contains a number of excellent individual chapters that offer a new and interesting perspective on the field. Although some of the work has been previously reviewed, it is helpful to have a resource with numerous topics in one place. The range and diversity of topics will benefit many readers. In particular, I believe that this book will be an excellent resource for synthetic chemists looking for summaries of existing strategies to generate a wide range of modified nucleosides. Along that line, the more clinically based chapters provide good summaries of the biological activities of the modified nucleotides. There is a nice balance of older and newer literature that should be of use to established as well as novice researchers, and most of the chapters are well referenced and up-to-date. I would certainly recommend this book to anyone interested in the bioorganic and medicinal chemistry of modified nucleosides and nucleic acids.

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