

## Book Reviews \*

**Fractal Concepts in Surface Growth.** By A.-L. Barabási (IBM T.J. Watson Research Center, New York) and H. E. Stanley (Boston University). Cambridge University Press: New York. 1995. xx + 366 pp. \$27.95. ISBN 0-521-48318-2.

Fractal geometry has fueled a wealth of activity across a broad range of scientific disciplines. Of these applications, perhaps none are more fitting than in the area of growth phenomena. The goal of this book is to show how fractal concepts can be used to understand interface roughening that results from nonequilibrium processes. In a sense, this book marks the maturing of a field. Previous treatments in this area include the popular *Fractal Growth Phenomena* by Vicsek, and it is interesting to compare the two books. Vicsek's book is essentially a book about fractals and serves as a good introduction to these concepts. The present volume is about surface growth, and fractals are used as a mathematical tool to explore such phenomena. Also, the book by Vicsek is primarily concerned with growth phenomena that generate self-similar fractals. A broader class of fractals known as self-affine fractals is the focus of the Barabási-Stanley work. These fractals show a directional dependence to their morphology and are generally more applicable to surface growth phenomena.

This book is an excellent introductory text and could be used for advanced course work in a number of areas. It should be of interest to materials scientists, condensed matter physicists, and physical chemists working on surface phenomena. The first three introductory chapters cover basic concepts in scaling and fractals with emphasis on their relationship to surfaces. Chapters 4-8 provide a general theoretical background to the modeling of surface disorder. These chapters introduce the Kardar-Parisi-Zhang (KPZ) equation that provides the framework from which the scaling and renormalization approaches are hung. This equation will be used throughout the book in various guises. This section, also introduces computer modeling and demonstrates the utility of these simulations. For the uninitiated, parts of this section could be mathematically heavy going. However, this section of the text recaptures some of the effortless flow that marked Stanley's award winning *Introduction to Phase Transition and Critical Phenomena*. More difficult material is buried in appendixes at the end of the book. While some may find this annoying, it makes good pedagogical sense. The next section (Chapters 9-11) shows that new nonlinearities can arise in the KPZ equation when considering interfaces in random media. These effects result in different scaling laws and universality classes. While this is a nice progression from the previous section, the experimental topics are probably not of wide interest to chemists. The following and largest section, on the other hand, deals with molecular beam epitaxy (MBE) and should have a much stronger appeal to a chemical audience. This section nicely builds the complexity of the theory from linear to nonlinear to computer simulations. A direct connection with experiment is then made. Finally, a number of special topics are covered. One even sees some chemical kinetics in the discussion of aggregation and island formation in deposition. The final two sections of the book are of a more advanced and theoretical nature. The three chapter sections on noise (Chapters 21-23) will appeal to the theoretically inclined. Advanced topics, multifractal structures, variants of the KPZ equation, and directed polymers, are treated in three successive chapters. The book concludes with a summary chapter that brings together results and topics discussed in the book.

The strength of this book is that it links results from theory, computer simulation, and experiment in one unified exposition. It provides an excellent entree into this literature and will be a valuable aid for both teaching and research. I anticipate that this book will be cited long after its contemporaries are out of print.

T. Gregory Dewey, University of Denver

JA9552930

**Ketenes.** By Thomas T. Tidwell (University of Toronto). Wiley-Interscience: New York. 1995. xv + 665 pp. \$69.95. ISBN 0-471-57580-1.

*Ketenes* represents a major work on almost all aspects of this important class of synthetic intermediates. Not since Staudinger's

classic book *Die Ketene* published in 1912 has there been such an extensive coverage of this functional group, one that is of interest to theoreticians and physical organic as well as synthetic chemists. The coverage emphasizes the substituent effect on ketene reactivity which the author takes a special interest in having been responsible for the prediction of stable ketenes and bisketenes by theoretical calculations and eventually the synthesis of some of these for the first time. A brief introduction surveys the early history of ketene discovery. This is followed by an extensive coverage of the structure and thermochemistry of these derivatives based on both theoretical and experimental studies, the latter material being somewhat limited by the very few known stable ketenes which permit such examinations. The same comment applies to the section on spectroscopic data. Nevertheless, the essential characteristic spectral data of this functional group and evidence for its unique electronic structure are clearly pointed out. The most extensive coverage is found in the last three chapters on the preparation of ketenes, types of ketenes, and reactions of ketenes. There is some unavoidable overlap in the last two chapters. In the chapter detailing the types of ketenes which have been observed, the instability of many of these derivatives permits their observation only as secondary reaction products, reactions which are covered in the last chapter. The section on [2 + 2] cycloadditions is documented very effectively and exemplifies the cross-disciplinary approach involving theoretical, physical-chemical, and stereochemical product analysis in attempts to unravel this controversial mechanism. Although most of the references cited are from the 1970s and 1980s, the period regarded as the second "golden age" of ketene chemistry, citations from the older as well as the most recent literature (up to 1994) are also included. The illustrations, chemical structures, and tables are clear and concise. This book will be of interest to the general chemical community as well as to specialists in synthetic and physical organic chemistry. It is certainly a timely, well-written treatise and makes a valuable addition to any technical library.

E. Lee-Ruff, York University

JA9552331

**Packed Towers (In Processing and Environmental Technology).**

By Reinhart Billet (Ruhr University, Bochum, Germany). Translated by James W. Fullerton. VCH: Weinheim and New York. 1995. xvi + 382 pp. \$135.00. ISBN 3-527-28616-0.

This book is concerned with chemical processing in packed towers. Packed towers, especially for gas absorption, are a basic unit operation of the chemical process industry. They are used in diverse areas, like ammonia manufacture, ethylene production, and natural gas upgrading. Absorption in packed towers is the way in which sulfur oxides are removed from flue gas by reaction with aqueous amines. It is a very important process.

The basic process is simple to explain. The equipment fundamentally consists of a piece of pipe stood on its end and filled with some inert material which has a high surface area per volume. In many cases, this inert material looks like ceramic macaroni. Gas is pumped into the bottom of the column and comes out of the top. Liquid, poured into the top of the column, trickles over the inert material and flows out the bottom. Because the inert material or "packing" has a large surface area per volume, the contact between gas and liquid is intimate and gas adsorption occurs rapidly.

However, this basic process can be hard to analyze. The literature is dense and confusing and fits tightly into a sequence of engineering classes. Those who lack part of this sequence often have trouble understanding what is happening. Moreover, most undergraduate and graduate texts give a misleading simple description of the process. They ignore chemical reaction, which, for example, is basic to the absorption of sulfur dioxide. They downplay the constraints of fluid mechanics. While these texts are adequate as a superficial introduction, they are risky for design.

Other reliable books are thus required. For systems involving chemical reactions, the book *Gas Treating With Industrial Solvents* by Astartia *et al.* is the best source. However, for the constraints of fluid flow, no current book is successful. Some books on distillation, by

\*Unsigned book reviews are by the Book Review Editor.

Kister and by Strigle, are helpful but do not detail mass transfer. Traditional texts like Treybal are critically limited because the mass transfer correlations and tower packing discussed are 20 years out of date.

Billet's book fills this void. It is focused on packed towers for gas-liquid systems, although liquid-liquid systems are also discussed. Its emphasis is on the fluid mechanics and, in particular, on loading and flooding. It stresses modern packing. On the aspects of fluid mechanics, Billet's book is superb.

It seems more limited on aspects of mass transfer. Billet sensibly adapts the approach of Higbee and suggests mass transfer correlations roughly consistent with those used by other authors. (In the key Eq. 5.5, the exponent on the term including the diffusion coefficient should be one-half, not one-sixth.) Because he does not discuss why he has chosen Higbee, one must adopt his recommendations blindly. He ignores the effect of chemical reaction. On the other hand, Billet clearly intends his book to be largely used with existing pilot plant data, where differences between mass transfer correlations will be minor. For this purpose, this book fills a real need.

E. L. Cussler, *University of Minnesota*

JA9551906

### Heterocyclic Compounds. Volume 38. Isoquinolines. Part 3.

Edited by Gary M. Coppola and Herbert F. Schuster (East Hanover, New York). John Wiley: New York. 1995. xi + 552 pp. \$225.00. ISBN 0-471-62855-7.

Because the isoquinoline field is very large and includes many compounds of pharmaceutical interest, a four-part series of books was originally proposed to examine various facets of the chemistry of the isoquinolines. Part 1 was published in 1981 and Part 2 in 1990. Unforeseen circumstances and delays necessitated a reorganization of remaining chapters and has led to the present volume, Part 3, being issued as the final volume in this series. This volume is divided into two chapters describing the chemistry of two major groupings of isoquinolines: (1) those with basic-containing substituents in the side chain and (2) those possessing hydroxyl or thiol substituents.

Chapter 1, authored by Schuster and Kathawala, is 224 pages in length and focuses on isoquinolines and hydrogenated isoquinolines that possess side chains that contain basic functionalities that are not attached directly to the isoquinoline ring system. Motivation for design and synthesis of such compounds has been their potential pharmacological activity. Chapter 2, which reviews isoquinolinols and their hydrogenated derivatives, is 319 pages in length and was authored by Hara, Oshino, and Umezawa. Each chapter includes a detailed description of synthesis, reactions, properties, structures, physical data, and tables of structures with physical constants. Pharmacological data is included for some compounds along with some structure-activity relationship (SAR) correlations. Chapter 2 also includes 58 pages of tabulated compounds with their spectroscopic data. There is an 8-page index to the entire volume.

Although some effort was made to include additional references from the mid-1980s, only nine references date from 1985 and later of a total of 419 references of Chapter 1. Chapter 2 contains a total of 1083 references with only nine dated 1988 and later. Although the publication date is 1995, this book covers the literature of these classes of isoquinolines to the early or mid 1980s.

The text is well written and the illustrations are excellent. In short, the quality of the book measures up to our expectations for the series of monographs that comprise *The Chemistry of Heterocyclic Compounds*, published under the initial editorship of Arnold Weissberger. This volume, which rounds off the series on isoquinolines, will be welcomed by organic and medicinal chemists involved in isoquinoline research as a useful reference book for their institutional libraries.

Alice Jean Matuszak, *University of the Pacific*

JA955237N

**Quality Assurance in Analytical Chemistry.** Edited by W. Funk, V. Dammann, and G. Donnevert (Fachbereich Technisches Gesundheitswesen der Fachhochschule Giessen-Friedberg, Giessen, FRG). VCH: New York. 1995. xxii + 238 pp. \$80.00. ISBN 3-527-28668-3.

This book presents a unique, four-phase strategy for quality assurance in analytical chemistry. It describes all measures of quality assurance for analytical procedures from development of analytical procedure, to implementation in routine analysis, to internal and external quality control of a laboratory. Examples for the necessary statistical calculations are supplied as well as interpretations for quality parameters and statistical data.

JA9553314

### Immunoanalysis of Agrochemicals: Emerging Technologies.

Edited by Judd O. Nelson (University of Maryland), Alexander E. Karu (University of California-Berkeley), and Rosie B. Wong (American Cyanamid). American Chemical Society: Washington, DC. 1995. xi + 366 pp. \$99.95. ISBN 0-8412-3149-4.

ACS Symposium Series No. 586. Developed from a symposium sponsored by the Division of Agrochemicals at the 207th National Meeting of the American Chemical Society, San Diego, CA, March 13-17, 1994.

Discusses advances in antibody engineering and recognition of small molecules. Focuses on new basic and applied science in hapten and assay chemistry and formats. Explores developing methods that improve sensitivity, allow real-time repeated analyses, and allow multi-analyte analysis. Presents data validation guidelines and quality standards for immunoassay methods. Includes introductory chapter by Bruce D. Hammock and Shirley J. Gee.

JA955338L

### Fire and Polymers II: Materials and Tests for Hazard Prevention.

Edited by Gordon L. Nelson (Florida Institute of Technology). American Chemical Society: Washington, DC. 1995. x + 662 pp. \$129.95. ISBN 0-8412-3231-8.

ACS Symposium Series No. 599. Developed from a symposium sponsored by the Division of Polymeric Materials: Science and Engineering, Inc., at the 208th National Meeting of the American Chemical Society, Washington, DC, August 21-26, 1994.

Presents approaches to increasing the effectiveness of flame retardancy in polymers. Discusses non-halogen flame retardants, including phosphorus, metals, and metal compounds. Describes the use of char forming materials and the effects of surface changes on flammability. Provides a discussion on the state-of-the-art of smoke and toxicity issues. Reviews the latest tools and models for fire performance assessment. Examines regulation, corrosivity, recycling, environmental questions, and real scale performance assessment issues in the U.S. and Europe.

JA955332W

### Hybrid Organic-Inorganic Composites.

Edited by J. E. Mark (University of Cincinnati), C. Y.-C. Lee (U.S. Air Force), and P. A. Bianconi (Pennsylvania State University). American Chemical Society: Washington, DC. 1995. xi + 378 pp. \$109.95. ISBN 0-8412-3148-6.

ACS Symposium Series No. 585. Developed from a symposium sponsored by the Division of Polymeric Materials: Science and Engineering, Inc., at the 207th National Meeting of the American Chemical Society, San Diego, CA, March 13-17, 1994.

Presents novel research demonstrating some of the ways in which the unique properties of organic and inorganic materials can be synergistically combined. Discusses the development of composites with enhanced properties through the use of biomimicry and nanostructured materials. Examines the synthesis of composites with improved high-temperature stability and compounds with greatly increased resistance to impact failure. Looks at new materials offering increased electrical conductivity, nonlinear optical properties, and novel interfacial properties.

JA955334G

**Reduction of Nitrogen Oxide Emissions.** Edited by Umit S. Ozkan (Ohio State University), Sanjay K. Agarwal (Exxon Chemical Company) and George Marcelin (Altamira Instruments). American Chemical Society: Washington, DC. 1995. x + 237 pp. \$79.95. ISBN 0-8412-3150-8.

ACS Symposium Series No. 587. Developed from a symposium sponsored by the Division of Petroleum Chemistry, Inc., at the 207th National Meeting of the American Chemical Society, San Diego, CA, March 13–17, 1994.

Includes two overview chapters covering both technical and regulatory aspects of nitrogen oxide emissions from stationary sources. Discusses new directions in the field such as direct composition of NO<sub>x</sub>, different reducing agents, new catalytic materials, and two new noncatalytic techniques. Provides a thorough insight for the phenomena involved in existing technologies; offers a broad spectrum of studies tackling the problem of NO<sub>x</sub> reduction.

JA9553359

**Surfactant-Enhanced Subsurface Remediation: Emerging Technologies.** Edited by David A. Sabatini, Robert C. Knox, and Jeffrey H. Harwell (University of Oklahoma). American Chemical Society: Washington, DC. 1995. x + 300 pp. \$84.95. ISBN 0-8412-3225-3.

ACS Symposium Series No. 594. Developed from a symposium sponsored by the Division of Environmental Chemistry, Inc., and the Division of Colloid and Surface Chemistry at the 207th National Meeting of the American Chemical Society, San Diego, CA, March 13–17, 1994.

Provides a timely and thorough review of surfactant-based remediation technologies. Covers fundamental mechanistic studies to scale-up and process modeling and full-scale field implementation studies. Summarizes the technical, economic, and sociopolitical issues affecting widespread implementation of these technologies. Includes contributions from academic and industrial researchers as well as regulatory personnel.

JA955337T

**Flow-Induced Structure in Polymers.** Edited by Alan I. Nakatani (National Institute of Standards and Technology) and Mark D. Dadmun (University of Tennessee). American Chemical Society: Washington, DC. 1995. xii + 364 pp. \$99.95. ISBN 0-8412-3230-X.

ACS Symposium Series No. 597. Developed from a symposium sponsored by the Division of Polymeric Materials: Science and Engineering, Inc., at the 208th National Meeting of the American Chemical Society, Washington, DC, August 21–25, 1994.

Examines recent advances in understanding the structures of polymer melts, block copolymers, liquid crystalline polymers, colloid suspensions, and multiphase systems subjected to flow. Reports on advances in instrumental techniques, characterization, theories, and applications. Provides an overview chapter as a guide and reference source to related reviews and identifies similarities in flow behavior between various materials science disciplines.

JA955333O

**Peptide-Based Drug Design: Controlling Transport and Metabolism.** Edited by Michael D. Taylor (TSRL, Inc.) and Gordon L. Amidon (University of Michigan). American Chemical Society: Washington, DC. 1994. xviii + 567 pp. \$99.95. ISBN 0-8412-3058-7.

This ACS Professional Reference Book provides a framework for designing peptide-based therapeutic agents with improved transport and metabolism properties for optimal *in vivo* activity. Covers recent advances in molecular biology of transporters as well as what is more classically known about drug metabolism and drug transport of amino acids and peptides. Focuses on intestinal peptide transport, liver peptide transport, peptide delivery to the brain, peptide transport in microorganisms, and approaches to limiting peptide metabolism. Reviews the state of knowledge in the field and provides examples of how knowledge

of peptide transport was used to design strategies for improved delivery of specific classes of agents. Details experimental systems that can be used to evaluate transport and metabolism of peptide-based drugs.

JA955339D

**Theoretical and Computational Chemistry. Volume 1. Quantitative Treatment of Solute/Solvent Interactions.** Edited by P. Politzer and J. S. Murray (University of New Orleans). Elsevier: Amsterdam and New York. 1994. xi + 368 pp. \$228.50. ISBN 0-444-82054-X.

This book is concerned with theoretical methods for the prediction of the properties of organic molecules in solution. Each chapter is written by a different set of authors, who describe in some detail their own approach to the calculation of solvation interactions. While the chapters themselves are reasonably self-contained, there is a minimal amount of low-level introductory material; some degree of expertise is required from the reader to follow the presentations.

The first chapter, by Chris Cramer and Don Truhlar, describes their methods for computing solvation free energies using semiempirical quantum chemistry (e.g., AM1) combined with a version of the generalized Born model of Still and co-workers which treats the solvent as a dielectric continuum. The model has been extensively parametrized to experimental data on solvation free energies of a wide variety of small organic molecules and offers good predictive accuracy for these molecules at a modest computational cost. Applications to more complex systems such as sugars and nucleic acids are also presented.

Cramer and Truhlar's approach, while relying upon fitting to experimental data to achieve accuracy, is based upon a detailed molecular level description of the solute and a microscopic (although not molecular) model for the solvent. The remaining chapters in the book, in contrast, are principally concerned with the development of empirical models for physical properties in which simple functional forms are fit to large bodies of experimental results. These approaches include linear solvation energy relationships (LSER), linear free energy relations (LFER), quantitative structure–activity relations (QSAR), and general interaction properties function (GIPF). Some of the properties addressed by the methods are solvatochromatic shifts, pK<sub>a</sub>'s, hydrogen bonding strengths, solute partition coefficients for various pairs of gas, solid, and liquid phases, boiling points, heats of vaporization, and activity coefficients. Inputs into the predictor equations include both experimental data characterizing the solute and solvent and theoretical data, for example the electrostatic potential at the molecular surface as utilized by Murray and Politzer.

In general, these models display quite good performance, at minimal computational cost, for compounds that are structurally similar to some molecule in the data base used for parametrization. There is little discussion of the limitations of these approaches with regard to larger, more complex systems, nor is there consideration of self-consistent reaction field methods based on *ab initio* quantum chemistry or of approaches based upon molecular dynamics simulations. Thus, readers cannot expect to obtain a global perspective on how the empirical models fit into the entire spectrum of computational approaches to molecular solvation.

Overall, this is a very useful book for learning about empirical approaches to the calculation of the physical properties of molecules in solution. The articles are in general clear and well written, and substantial comparisons of theory and experiment are presented by the developers of each method so that the reader can make an intelligent evaluation of the value of the approach for his or her problem. The references are current and relevant and will serve to provide detailed descriptions of the various approaches should the reader wish to obtain a more in depth understanding.

Richard A. Friesner, Columbia University

JA955133C

**Regulation and Control of Complex Biological Processes by Biotransformation—Frontiers in Biotransformation, Volume 9.** Edited by Klaus Ruckpaul and Horst Rein (Max-Delbrück-Centrum, Berlin). VCH: New York. 1994. x + 253 pp. \$135.00. ISBN 3-05-501367-0.

*Regulation and Control of Complex Biological Processes by Biotransformation* is the last in a nine-volume treatise, *Frontiers in Biotransformation*. Its 245 pages comprise seven chapters with selected material pertaining to the regulation of renin, P-glycoprotein, and phase I and phase II drug metabolizing enzyme systems. The general aim of the book seems to be to illustrate the complex nature that the regulation of homeostatic processes can take by the presentation of current research for selected proteins and enzymes with, in some cases, unrelated *in vivo* function.

In Chapter 1, there is a thorough summary of current knowledge about the complex molecular mechanisms of renin regulation. It is carefully crafted to impart an understanding of key points for the control of renin biosynthesis and other enzymes of the angiotensin system. To this reviewer, a most welcome aspect of the chapter was the inclusion of a clear and measured interpretation of various experimental approaches taken by investigators in the field to elucidate the relevant mechanisms of regulation. Study designs presented include quantitative analysis of mRNA in animal and human tissues and more elaborate experiments with transfected cells and transgenic animals. The authors of Chapters 4 and 5 provide an excellent overview of the status of P-glycoprotein research that includes both molecular control of gene regulation and a complementary discussion of clinical relevance and challenges for anti-tumor chemotherapy. Again, a lucid presentation of technical data and extensive reference lists make these chapters a good starting point for the novice as well as valuable reference material for the more knowledgeable investigator.

The remaining four chapters of the book are devoted to the regulation of one or more enzymes of drug metabolism, principally, the cytochromes P450. The scope of each chapter is variable. The authors of Chapters 2 and 3 explore molecular aspects of CYP2B1/2 and CYP1A1 gene regulation, respectively. The review of CYP1A regulation has been restricted intentionally to investigations to elucidate Ah receptor binding domains of the CYP1A1 and CYP1A2 genes and identification of potential sites for other constitutively expressed binding proteins that may exert repressive or enhancing effects on CYP1A1 gene transcription. There is a more limited discussion of probable points of CYP1A regulation at the level of the cytosolic Ah receptor, with additional references for the interested reader. Because of the relative paucity of significant advances in our understanding of the molecular mechanism of P450 induction by phenobarbital-like compounds, in contrast to the TCDD inducible CYP1A genes, Chapter 2 is understandably less definitive in its content. Further, the presentation is also almost completely restricted to rat CYP2B and CYP2C gene expression and does not acknowledge or address known or suspected human phenobarbital inducible P450 enzymes, CYP3A4, CYP3A7, CYP2C, CYP2A6, and CYP2B6. However, the authors do provide a good synopsis of avenues of active investigation: identification of nuclear binding proteins, gene regulatory domains, the search for a phenobarbital receptor, and the involvement of endocrine hormones as constitutive modulators of gene expression.

Moving away from mechanisms of control of gene expression, Chapter 6 provides a very thorough review of most enzymes of biotransformation (phase I and phase II) that can be found in the developing fetus and neonate. There are several excellent well-referenced tables that summarize the current literature available for rodent and primate species which make this a worthwhile read for the interested investigator. The same can be said for Chapter 7, a summary of the clinical impact of genetically based, polymorphic expression of human drug metabolizing enzymes (i.e., CYP2D6, CYP2C<sub>meph</sub>, and NAT). The authors do not attempt to present the well-studied molecular aspects of genetic polymorphism; instead they focus on the presentation of classes of drugs in which metabolic disposition and efficacy *in vivo* can be compromised by the presence of polymorphic gene expression in the human population. Their discussion centers around case reports and retrospective and prospective studies that correlate readily observed inter-individual differences in drug effect with genetic differences in metabolic enzyme expression. For the administration of a drug racemate, the added complexity of pharmacologic and metabolic differences of each enantiomer is also discussed.

In summary, this compendium provides technical information and an intellectual perspective on a number of important topics that should be of interest to bioscientists. However, the limited size of the book and wide diversity of topics presented probably do not warrant its purchase for the personal library. Volume 9 represents a good addition to the *Frontiers in Biotransformation* series. For those interested in

one or more of its topics, it and its companion volumes should be found at a university or regional library.

Kenneth E. Thummel, *University of Washington*

JA955146Q

**Spectroscopy of Molecular Rotation in Gases and Liquids.** By A. I. Burshtein (Weizmann Institute of Science, Israel) and S. I. Temkin (Institute of Chemical Kinetics and Combustion, Russian Academy of Science). Cambridge: Cambridge, U.K. 1994. 294 pp. \$64.95. ISBN 0-521-45465-4.

This monograph addresses the theoretical description of molecular motions of simple molecules in liquid and dense gaseous phases and the experimental characterization of such motions, principally through line-shape measurements in optical (Raman and IR) spectra and in Brillouin scattering experiments. While the subject is of somewhat limited scope, the treatment is authoritative, comprehensive, and well organized. The monograph is intended for the research specialist and for graduate students entering the field, for whom it is likely to be of seminal importance.

The central theoretical problem here is the calculation of the molecular time correlation functions which describe the ensemble-averaged reorientational motions (Brownian motions) of molecules in fluid phases. Simple theories for the limiting physical cases of gases at low densities and for diffusive molecular motions in classical liquids have been known for many decades, as for example, Debye's theory describing reorientational motion of polar molecules in liquids, which dates from 1924. The intermediate regime is much more complex and less well understood. In passing from gas to liquid phase the nature of reorientational motions changes qualitatively. In the former, the rotational motion of essentially free rotors is interrupted by sudden intermolecular impacts, while in the latter, molecular reorientation is diffusive, i.e., the molecule-fixed coordinate frame reorients much more slowly than does the angular momentum vector. Also important in dense phases is the physical character of molecular collisions, which are not necessarily "sudden" but rather may have durations comparable to a free path. The theory of Brownian motions in phases of intermediate density is developed in a comprehensive and rigorous fashion in Chapter 1, culminating in general integral expressions for the time correlation functions of the molecule-fixed coordinate axes, for the molecular angular momentum vector, and for intermolecular torques. Specific applications of these general expressions to the analysis of spectroscopic data require the use of appropriate simplifying physical models, the more widely used of which are described in some detail in the remainder of the text. The theoretical development is complemented by a discussion of selected experimental data taken principally from Raman and IR spectroscopy and from Brillouin scattering experiments. Also discussed are recent molecular dynamics calculations, which provide a uniquely detailed source of "data" for the test of theory in this field. The text is well referenced from the 1950s to the present.

The authors disclaim practical applications of their topic and present the subject entirely from an academic standpoint. It is perhaps worth pointing out, however, that supercritical phases of intermediate density are finding an increasingly important niche in chemical catalysis and in chromatographic separations. The neighborhood of the critical point is a region of very rapid and continuous change in density that is accompanied by dramatic and fascinating variations in chemical properties (e.g., in solvent polarity, dielectric constant, solvation number, molecular clustering, etc.). It seems reasonable to hope that the theory and experimental techniques described by Burshtein and Temkin will ultimately contribute to our understanding of molecular dynamics and chemical processes in these more complex systems. In any event, the authors are to be congratulated on having produced an excellent monograph for research workers in one of the more abstruse and difficult areas of physical chemistry.

Robert R. Sharp, *The University of Michigan*

JA945115F

**HPLC. A Practical User's Guide.** By Marvin C. McMaster (University of Missouri—St. Louis). VCH: New York. 1994. xiv + 340 pp. \$55.00. ISBN 1-56081-636-8.

Overall the book has useful information for a beginning chromatographer. It is presented in a very informal manner that is easy to read without feeling intimidated by the material, as some scientific texts make the reader feel.

The dates on the reference list are certainly not recent, but the technology behind HPLC is not new either. Pumps and hardware have not changed significantly in the past 10 or 15 years. New advances are made most often in detectors and data handling. The author discusses both of these areas adequately.

The author's apprehension toward using computer-based data acquisition systems is strongly conveyed to the reader. I believe it is not completely founded. Computer costs are constantly dropping, and software continues to be developed. The reader should decide for himself whether an integrator or computer will meet his needs, and which he is comfortable working with. This discussion should be presented less as a personal opinion and in a more informational context.

A cost analysis is out of place in this book. If a reader is thinking about buying an HPLC, she can definitely use this book as a guideline for choosing the instrument components that correspond to her application. A relative cost factor may be useful, but an absolute dollar value or even a dollar range will probably be out of date before the book goes to print. Let buyers talk to distributors about absolute costs; they will quickly find out what is within their budget.

Finally, someone must *edit* the text. Spelling errors abound, as do misuses of past and present text and pluralization where it should not be. These mistakes detract from the flow of the book. Also, some of the figures look very cluttered, especially those with great detail such as the mass spectrometer figures. They might be better represented in figures with more resolution and depth. I only point these out because it takes the reader's mind off of what is being presented.

The book as a whole contains very useful information for the beginner. An experienced chromatographer, trying to realize more of the capability of an existing HPLC system, might turn to this book when researching new applications. However, I believe the information discussed is basic in nature and may not be useful in that instance.

Martin L. Spartz, *Central Michigan University*

JA9450566

**Surface Electron Transfer Processes.** By R. J. Dwayne Miller (University of Rochester), George L. McLendon (University of Rochester), Arthur J. Nozik (National Renewable Energy Laboratory), Wolfgang Schmickler (Universitat Ulm), and Frank Willig (Frits-Haber-Institut der Max-Planck-Gesellschaft). VCH Publishers: New York, Weinheim, and United Kingdom. 1995. viii + 370 pp. \$79.95. ISBN 1-56081-036-X.

This book will be most valuable to fairly advanced scientists (graduate school and beyond) who are interested in fundamental aspects of electrochemistry and photoelectrochemistry. The overall organization and continuity are excellent. As stated in the preface, the book is tutorial in nature rather than a collection of specialized reviews. For readers who are not familiar with basic concepts of electron transfer theory, properties of solids, and electrochemistry, Chapters 1 (Miller) and 2 (Nozik) provide the background material on these topics that is necessary for understanding the more in-depth topics that follow. In general, terminology introduced in these chapters is utilized throughout.

Chapter 3 (Schmickler) is a review of electron transfer theory at metal electrodes that includes a discussion of selected experimental results. It is a useful compliment to reviews on this topic by other authors. Chapters 4 and 5 are the strongest features of the book. Chapter 4 (Miller, 65 pages) is an in-depth discussion of electron transfer between solids and molecular states. A variety of key experiments involving homogeneous and heterogeneous systems are discussed within the theoretical framework developed in earlier chapters. Of particular importance is inclusion of pertinent results from the solid-state physics community. Chapter 5 (Willig, 135 pages) is the most thorough discussion of electron transfer involving adsorbed dyes molecules that I have encountered. Many nuances related to the interpretation of time-resolved experiments are considered as well as the implications of these results to photography and efficient photoelectrochemical cells. Chapter 7 (McLendon and Nozik) is an introduction to the emerging field of electron transfer in size-quantized systems. The somewhat controversial issue of hot electron transfer

processes is considered in Chapters 4 and 6. All chapters contain useful references through 1993.

Carl A. Koval, *University of Colorado*

JA9552048

**Clean Technology and the Environment.** Edited by R. C. Kirkwood (University of Strathclyde, Glasgow) and A. J. Longley (English & Physical Science Research Council, Swindon). Blackie Academic: London. 1995. xiv + 350 pp. \$129.95. ISBN 0-7514-0037-8.

The editors have compiled a volume of 11 chapters by 16 contributors which objectively presents the complex and serious issues of environmental pollution. This volume moves beyond recycling and landfill agendas and deals with the comprehensive issue of sustainable production of the goods and services our society expects. Realistic proposals utilizing clean technology are made which would allow effective and efficient use of resources. However, government involvement is critical to ensure long-term planning and a total cost rather than production cost analysis. The contributors provide the analysis which demonstrates that it is ultimately unwise to ignore environmental pollution on both ecological and economic grounds. This should be used effectively in countering short-sighted "cost-benefit analysis" which has been wielded to excuse environmental contamination.

Chapter 1 is essentially an introduction to environmental concepts and the problems of environmental pollution. It provides an overview of the text. Chapters 2, 3, and 4 describe air, water, and soil pollution and various means addressing the problems. Chapter 2 presents a comprehensive picture of types of atmospheric pollutants and their sources. The mechanisms by which atmospheric pollutants have global impact as well as the specific impact are described of certain pollutants. Methods to cope with this are discussed both in terms of the technology available and national and international regulation.

Chapter 3 summarizes the state of water pollution and presents a concise picture of the environmental consequences of fouling waters whether it be directly by organic waste or industrial discharge or indirectly by contamination of the soil or air. Control of this pollution is largely dependent upon regulation of discharges.

Chapter 4 is a rather encouraging chapter in that there are clearly existing methods of cleaning already fouled sites as well as means of reducing further pollution. Bioremediation is the use of organisms to reduce or eliminate pollutants. Several types of bioremediation are discussed with respect to cleaning contaminated soil and ground water. The advantages and disadvantages of these methods are discussed as are the circumstances in which they are most appropriate.

Although each of these chapters is written by different authors, together they present a picture of the interrelated nature of our environment. From these chapters a compelling argument can be made that both regulation of the amount of waste discharged and technology to neutralize waste are required.

Chapters 5 and 6 focus on the importance of viewing pollution in a comprehensive context. Chapter 5 is an introduction to the application of economics to pollution. This provides some insights to the complexities of determining the real cost of a pollutant that must be borne by society. Chapter 6 continues the theme of total cost and introduces "clean technology". This urges consideration of the total cycle of providing a service or product from its manufacture to its ultimate disposal.

The remainder of the text centers on specific examples of clean technology. Chapters 7, 8, and 9 detail specific examples of the technologies in agriculture and pharmaceuticals, plastics, and the food industries. Chapter 10 is the chemist's chapter. Here a number of methods are explored for cleaner synthetic processes. Chapter 11 provides an excellent final chapter in that the central issue of energy is explored. It makes a clear case for the ultimate need for efficient and sustainable energy sources.

The theme which emerges is that society must come to terms with its profound impact on the environment. Methods to deal with this problem already exist, and additional methods are under development. There must be a multifaceted approach: regulation, reduction of wastes, cleanup of existing pollutants. Environmental pollution is complex in that fouling either air, water, or soil potentially contaminates the others. Furthermore, the total impact of industrial products must be considered

from production to disposal. Economics can be presented as a powerful incentive favoring clean technology.

This book is quite readable and should be of interest to anyone concerned with environmental issues. There are sections which detail government policies or specific technologies which are rather dry for the casual reader, but which should make it quite useful as a reference book.

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**Modern Density Functional Theory: A Tool for Chemistry.** Edited by J. M. Seminario and P. Politzer (University of New Orleans, Louisiana). Elsevier: Amsterdam, 1995. xi + 405 pp. \$235.25. ISBN 0-444-82171-6.

Modern density-functional theory (dft) is a useful tool for chemistry, and so another good book on this subject is welcome. This book is good. It is unusually well organized and well referenced for an edited volume.

Just a few years ago one might have thought that the understanding of molecular electronic structure was becoming a closed subject. It seemed to be a matter of directing an appropriate computer program to generate whatever you wanted to know about a molecule of interest. The situation in fact was not so rosy, however. The calculations were terribly consuming of computer capacity and could not be taken to truly large molecules. Furthermore, a computer output of itself does not constitute or easily provide simple understandings transferrable from molecule to molecule.

The advent of the density-functional method for describing electronic structure changed all this. Accurate calculations on very large molecules have become possible, and the density-functional language appears to be uniquely suitable for qualitative description of molecular electronic structure and chemical reactivity. The aptness of dft is due to the fact that the basic descriptor in the theory is the single-particle electron density instead of the many-particle wave function. The subject is awkward to penetrate, as much as anything because of the surprise element in it for those with conventional training in quantum chemistry. The first single-authored text appeared in 1989; now there are three. A dozen or so edited multiauthored books have appeared. This book of Seminario and Politzer is one of the best of the edited volumes.

Seminario and Politzer have done a careful job of putting together in a disciplined way a coherent presentation of contemporary dft. Seminario is to be particularly complimented for writing an excellent 74-page introduction and coauthoring two other chapters. Otherwise, the authors mostly are leaders in the field and write well. The emphasis is on the computational applications of the method, not the conceptual implications of the subject.

There are 12 chapters, with topics and authors as follows: introduction (Seminario), semilocal functionals for exchange and correlation (Burke, Perdew, and Levy), local scaling version (Ludena, Kryachko, Koga, López-Boada, Hinze, Maldonado, and Valderrama), large molecules via divide and conquer (Zhou), symmetry and exchange and correlation (Dunlap), efficient methodologies (Johnson), D. Mol review and advances (Delley), transition states and reaction pathways for isomerization reactions (Abashkin, Russo, Sicilia, and Tuscano), NMR and ESR parameters (Malkin, Malkina, Eriksson, and Salahub), transition metal oxides (Broclawik), decomposition processes of

energetic molecules (Politzer, Seminario, and Grice), further applications (Balbuena and Seminario). There follows a three-page subject index.

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JA955184+

**Ion Chromatography, 2nd Edition.** By Joachim Weiss (Dionex GmbH). VCH: Weinheim, Germany, 1995. xi + 463 pp. DM164.00. ISBN 3-527-28698-5.

This book describes in a rigorous but readable manner the fundamental ion chromatography (IC) research done not only in academics but also in industry with over 400 reference citations. Although the author of this book is affiliated with Dionex, the coverage of IC is quite balanced and objective. Both nonsuppressed as well as suppressed IC are discussed with a major emphasis as expected toward anions. Detection techniques other than conductivity such as spectroscopic, electrochemical, and indirect methods are reviewed. Although the evolution of stationary phases (latex agglomerated materials) by Dionex is probably treated more completely, other nonpolymeric ion exchange materials such as silica-based supports are discussed. Several topics are explained in more detail than what is normally found in most books. For example, the mechanism of the chloromethylation reaction of polystyrene-divinylbenzene using formaldehyde and HCl in the presence of an acid catalyst is given. In addition, the theory of electrochemical detection (both conductivity and amperometry) is rigorously treated. Besides the necessary treatment of anion and cation exchange chromatography, two other types of HPLC for ionic substances are included. A separate chapter on ion exclusion chromatography although short is clearly written with respect to retention mechanism, and applications pertaining to amino acids as well as organic acids are shown. The major chapter on ion-pair chromatography is unusual since often this subject is only extensively considered in HPLC books emphasizing reversed phase chromatography. A thorough treatment of the various proposed retention mechanisms is given and chromatograms of both surface inactive ions (inorganics and drugs) and surface active anions (surfactants) are given.

This book is not intended to be a textbook for those interested in learning the basics of chromatography. Although the thermodynamic aspects of IC are covered, the chapter on the theory of chromatography only briefly outlines column efficiency. The short chapter on quantitative analysis and statistics is really not needed in this book and is a subject more appropriately covered in a standard analytical chemistry textbook. It would of been nice if more attention had been directed toward sample pretreatment and particularly instrumental troubleshooting. Certainly the variety of separation problems that have been solved by IC is a major emphasis (about 20%) of this book. Numerous chromatograms based on environmental analysis, clinical chemistry, and chemical industry such as detergents, food and beverage, and pharmaceuticals are included. Besides examples of chromatograms showing inorganic anions and cations, stronger than usual emphasis of ion chromatography for polyvalent anions (i.e., polyphosphates) and carbohydrates is noted. Although very few references are from the 1990s, this did not seem to be a major problem since IC is quite a mature field. This book is an excellent reference for someone starting out or practicing IC, particularly in the suppressed mode.

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