

## Book Reviews

**Determination of Trace Elements.** Edited by Zeev B. Alfassi (Ben Gurion University). VCH: Weinheim, 1994. xiv + 608 pp. \$165.00. ISBN 3-527-28424-9.

This book has 13 chapters, each written by an expert in the area covered by the chapter. Chapters 1–4 cover the background involved in trace analysis, i.e., error analysis; limits of detection; sample and sample preparation; and preconcentration techniques. Chapters 5–11 discuss specific instruments used in trace analysis. They are atomic absorption; plasma optical emission and mass spectrometry; instrumental neutron activation analysis; radiochemical neutron activation analysis; electron spectroscopic methods; and electrochemical methods and chromatographic methods using atomic plasma emission and radioanalytical methods. The last two chapters discuss speciation of trace metals and trace metals in the environment and health sciences. The bibliographies at the end of the chapters range from 21 references on AAS to 433 on radioanalytical methods. For the most part the references are from 1992 or older.

This book would be useful to those people who are just starting work in the field or who would like to examine the various techniques available in the field. The first four chapters are particularly useful. There are some interesting discussions on the types of problems encountered in trying to do trace analysis work. The effect of different types of glassware on the results and the handling of samples are very important chapters for beginners. Chapters 5–11 give a limited perspective of various analytical techniques and in most cases the limits of detection of the various elements analyzed by each technique. The emphasis in the chapters is on the nature of the instruments used in the analysis more than a comparison of the different techniques. The approach is a survey of the field and not depth in any particular area. There are references though as to where to get further information in a particular area.

Because of the cost and other problems listed below, I cannot recommend the book as a part of one's library. The book is too expensive to be used as a textbook, and what appears to be a translation problem for some of the chapters leads to stilted and complex sentences. For instance p 18 says, "Alarming is not the real value of the blank of one single step but the fact that blanks occur even during very simple operations and accumulate during the whole analytical procedure to amounts in the ng/g range". There are also typos throughout the book, some chapters have many more than others. For instance, p 24 lists nitric acid as  $\text{NHO}_3$ ; p 159 "simpl" for simple; p 168 "lame" for flame; and p 190 "atoic" for atomic.

The last two chapters are interesting, but the references date from 1992 or older and are of limited use.

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**From Chemical Topology to Three-Dimensional Geometry: Topics in Applied Chemistry Series.** Edited by Alexandru T. Balaban (Polytechnic University, Bucharest, Romania). Plenum Press: New York, 1997. xxiii + 420 pp. \$125.00. ISBN 0-306-45462-9.

The aim of this book is to provide the reader with an up-to-date account of how one can provide mathematically nonsophisticated molecular descriptors encompassing three-dimensional aspects of molecules. The advantages of such descriptors are an easy intuitive grasp of their significance, the possibility to compute them for any imaginable structure, and their power to be used in structure–activity studies (QSAR) and in molecular modeling for drug design. This book thus focuses on mathematical methods, including topological ones, for taking into account the third dimension of the chemical world. The contributors to this book are the leaders in the field, who are personally responsible for having made significant advances in their respective areas.

The first four chapters and Chapter 6 are concerned with three-dimensional molecular descriptors and their use for QSAR and molecular similarity studies associated with molecular modeling of

agonist–receptor interactions, with drug design, and with the discovery of new lead compounds for various types of biological activities. These include chapters entitled From Chemical Graphs to 3D Molecular Modeling (Balaban), Descriptors of Molecular Shape in 3D (Mezey), 3D Molecular Design: Searching for Active Conformers in QSAR (Mekeny and Veith), Use of Graph-Theoretic and Geometrical Molecular Descriptors in Structure-Activity Relationships (Basak, Grunwald, and Niemi), and On Characterization of 3D Molecular Structure (Randić and Razingar). Chapter 5 (Recognition of Membrane Protein Structure from Amino Acid Sequence by Lučić, Trinajstić, and Juretić) discusses problems associated with the poorly understood correlation between the primary structure of proteins which determine their biological activities.

Chapters 7–9 discuss topological methods applied to the area of fullerenes and congeneric structures, some of which have not yet been obtained experimentally, but which are predicted to be as stable as fullerenes. These chapters include Chemical Graph Theory of Fullerenes (Fowler), Recent Work on Toroidal and Other Exotic Fullerene Structures (Kirby), and All-Conjugated Carbon Species (Klein and Zhu). The final chapter (Applications of Topology and Graph Theory in Understanding Inorganic Molecules by King) is dedicated to the application of graph theory to polyhedral boranes, metal carbonyl clusters, coinage metal clusters, post-transition element clusters, and polyoxometalates.

This book provides an excellent view of the current status of the use of mathematical methods to study the three-dimensional aspects of chemical structure and properties. The combination of fundamental and applied research in the chapters in this book will make it especially valuable to its intended audience, namely graduate students and research scientists of various profiles (chemists, biochemists, medicinal chemists, mathematicians, and statisticians) who are interested in molecular modeling, in fullerene research, in drug design, and in modern mathematical chemistry.

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**Advances in Chemical Physics, Volume XCVI.** Edited by I. Progogine (The University of Texas at Austin) and Stuart A. Rice (The University of Chicago). Wiley: New York, 1996. ix + 330 pp. \$125.00. ISBN 0-471-15652-3.

Volume 96 of the venerable *Advances in Chemical Physics* continues to deliver the high impact, up-to-date and expert's summary type of articles it has been known for. I read through the whole monograph in the order closest to my chemical physics experience. First was Winstead and McKoy's article on electron scattering by small molecules and Lester's piece on vibrational predissociation dynamics of van der Waals complexes. Then I ventured into Sepulveda and Grossman's article on time-dependent semiclassical mechanics and, finally, Gordon and Hall's paper on applications of Doppler spectroscopy to photofragmentation.

Winstead and McKoy pick up from the classic review of Lane published in 1980 of low-energy electron-molecule scattering with their goal of describing the current state of the field. This they accomplish very well. The authors focus on the few groups engaged in theoretical studies of electron-molecule scattering, in particular the Livermore group and their own group at JPL/Caltech. I found their comparison of theoretical calculations and experimental cross sections very informative. For one, all comparisons are done consistently with the same units ( $10^{16} \text{ cm}^2$ ) and on a linear scale. It would be particularly annoying if we had to view 100 different cross section plots and some are in linear scales while others are in logarithmic scales! Winstead and McKoy has done the electron scattering community a good service. My only wish is that the cross section data for the next 100 molecules be plotted in similar fashion. Extensive discussion also exists on the Schwinger Multichannel Method (SMC) for electron-molecule scattering. In particular, the authors describe very recent developments in parallelizing their computer codes using the distributed-memory,

multiple-instruction, multiple-data design. Overall, the electronically elastic and inelastic cross sections for about 20 molecules are reported ranging from  $\text{CH}_4$  to  $\text{Si}_2\text{H}_6$ . This review has 248 references.

Marsha Lester starts her review of the dynamics of van der Waals (vdW) complexes by pointing out the scientific rationale for these types of experiments. In general, the dissociation dynamics of vdW complexes are nonstatistical due to the small number of states involved. Furthermore, the binding of the constituent monomers are relatively weak and require only IR photons which are sufficient to provide one vibrational quanta of energy—just enough to break the bond. The main mechanisms for dissociating vdW complexes are therefore: vibrational predissociation and internal rotation predissociation. For example, energy transfer between vibrational excitation and translational motion along the vdW bond leads to breakage of the chemical bond. Unraveling the dynamics involves careful study of the rotationally resolved absorption spectrum and lifetimes (i.e., line widths) of the vdW complexes as well as the final state distribution of the product molecules. Clearly, this will involve a concerted joint effort by experimentalists and theoreticians. The former provide insights into the magnitudes of the coupling terms whereas the latter provide the accurate potential energy surfaces. This review has 107 references.

Sepulveda and Grossman provide a very readable introduction to semiclassical approximations to the time dependent Schrodinger equation. The authors use a subtle change of wording: time-dependent semiclassical mechanics. But apart from this semantic detail, the article draws effortlessly from Wentzel–Keller–Brillouin (WKB) theory, to Maslov, to Gutzwiller, and finally to Heller all in 114 pages! The length is justified considering the care the authors took in collecting a set of equations with consistent notation that is readable to an average experimentalist. For this Sepulveda and Grossman can be forgiven for not showing a single experimental spectrum. What they do show are several comparisons of theoretical spectra calculated using quantum mechanics and using semiclassical methods of various kinds (Gaussian wavepacket dynamics and cellular dynamics). These comparisons not only provide inexpensive numerical methods for obtaining quantum properties in the time domain but more importantly provide insight into the correspondence between classical and quantum mechanics. This review has 106 references.

Gordon and Hall's review of Doppler spectroscopy starts from Zare and Herschbach's original suggestion in 1963 that the angular distribution of atomic fragments resulting from diatomic photodissociation can be derived from the Doppler line shape. Much of the recent developments have been in extending this to molecular fragments in which case the theoretical interpretations become nontrivial. For molecular fragments, the rotational polarization of the fragments and its correlation with recoil velocity become important. Just as the dissociation (pump) photon pulse is sensitive to the original molecule's transition dipole, the probe photon pulse is also sensitive to the molecular fragment transition dipole. Gordon and Hall collect the relevant mathematical tools to make Doppler profile analysis a central field of study rather than simply being a "spectroscopist's tool". This review has 94 references.

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**The Chemistry of Free Radical Polymerization.** By Graeme Moad (CSIRO, Division of Chemicals and Polymers) and David H. Solomon (University of Melbourne). Elsevier: Oxford, U.K., 1995. xvi + 408 pp. \$120.00. ISBN 0-08-042078-8.

The development of new techniques over the past quarter century has allowed the determination of reaction mechanisms and polymer structure in ever more detail. This has resulted in the revision of the early simple notion that initiation and propagation proceed almost exclusively by addition of radicals to the less substituted (tail) end of the double bond of a monomer molecule. Abstraction, head addition to the double bond, chain transfer, and intramolecular atom transfer are more prevalent than originally thought. These processes have a considerable effect on polymer properties.

This book reviews the advances in our knowledge of all aspects of free radical polymerization from initial concepts to the most recent developments. Emphasis is on the mechanism of each stage of the polymerization process: initiation, propagation, and termination. A

brief introductory chapter is followed by a short chapter on free radical reactions featuring those involved in free radical polymerization: addition to double bonds, atom transfer, and radical–radical reactions. Initiation, propagation, and termination are treated in a very comprehensive way in the three ensuing chapters, as are the techniques used in determination of the mechanisms of these reactions. The sixth chapter discusses copolymerization, and the final chapter, utilizing the material presented previously, describes how to control the polymerization process to produce polymers with predetermined characteristics.

The book is clearly written with very few errors. The literature is covered to early 1995; about 25% of the references are after 1990. There is a very good index. This is an excellent source of information and should be on the desk of everyone involved in the field. Together with supplemental material, this would be a good text for a course in polymer chemistry.

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**Modern Aspects of Electrochemistry, No. 29.** Edited by J. O'M. Bockris (Texas A&M University), B. E. Conway (University of Ottawa), and R. E. White (University of South Carolina). Plenum Press: New York, 1996. xi + 490 pp. \$110.00. ISBN 0-306-45162-X.

This collection of five review chapters on diverse aspects of interfacial electrochemistry and related disciplines follows the general pattern seen in earlier volumes of this long-established review series. Since the publication of the first (and now classic) volume in 1954, this series has contributed importantly, although decidedly unevenly, to the review literature in electrochemical science. A variable quality of the review chapters is also evident in the present volume. The first chapter (by D. B. Sepa) is concerned with the much-discussed issue of the meaning and significance of activation energies in electrochemical kinetics. In the reviewer's opinion, this topic has been subjected to more than its share of confused (and confusing) essays over the years. Unfortunately, the present review, although detailed and apparently thoughtful, adds little to clarify the fundamental significance of electrochemical activation parameters. Rather, it conveys (and possibly perpetuates) the impression that such quantities are intrinsically complex and ambiguous to interpret, which they are not.

The second chapter (by C. G. Vayenas et al.) reviews at great length the extensive research by this group and others into the intriguing phenomenon of "electrochemical activation" of heterogeneous catalytic processes at solid–gas interfaces. This so-called "NEMCA" effect ("non-Faradaic electrochemical modification of catalytic activity") usually utilizes solid electrolyte–metal junctions to alter the surface potential,  $\Delta V_m$ , of the latter metal–gas interface. Substantial changes in catalyst performance are often seen upon altering  $\Delta V_m$  in this fashion. The findings are well-known to the gas-phase heterogeneous catalysis community; the appearance of the present review is especially welcome in view of the relevance of the phenomenon (or phenomena) to electrochemical science. This electrochemist reviewer, however, is concerned that seemingly inadequate attention has been given to the interpretation of the intriguing catalytic effects. The "matter-of-fact" assertion by Vayenas et al. that "NEMCA" is due to potential-induced variations in chemisorbate bonding seem unproven and possibly quite inadequate.

The third review (by I.-H. Plonski) considers the interpretation of electrochemical measurements of ion dissolution in acidic media in terms of adsorptive factors. Although restricted to conventional electrochemical results, and thereby giving little attention to recent findings with microscopic-level techniques, the review is a useful contribution to an important area. The fourth chapter (by S. G. Roscoe) provides a detailed assessment of recent results from various optical spectroscopic, microscopic, and other methods toward understanding the behavior of proteins at electrochemical and related interfaces. The reviewer appears to have been thorough in covering this somewhat diffuse yet important topic. The last chapter (by R. Woods) discusses the nature of chemisorption of thiols on metals and metal sulfide surfaces. The review appears to be a good survey of work involving the latter type of interfaces. However, discussion of the very well-publicized area of thiol adsorption on metals, especially monocrystalline

gold surfaces, is remarkably incomplete, omitting references to numerous important recent studies regarding chemical applications as well as the structure of thiol films.

Overall, then, the flaws in presentation and scholarship that are evident in the present volume detract significantly from its usefulness as a review/reference source. Nonetheless, most libraries will (and should) continue to subscribe to this significant review series, reflecting its continuing value to electrochemical science.

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**Principles and Practice of Heterogeneous Catalysis.** By J. M. Thomas (University of Cambridge) and W. J. Thomas (University of Bath). VCH: Weinheim, 1997. xxiii + 669 pp. DM88.00. ISBN 3-527-29239-X.

The eight chapters of this excellent book reflect a good portion of the modern heterogeneous catalysis principles, techniques, and applications. The material covered by the authors will constitute a stimulating reference source for a broad audience such as industrial and academic researchers and chemical engineering and chemistry graduate students. This book is also perfectly suitable as required reading in graduate heterogeneous catalysis courses, given the many interesting "standard" and "thought" problems included at the end of each chapter. There is a good balance between classic and new (less than 4 years old) bibliographic references, the latter being about 20–30% of all citations included, and generally referenced by the authors to introduce state-of-the-art research topics.

In Chapter 1, the authors opt for a historical approach to the evolution of the basic concepts in catalysis, flowing naturally toward the presentation of relevant examples (e.g., immobilized metal clusters and enzymes) and more specific principles such as the meaning of turnover frequencies, activity, selectivity, and volcano plots. The authors then discuss adsorption phenomena, with the clever incorporation of both statistical mechanics and kinetics principles to address this issue. Readers will likely postpone the study of Chapter 3 on catalyst characterization to proceed with Chapter 4 (significance of pore structure and surface area), which seems to be the natural extension of Chapter 2 on adsorption phenomena. The two key misses on adsorption are the lack of mathematical discussions on the widely popular Barret–Joyner–Halenda (BJH) and Horváth–Kawazoe methods for the modeling of meso- and microporosity in solid catalysts. In addition, a simple drawing of an automatic adsorption instrument (rather than the conventional and old volumetric apparatus shown in Figure 4.1) would be more relevant to the modern experimental methods. At this point in their work, the authors introduce the fundamentals of diffusion in porous catalysts, through two subsections containing a wealth of information on the effect of diffusion on reaction rates and on some very useful experimental methods to determine the occurrence of diffusional limitations. Some attractive engineering flavor is now added, as mathematical models for catalyst deactivation and reactor design are also incorporated in Chapters 6 and 7.

Chapter 3 deals with the physicochemical characterization of catalytic surfaces, with special emphasis on ideal systems such as metal and metal oxide single crystals. Only half a page is devoted to Raman spectroscopy, a technique that has proven very useful for the *in situ* characterization of surfaces and adsorbed species (see, for example, the work by the groups of Knözinger, Wachs, and Stair, to name a few).

The final chapter of the book presents a number of important industrial applications of heterogeneous catalysis. These include the well-established Fischer–Tropsch and methanol synthesis processes, some that have caused renewed interest (photocatalysis, catalytic distillation, etc.) and also a few new research avenues such as the potential use of mesoporous catalytic materials.

As it is often the case, even with high-quality books such as this

one, dealing with a rather broad area of scientific research sometimes causes the reader to experience the feeling that some crucial topic has been left out or has not been presented in detail. For example, the current knowledge on acid and base catalysis deserves perhaps more attention, as the authors briefly discuss the chemistry essentials of catalytic cracking processes in just one page of their final chapter. For example, one of the main contributions of computational *ab initio* methods in catalysis has been the modeling of zeolite acidity (see, for example, the work by the groups of Sauer and van Santen and more recently by Haw and Nicholas). This could have been introduced in Chapter 5 (where solid state and computational aspects are presented) to set the tone for a more thorough discussion on acid–base catalytic chemistry.

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**Advances in Dendritic Macromolecules, Vol. 3.** Edited by George R. Newkome (University of South Florida). JAI Press: Greenwich, CT, 1996. xii + 201 pp. \$109.50. ISBN 0-7623-0069-8.

This edition in the series consists of five chapters, all of which have some concern for synthetic techniques, but with the exception of the first chapter, Dendrimers and Hyperbranched Aliphatic Polyesters Based on 2,2-Bis(Hydroxymethyl)propionic Acid (Bis-MPA), the major point of attention is the characteristics of specific types of dendrimers and hyperbranched polymers. (In the first chapter, the concern is with dendrimer syntheses and their more-or-less classical evaluation as polymer materials.) In the other chapters, particular attention is given to magnetic, photochemical, electrochemical, and redox characteristics of species. As with all such edited works having numerous contributors, the quality of the presentations varies from chapter to chapter. Some particularly good points might here be noted where there is notable value to the readers, both those who are already experienced in studies on dendrimers and hyperbranched polymers and those interested in entering the field or using such species for particular purposes.

The chapter Consequences of the Fractal Character of Dendritic High-Spin Macromolecules on Their Physicochemical Properties provides a very good analysis of the difficulties in constructing and using dendrimers with open-shell electronic states, including stereochemical and conformational consequences. This chapter is notable in its value in that it provides reasonable cautions as well as points to areas that are ripe for investigation.

Similarly, the chapter Redox-Active Dendrimers, Related Building Blocks, and Oligomers, building on a proper mix in the discussion of synthesis and electrochemistry, both explicitly and implicitly points to areas for further intriguing investigations. The chapter Organometallic Dendritic Macromolecules: Organosilicon and Organometallic Entities as Cores or Building Blocks also gives a mix of synthesis and physical chemical (electrochemical) studies, pointing to continuing areas for investigation and providing useful guidance for the experimentalist.

The chapter Dendrimers Based on Metal Complexes is a survey of a variety of multi-transition-metal-centered dendrimers, particular attention being given to their electrochemical behavior and energy transfer processes. Difficulties associated with detailed structural analyses for such species are noted.

While the concentration of the volume is with dendrimer (hyperbranched polymer) physical characteristics and behavior, and investigators in these areas or thinking of moving into these areas will find it particularly useful, there is sufficient attention given to syntheses and suggestions of target species that synthesizers will find it of use.

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