Computer Software Reviews

Chemcal. Program Version 2.01.00. Copyright 1985 by B&B Scientific Software: 1124 East Portland Street, Phoenix, Arizona 85004. $89.95.

Chemcal is a single-disk, noncopy-protected program that is most useful for the calculations needed for chemical analyses. The software is IBM compatible. (This reviewer found that it will also run on a Texas Instruments Professional Computer with use of the "Emulate" program provided on MS-DOS.) From the main menu that appears after loading the program, one has a choice of four subprograms: one that allows the calculations of elemental percent weights from a molecular formula, one that allows the reverse process, a third that is a slight variation of the latter, and a fourth subprogram that is a listing of atomic weights. The calculations are most readily done for programs containing any of the following elements: C, H, N, O, S, P, Cl, F, Br, and I. (Although slightly more tedious, it is possible to make determinations when other elements are present.) The software also allows one to take into account in such calculations the presence of solvent molecules.

This reviewer found the program to be simple to learn and use. If one has a compatible computer readily available, the program can easily take the place of a tabular listing of the elemental percent weights for various molecular formulas or of a calculator needed to make such calculations.

David Wenkert, *North Texas State University*

Book Reviews*

Progress in Analytical Atomic Spectroscopy. Volume 7. By C. L. Chakrabarti (Carleton University). Pergamon Press: Elmsford, NY. 1986. v + 421 pp. $132.00. ISBN 0-08-034141-1.

This volume is a compilation of papers originally published in 1984 in the journal of the same name. This journal is aimed at the rapid publication of comprehensive reviews authored by some of the leading analytical spectroscopists in the world (Note: As of 1986, the journal has broadened its scope to include analytical molecular spectroscopy and has, thus, changed its name to Progress in Analytical Spectroscopy). Since its inception in 1978, this journal has been an authoritative reference guide for analytical spectroscopists—this volume is no exception. Although the nine review articles included in this volume range from 13 to 71 pages in length, all present a detailed account of their respective subjects. Generally, the articles are more than just reviews based on previously published papers and include a wealth of previously unpublished data from the authors' laboratories as well.

Two of the most popular high-power transient plasma sources (spark and laser plasmas) are covered separately by Scheeline (High Voltage Discharges: Diagnostics and Opportunities) and Dittrich and Wennrich (Laser Vaporization in Atomic Spectroscopy). Scheeline limits his presentation primarily to modern spark source production and diagnostics, but he closes with a discussion of some of the more promising new transient plasma sources produced by high-voltage capacitive discharges. Dittrich and Wennrich's treatment of laser atom/ion cells is exhaustive in its scope, including no less than 432 references!

An excellent review/tutorial on microwave plasma sources is presented by Matousek, Orr, and Selby (Microwave-Induced Plasmas: Implementation and Application). Coverage of electrothermal atom cells includes theoretical modeling of platform atomizers in a paper by Paveri-Fontana and Tessari (Models in Electrothermal Atomization: The Platform Atomizer) as well as Sedykh and Belyaev's discussion of the use of molecular absorption measurements for graphite furnace diagnostics (A Study of Sample Volatilization in a Graphite Furnace by Means of Atomic and Molecular Absorption Spectra).

A comprehensive tutorial on noise and noise reduction schemes in optical spectroscopy is given by Epstein and Winefordner (Summary of the Usefulness of Signal-to-Noise Treatment in Analytical Spectrometry). A detailed theoretical treatment of the technique of laser-enhanced ionization is given by Travis and co-workers (Principles of Laser-Enhanced Ionization Spectrometry in Flames) along with a discussion of the future prospects of the method.

Finally, the volume contains two articles on detection strategies in analytical spectroscopy. McGeorge and Salin (Image Sensor Applications in Analytical Atomic Spectroscopy) present a framework for the evaluation of multiwavelength detection systems with discussion of a variety of electronic multichannel detection devices. A very different perspective is presented by Dittrich and Niebergall in their comprehensive presentation of an extremely powerful plasma diagnostic technique called equidensitometry (Equidensitometry—A Method for Plasma Diagnostics in Atomic Spectroscopy). This method is actually just a means of presenting spatially resolved spectrographic information, but its visual impact is impressive—the potential of equidensitometry as a plasma diagnostic tool is amply demonstrated by the authors.

Unfortunately, space limitations preclude more than a terse commentary on the papers included in this volume—suffice it to say that this compilation is an essential addition to the library of any analytical atomic spectroscopist who is without access to the original journal.

Joel M. Goldberg, *University of Vermont*

Practical Organic Mass Spectrometry. By J. R. Chapman (Kratos Analytical Instruments Ltd.). John Wiley & Sons: New York. 1985. ix + 197 pp. $34.95. ISBN 0-471-90696-4.

This book is directed toward the practicing mass spectrometrist and aims to review the principles, practical details, and applications of a number of newer methods. Theoretical presentation is deliberately limited to providing the basic understanding necessary for employing or evaluating a technique.

The first chapter (24 references) is an introduction covering the standard instrumentation. Included in this chapter is a discussion of multiplier gain measurements and methods for determining the basic instrument sensitivity. There is no discussion of FTMS or TOF instruments or their performance relative to the more common types of mass analyzers.

The second chapter (56 references) deals with sample introduction and concentrates on GC and probe inlets. The major LCMS systems are concisely described in this chapter, but the reader is referred to other literature for applications and practical details.

The third and fourth chapters give authoritative yet concise reviews of the major ion–molecule reactions employed in positive and negative chemical ionization methods, respectively. Practical details are presented on CI operation and the introduction of reagent gases into high-voltage sources of magnetic instruments. Both chapters give separate tables listing applications along with reference lists organized by the reagent gas employed and the compound classes studied. Chapter 3 contains 69 general references plus 276 application references while Chapter 4 gives 49 and 80 references, respectively.

Chapter 5 covers methods for analysis of labile molecules including FC, DCI, DEI, and FAB. The theoretical and practical discussion emphasizes FD following the author's belief that this technique provides a common background in ion formation processes and sample preparation methods for the use of other, newer methods. This chapter contains 121 general plus 46 DCI and DEI application references.

Chapter 6, on metastable ions, gives a complete set of equations describing the required field relations for implementing various metastable scans on magnetic instruments. A lucid discussion is given on the precursor or fragment ion resolutions obtained with these scan modes. While some bias may be noted in the author's preference for IFFR studies on forward geometry magnetic instruments, the treatment of the advantages of triple-stage quadrupole instruments is brief but objective. A table with 98 references summarizes analytical applications to 1983 and 84 references are given.

*Unsigned book reviews are by the Book Review Editor.

The final chapter (73 references), on quantitative analysis, is not as complete as the other chapters and is misleading on at least two points. The large body of work on computer-automated target-compound analysis is not mentioned, while oil analysis by batch inlet is cited as the leading example of quantitative work under scanning conditions. The discussion of sensitivity based on the detection of less than 100 ions is by the author's own admission not often achieved in practice. The reader would have been better served in this chapter if the rather limited discussion on detection limits established by the standard deviation of the blank had been given a more complete presentation.

This volume is efficiently illustrated and the text is written with a concise, uniform style that manages to accurately and thoroughly cover the salient points of the chosen subjects. The organization of the chapters by theory, practical details, and applications is convenient. The lack of current references is somewhat disappointing, but those provided are useful and extensive. On the whole this book meets the author's stated aims of giving the informed user a practical basis for evaluating and using the methods described. As a concise guide to a number of current methods, this book should be a useful resource to spectrometrists dealing with diverse analytical projects.

James H. McReynolds, *State University of New York at Buffalo*

Chemistry of Organo-Zirconium and -Hafnium Compounds. By D. J. Cardin (University of Dublin), M. F. Lappert (University of Sussex), and C. L. Raston (University of Western Australia). Ellis Horwood Limited: Chichester (distributed by John Wiley & Sons: New York). 1986. 451 pp. $120.00. ISBN 0-470-20204-1.

I thought I had a good overview of the chemistry of organozirconium compounds ... at least I thought I did until I read this book! The authors have managed to pull together, in remarkably comprehensive fashion, the organometallic chemistry of zirconium and hafnium, but they have done so not simply in an encyclopedic way (as is all too typical these days for reviews and monographs). Rather they have accomplished this in a way which makes sense to the reader. The book follows a typical format for volumes of this type, and data are organized around ligand types and formal oxidation states for the metals. Consider, for example, Chapter 2 (Monocyclopentadienyl Compounds of Zirconium(IV) and Hafnium(IV)), Chapter 3 (Monocyclopentadienylzirconium(III) and -hafnium(III) Compounds), Chapter 5 (Bis(cyclopentadienyl)metal Halides, Pseudohalides, and Compounds with Oxygen-, Sulfur-, Selenium-, Nitrogen-, Phosphorus-, Arsenic-, or Antimony-centered Ligands), Chapter 7 (Metallocene(IV) Dialkyls and Related Compounds), Chapter 8 (Metallocene(IV) Monoalkyl Derivatives and Related Compounds), Chapter 9 (Metallocene(IV) Diaryl, Dialkenyl, Diallyls, Dialkynyls, and Metallacycles), Chapter 11 (Metallocene(IV) Compounds with Triorgano-silyl, -germyl, or -stannyl Ligands, or with Zr-M Bonds (M = a Transition Metal)), Chapter 12 (Metallocene(IV) Tetrahydridoborates, Hydrides and Hydridoaluminates), Chapter 13 (Zirconocene(III) and Hafnocene(III) Compounds), Chapter 14 (Metallocene(II) Compounds), Chapter 15 (Triscyclopentadienyl and Tetrakis(cyclopentadienyl) Compounds of Zirconium and Hafnium), Chapter 16 (Complexes of Anionic π-Ligands other than Cyclopentadienyls), Chapter 17 (Homoleptic Complexes with σ-Bonding Ligands and Heteroleptic Alkenyl and Iminoacyls), Chapter 18 (Heteroleptic Complexes with σ-Bonding Ligands), and Chapter 19 (Complexes with Neutral π-Ligands). However, several chapters are rather unusual for this type of volume and are especially welcome. For example, Chapter 1 (Organo-zirconium and -hafnium Chemistry: Introduction) contains a discussion on "comparisons" with neighboring elements. Here, trends are shown linking the chemistries of zirconium and hafnium systems to those of other metals in the Periodic Table. Bond-dissociation enthalpies are presented in a very useful table. The authors draw upon their expertise in the field to provide insight into, for example, "general factors affecting stability". They also offer some interesting historical perspective on the evolution of topics discused. Chapter 4 (Stereochemistry and Molecular Structures of Metallocene Derivatives) and Chapter 10 (Molecular Structures of the Metallocene(IV) Alkyls and other Hydrocarbyls, including Ylides, and Alkylidene-Zirconium-aluminum Complexes) concentrate on structural data; the collation of such information, which draws heavily on the crystallographic literature, is especially useful for comparison-making purposes. Finally, Chapter 6 (Introduction to the Metallocene(IV) Alkyls, and other Hydrocarbyls, with Some General Comments on σ-Bonded Organic Groups) and Chapter 20 (Organo-zirconium and -hafnium Complexes in Organic Synthesis and Catalysis) focus on the chemistry of compounds many of which find use as intermediates in organic synthesis. A broad variety of illustrations is provided. Each chapter is augmented with an addendum containing recent literature through 1984.

I hope that this work will someday reappear in a second edition. Apart from that hope, I would have to say that this book is definitely the "last word" in this field.

Jeffrey Schwartz, *Princeton University*

Methods in Enzymology. Volume 112. Drug and Enzyme Targeting. Part A. Edited by Kenneth J. Widder (University of California, San Diego) and Ralph Green (Cleveland Clinic Foundation). Academic Press: Orlando. 1985. XXV + 589 pp. $69.00. ISBN 0-12-182012-2.

This book represents a broad overview of the various technologies available for the targeting of drugs and enzymes. Part A of this comprehensive topic is treated in Volume 112 and is divided into four sections that represent the major physical, chemical, and biochemical approaches to targeting. Section I deals with microencapsulation techniques and is concerned exclusively with various technologies on microspheres, including their preparation, entrapment of drugs, stability, drug release, and storage characteristics. Interesting examples where microspheres are used for drug targetting include microsphere–antibody combinations (immunospheres) and magnetically responsive microspheres. The methodology to prepare each of these interesting species is adequately discussed as are other methods of preparing such microspheres. Recent literature references are cited.

Secion II on drug conjugates represents the biochemical approach to drug targeting and contains eight chapters detailing a variety of approaches such as antibody–toxin conjugates and various other polymer–drug conjugates, e.g., polylysine, dextran, insulin, and glycoprotein conjugates. Most such conjugates are prodrugs and require hydrolysis to free the bioactive drug. Resistance to complete hydrolysis plus difficulty in transporting such large molecules to specific cells and tissues within the organism account for their limited success as site-specific drug delivery agents, but such issues do not receive adequate treatment in this section.

Section III on prodrugs contains chapters on prodrug pharmacokinetics, prediction of prodrug stability, prodrug influence on metabolic pathways, and prodrug design for enhancement of GI absorption and targeting to the brain. All chapters are written by active investigators in the field and cover specific topics in a thorough manner.

The final section contains eleven chapters on the use of polymer systems for the controlled release of enzymes and drugs. Included are discussions on the use of biodegradable polymers to modulate the release of macromolecules such as interferon and insulin. Others treat transdermal drug delivery systems and osmotic drug delivery—both by the use of rate-controlling microporous polymeric membranes designed to regulate release of drug from the device in a predictable manner. Chapters on the theory and application of membrane systems are also included and complement the chapters that discuss applications of specific polymer systems.

Most chapters contain sections on methodology and materials that are useful for the synthesis and fabrication of the delivery systems being discussed.

In this book the subject of drug and enzyme targeting is treated from an interdisciplinary viewpoint and represents a good "how-to" approach in dealing with a wide variety of drug and enzyme delivery systems. The book should appeal to those desiring a general knowledge of the field. References cited in most of the chapters are comprehensive and current enough to allow investigators access to relevant drug delivery literature.

A companion volume is in preparation and will address drug and enzyme delivery issues by the use of liposomes, cell carriers, and receptor mediation.

Anthony A. Sinkula, *Upjohn Company, Kalamazoo*

Lecture Notes in Chemistry. Volume 39. Electrochemistry on Liquid/Liquid Interfaces. By P. Vanýsek (Northern Illinois University). Springer-Verlag Publishers: New York. 1985. 106 pp. $15.20. ISBN 3-540-15677-1 (paperback); ISBN 0-387-15677-1 (hard cover).

The author has certainly met the aim of the *Lecture Notes in Chemistry* series by providing, at a very high level, a timely, well-organized monograph on new developments in electrochemistry on liquid/liquid interfaces. This publication is extremely well referenced with 344 references (through 1985) collected in alphabetical order at the end of the monograph. A table of contents and a complete list of symbols are also included.

A comprehensive summary of the principal studies of liquid/liquid interfaces is presented in a 5-page introductory chapter. Sufficient theoretical background for an experienced electrochemist is presented in Chapter 2. Topics covered are equilibrium conditions, Nernst potential, single-ion Gibbs energy of transfer, ideally polarizable liquid/liquid interfaces, and redox-system equilibrium.

In Chapter 3, the author discusses at length the experimental requirements for electrochemical measurements at liquid/liquid interfaces. Required electrode configurations, the quasi and conventional reference

electrodes used, a description of the four-electrode potentiostat, and the requirements of a suitable organic solvent for a water/organic solvent system are very well presented. Also included are descriptions of an electrolyte dropping electrode, an electrolyte hanging-drop electrode, and a typical cell for L/L measurements as well as discussions of chronopotentiometric and cyclic voltammetric measurements. The author includes useful examples of the techniques described. Problems which may be encountered in experimental measurements are noted. The reader is continuously reminded of the similarities of phenomena at the interface of two immiscible electrolyte solutions and that at a metal/electrolyte solution interface.

An excellent chapter on double layers at liquid/liquid interfaces is presented next. A good discussion of double-layer and inner-layer capacitances is included. Mention is made of the mean spherical approximation model to the interpretation of interface phenomena and of digital processing of a video image for measurement of surface and interfacial tensions.

A thorough discussion (13 pages) of current flow across the interface is presented in Chapter 5. A table of charge-transfer rate constants for 38 ions is included in this chapter. Chapter 6 deals with mediated properties. The author comments on the carrier properties of antibiotics, a study of ion-transfer facilitation by macrocyclic polyethers, and a model for the liquid/liquid kinetics of extraction of metals by organic acids. Suggestions for further work involving formation of precipitates at the L/L interface are also presented.

The use of equivalent circuits to gain an understanding of the laboratory results is discussed in the chapter on impedance measurements. The author includes a description of the use of AC bridges, Lissajous figures, and phase-sensitive detection. Problems associated with impedance measurements are nicely pointed out.

The monograph finishes with a brief (2 pages) discussion of phase-transfer catalysis and its possible use in research on interfacial catalysis from an electrochemical and physicochemical point of view.

A strong point of this monograph from an instructional point of view is the author's inclusion of a general description of the fundamental principles and techniques behind each type of experimental measurement presented. I did not find any serious errors. Minor, readily recognizable, and easily corrected errors were found. These do not, however, detract from the overall excellent quality of this publication.

Russell R. Bessette, *Southeastern Massachusetts University*

Vitamin B6 Pyridoxal Phosphate: Chemical, Biochemical and Medical Aspects. Parts A and B. Edited by David Dolphin, Rozanne Poulson, and Olga Avramovic. John Wiley & Sons: New York. 1986. Part A: 725 pp. $99.95. ISBN 0471-09783-7. Part B: 792 pp. $99.95. ISBN 0471-09785-3.

The two books constitute Volume I of a series of volumes to be published on coenzymes and cofactors. The volume on B6 is an ambitious survey with a truly international list of contributors. Authors from the USA, Canada, Europe, Japan and Russia are represented. The subject matter is vast with chapters ranging from historical aspects to enzyme mechanisms. There are also contributions on biochemical, nutritional, clinical, and pharmacological aspects. In general, the quality of the chapters (with one exception) is good to excellent, but there are a fair number of typographical errors and the nomenclature is not uniform throughout. Also, the subject matter overlaps in part. For example, Walsh has written a concise chapter on "suicide" inhibitors of pyridoxal 5′-phosphate (PLP) enzymes, but many of these examples are repeated in chapters on individual enzymes (e.g., in chapters dealing with aspartate aminotransferase and γ-cystathionase).

I was dismayed by one chapter that describes the mass spectral properties of PLP and related compounds. In this chapter the authors purport to show from mass spectral and UV absorbance data that, of all the commercial preparations of PLP available, only one (sample A) is authentic. They suggest that an "impure" sample (sample B) may contain 6-chloro PLP and then interpret the spectrum of B as if it were 6-chloro PLP; however, the authors later write that "the molecular species present in B should be chemically characterized". In my opinion the interpretation of the mass spectra shown for *both* A and B are unconvincing. I agree with the authors that the spectrum of B seems to show chlorine which from chemical tests does not appear to be chloride ion. However, the authors should have carried out a complete elemental analysis to determine the actual amount of chlorine present in B. Secondly, as evidenced from the rest of the book, very many chromatographic procedures are available for separating PLP analogues that should readily separate 6-chloro PLP from authentic PLP. Finally, as described in the current volume, many authors have made derivatives of PLP; others have carried out NMR and other physicochemical studies of PLP (in most cases obtained from commercial sources). Surely, one would think that other authors would have detected something wrong if their commercial sample contained 6-chloro PLP!

Volume 1 contains much new information on the role of PLP in a large number of enzymatic reactions (and the role of pyridoxamine 5′-phosphate (PMP) and other forms of the cofactor in a few cases). With the introduction of increasingly sophisticated analytical techniques within the last few years, the detailed mechanisms of the enzymatic reactions involving this extremely versatile cofactor are slowly being unraveled. I was particularly interested to note that the role of PLP in glycogen phosphorylase, after many years of debate, is becoming clearer. I also found it interesting that, despite the relative simplicity of the structure of PLP, the details of its biosynthesis have eluded investigators for over 30 years. Hill and Spenser have put together a fascinating chapter in which the mechanism (at least in outline) seems to be yielding to a determined effort at solution. The chapter is written, however, in a somewhat combative nature that may annoy some of the authors quoted. In conclusion, except with the reservations noted above, the volume is an excellent and important contribution to the fields of biochemistry, chemistry, pharmacology, clinical, and nutritive aspects of vitamin B6. I recommend the two books highly.

Arthur J. L. Cooper, *Cornell University Medical College*

Anleitungen für die chemische Laboratoriumpraxis. Volume XXI. UV–VIS–Spektroskopie und ihre Anwendungen. By H. H. Perkampus (University of Düsseldorf). Volume XXI: W. Fresenius, J. F. K. Huber, E. Pungor, G. A. Rechnitz, W. Simon, G. Tölg, and Th. S. West, Eds. Springer Verlag: Berlin, Heidelberg, New York, Tokyo. 1986. VIII + 208 pp. DM 148 (hardcover). ISBN 3-540-15467-1.

This little volume begins with a brief discussion of the physicochemical bases of electronic spectroscopy, primarily focusing on absorption, but with some attention to emission spectroscopy, and with a discussion of the equipment used. A comprehensive chapter deals with analytical applications, with extensive tables of methods available for the determination of metals (by complexation, and by acidic and basic extraction), anions, and organic compounds, for analysis of water, and for enzymatic analysis. A chapter on special methods deals with double-wavelength, derivative, reflection, photoacoustic, and luminescence excitation spectroscopies. Investigation of equilibria, including pK's, complex formation, H-bonded association, charge transfer, and metal complexes is discussed. A further chapter deals with the use of electronic spectroscopy in kinetics, emphasizing reacions of different order, sequential, parallel, and fast reactions, stop-flow and relaxation methods, and photochemistry. A final brief chapter focuses on various aspects of the evaluation of spectra: oscillator strengths and transition moments, band analysis involving Gaussian and Lorentzian functions and derivative spectra, and vibrational structure.

The volume is well illustrated with pertinent figures, carefully derived equations, extensive tables, and a considerable bibliography. It should serve as an introduction to any analytical chemist becoming involved in the use of electronic spectroscopy and as a reference volume in this general area.

H. H. Jaffé, *University of Cincinnati*

Progress in Physical Organic Chemistry. Volume 15. Edited by R. W. Taft (University of California, Irvine). John Wiley & Sons: New York. 1985. ix + 362 pp. $70.00. ISBN 0471-81474-1.

This volume meets the high standards one expects in this series, of which Volume 1 was published in 1963. It consists of four chapters.

The first chapter is on Structural Principles of Unsaturated Organic Compounds: Evidence by Quantum Chemical Calculations by S. Dähne and FL Moldenhauer. This deals with the triad theory and its applications to unsaturated organic compounds. Its stated goal is "...to provide experimental chemists with simple implements to design and fit new unsaturated organic compounds with special electronic structures". The primary emphasis is on polymethines, defined as systems of N atomic centers occupied by $(N + 1)$ or $(N - 1)$ π-electrons; these may have linear or branched conjugated units or aromatic units or combinations of these. Such systems generally absorb at long wavelengths, and a set of color rules which are helpful in inferring colors from electronic configuration is applied. Molecular diagrams with parameters derived from calculations are given and discussed for a wide variety of systems.

The second chapter is on Chemical Process Systemization by Electron Count in Transition Matrix by San-Yan Chu and Tieh-Sheng Lee. This is a brief (16 pages) review of a scheme for process codification which involves counting the electrons that are acted on by the operator in the ıransition matrix element. Applications to cation radicals, anion radicals, energy transfers, and aromaticity are included.

The succeeding chapter entitled Solvolysis Revisited is by M. J. Blandamer, J. M. W. Scott, and R. E. Robertson. This is an update of a review by Robertson on Solvolysis in Water in Volume 4 of this series. The focus is primarily on the consequences of different methods of

treating kinetic data and the significance of the derived activation parameters. Discussions of moderation of the reactions by solvent and the dependence of rate constants on temperature are followed by discussions of analytical approaches to interpretation of data. Models for solvolytic reactions are analyzed critically, and future directions in which research in this area might be directed are briefly considered.

The final, long, chapter is on the Collage of S_N2 Reactivity Patterns: A State Correlation Diagram Model by S. S. Shaikh. The purpose of the chapter is to introduce the state correlation diagram model in a form that unifies the concepts of physical organic chemistry and of theoretical organic chemistry as developed by the author and A. Pross. The application of the model is developed and applied to various examples to show how it accounts for substituent effects, breakdown in the well-known reactivity/selectivity and Bell–Evans–Polanyi principles, and the Leffler–Hammond postulates as well as changes in mechanisms from S_N2 to electron transfer.

As is true of so many volumes of this type, the price is likely to make purchase by individuals rare, but it should be found in any worthwhile institutional chemistry library.

Henry G. Kuivila, *State University of New York at Albany*

Enzyme Chemistry. Impact and Applications. Edited by C. J. Suckling (University of Strathclyde). Chapman and Hall: London and New York. 1984. 255 pp. $36.00. ISBN 0-412-25850-1.

This collection of essays explores, as the title of the volume implies, the role that enzymology has come to play in shaping and in certain instances even re-defining problems and approaches in both chemistry and the life sciences. The editor has chosen to restrict his selection of topics to a limited number of rather obvious cases of applied enzymology. These include the following: the use of enzymes in organic synthesis; chemical models for enzymatic catalysis; the development of enzyme inactivators as an approach to the problem of rational drug design; the role of metal ions in biology; the analysis of natural product biosynthesis elucidated at the level of enzyme reaction mechanisms. As a consequence of these choices, the book is by no means a comprehensive review, as the editor readily admits. Nonetheless, the seven articles collected here are scholarly and well written and provide the reader who is new to these areas considerable insight into the interplay of enzymology and a number of other fields of basic and applied science. In a brief but fascinating introductory chapter, the editor provides an especially revealing historical observation: applied enzymology is not a recent development. Enzyme chemistry began to impact substantially on laboratory and industrial science and on agriculture and medicine as early as the mid-nineteenth century. The pace in recent years has quickened, of course. And with the entry of enzymologists into such fields as fermentation technology, toxicology, and chemical carcinogenesis and genetic engineering, we can be assured that the continuing role of fundamental enzymology in allied areas of science will be substantial.

Michael Johnston, *University of Chicago*

The Vital Force: A Study of Bioenergetics. By Franklin M. Harold (National Jewish Center for Immunology and Respiratory Medicine). W. H. Freeman and Co.: New York. 1986. XVIII + 577 pp. $37.95. ISBN 0-7167-1734-4.

Mitchells' chemiosmotic hypothesis, which postulated a central role for proton currents in biological energy-conversion processes, has transformed the study of bioenergetics. Over the last two decades reversible proton pumps and proton-coupled transport systems were found to be a ubiquitous component in most cells and organelles. The concept of a primary ion pump and the associated coupled reversible symporters and antiporters has also been applied to sodium, calcium, and other pumps. Harold's book describes and summarizes recent advances in bioenergetics and related fields, which were brought about by the development of the chemiosmotic theory. The book discusses in detail the mechanism of energy conversion in such processes as oxidative phosphorylation, photophosphorylation, primary and secondary active transport, contraction and motility, signaling and morphogenesis. This is a much wider scope than previous books on bioenergetics, which traditionally dealt only with oxidative phosphorylation and photophosphorylation. Harold's style is exemplary for its clarity and simplicity; with the help of thoughtful figures and diagrams he succeeds in a lucid presentation of complex and often confusing issues. However, the author has chosen to dispense with rigorous physicochemical formulations and with much of the molecular detail in favor of qualitative descriptions and broad explanations. This would endear him to the more biologically oriented reader, but it does make the book less usefull to physical biochemists and to the researchers in this field. On the whole, Harold shows more respect to beautiful theories and models than to the ugly facts. An example is found in Chapter 7, where he describes the interconversion by the ionophores, valinomycin and nigercin, of the two components of the proton electrochemical potential in mitochondria. The diagram shown (Figure 7.7) illustrates the principle but bears little resemblance to the actual experimental data of Mitchell and Moyle, which Harold cites as a basis for this figure. In fact, for various complicated reasons, mitochondria do not show complete interconversion of the components of the proton electrochemical potential. Harold is also probably too zealous in advocating all the various ideas originated by Mitchell, even those ideas which overwhelming experimental evidence appears to refute. Nevertheless, despite its few shortcomings, this book, with its wide scope and special point of view, does fill a void and would be a welcomed addition to the very limited selection of books on bioenergetics.

Hagai Rottenberg, *Hahnemann University*

Catalysis. Volume 7 (A Specialist Periodical Report). Senior Reporters G. C. Bond (Brunell University) and G. Webb (University of Glasgow); Reporters R. Burch, A. D. H. Clague, P. J. Gellings, M. J. Ledoux, J. R. H. Ross, and C. J. Wright. The Royal Society of Chemistry: London. 1985. xi + 196 pp. $87.00 (£60.00). ISBN 0-85186-584-4.

This volume consists of six chapters; each is a high-quality review article. Chapter 1, Metal Catalysed Methanation and Steam Reforming with 206 references, by J. R. H. Ross, first reviews the title processes and some of their problems, then discusses the catalysts used, and finally, briefly mentions mechanistic aspects.

Catalyst Characterization with Neutron Techniques, by C. J. Wright, 90 references, composes Chapter 2. Covered are the characterization of surfaces of catalysts, of bulk properties of catalysts, and of adsorbent–adsorbate interactions. The author gives the reader a feeling about those areas in which neutron scattering offers unique information about catalysts.

Chapter 3 not only furnishes the expert a review of current events in catalysis studies with solid state NMR but also furnishes the student with enough background knowledge in language and equipment to understand experimental results. Therefore, its title, High Resolution Solid State N.M.R.—Theory and Applications, is highly appropriate. The 163 references cover NMR parameters, problems with solids, improving sensitivity, narrowing lines, shortening relaxation times, choosing equipment, NMR studies of the bulk and surface of catalytic materials, and NMR studies of adsorbed species and chemical reactions at catalytic surfaces.

P. J. Gellings' Oxidation by Catalysts Containing Vanadium, 150 references, highlights the use of vanadium in these catalyst systems by covering spectroscopic investigations, oxygen species in vanadium-containing catalysts, acid–base properties of vanadium oxide catalysts, some special oxidation reactions, mixed oxide catalysts, and supported vanadium oxide catalysts.

Hydrodenitrogenation, Chapter 5, by M. J. Ledoux, uses 68 references to bring an interesting perspective to this developing subject. This perspective is best seen in its divisions: economic aspects, origin and nature, industrial processes, kinetics and mechanism, and catalysts.

Finally, Chapter 6 is an elegant discussion of structure sensitivity. R. Burch treats this important topic under the title of Structure and Properties of Supported Noble Metal Catalysts. Its 354 references are divided between the basis of structure sensitivity, small metal particles, electronic properties of small metal particles, influence of particle size on the energetics of adsorption, change of structure of supported metals—sintering, and relevance of particle size effects to structure sensitivity.

Uniformly the chapters are well written; they cover the recent literature through 1983. The Senior Reporters have chosen the topics to be diverse, and in this respect they have made good choices. Consequently, this book will be a very timely addition to the libraries of specialists in catalysis. A sad note from the Preface is the specter of discontinuation of the series from lack of sales. Examination of the price explains the reason. Nevertheless, such scholarly work is worthy of support, and this reviewer hopes sufficient support will materialize and/or expenses will be reduced enough for continuation.

Gerard V. Smith, *Southern Illinois University at Carbondale*

Basic Tables for Chemical Analysis. By T. J. Bruno (National Bureau of Standards, Boulder, CO) and P. D. N. Svoronos (Georgetown University). U.S. Government Printing Office: Washington, D.C. 1986. v + 233 pp. $11.00. ISBN 003-003-02724-3.

This soft-bound book is a collection of mostly numerical data collected from a variety of sources and "is offered to the scientific community as a low-cost source of useful information for the practicing chemist." It is, indeed, useful to have such information gathered in one place, especially that which is hard to find elsewhere. The section on infrared spectroscopy, for example, includes tables of the transparent regions of a variety of cell-window materials, the full IR spectra of a wide selection of solvents, and unusually extensive tables of the characteristic IR frequencies of structural features. The NMR section is similarly compre-

hensive for ^1H NMR, but ^{13}C NMR is ignored except for a table of ^{13}C NMR shifts for a group of solvents. A section of 65 pages gives useful data on packings for chromatographic columns. Another section, on mass spectrometry, consists principally of a tabulation of fragmentation patterns of common structural types. Unfortunately, the tabulation that one would find most useful, and would reasonably expect to find in a book of this sort, is omitted: masses and isotope abundances for various combinations of atoms.

Unexpectedly, a section on "qualitative analysis" is included. It is not a collection of tables, but it contains a verbal description of classical wet tests for organic and inorganic substances, presented at the freshman/sophmore level. This section is certainly inadequate, and it is as archaic as the references cited (e.g., Oliver Kamm's classic book of 1932); important references on the subject, such as "The Systematic Identification of Organic Compounds", by Shriver, Fuson, Curtin, and Morrill, and the books of Cheronis and Entrikin, are omitted. The book concludes with a section of Miscellaneous Tables (drying agents and flammability of liquids). The table of drying agents could have been useful, but it is a disaster. Firstly, the entries in the table are not explained, so one does not know if the lines of dots in a given box mean that the drying agent is suitable for the given type of compound or is not suitable. Secondly, "never" is written in some boxes, such as for use of P_2O_5 for carboxylic acids, but does not appear where it seems essential, such as for use of KOH for drying acids!

The lack of an index is inconvenient. The nomenclature used in some tables is unprofessional (e.g., "amylmercaptan", "ethylacetone"), and the references are in many instances absurdly out of date and are secondary or tertiary (e.g., *The Handbook of Chemistry and Physics* for 1971). The aim of the authors is commendable, and their book will undoubtedly be useful, but it could have been so much better with a little more care.

Vibrational Spectra and Structure: A Series of Advances. Volume 14. Edited by J. R. Durig (University of South Carolina). Elsevier Science Publishers: Amsterdam and New York. 1985. xvii + 480 pp. $129.75. ISBN 0-444-42536-5.

Volume 14 of this series contains topical articles on IR laser spectroscopy, vibrational properties of layered materials, ab initio calculations of force constants, and calculations of IR intensities. Other chapters include the electronic spectra of polyatomic free radicals and FT-IR spectroscopy. Each review is prepared by authors chosen from the international community and distinguished in their respective subjects.

S. Nakashima, M. Hangyo, and A. Mitsuishi report on the vibrational spectroscopy and lattice dynamics of layered materials, defined here as crystalline structures with strong covalent or ionic bonding in two-dimensions. The authors present a well-organized in-depth review of the interlayer optical and accoustical phonon properties in these materials. They apply factor group analysis, consider the influence of hydrostatic pressure and low temperature, and include a discussion of charge density waves, commensurate and incommensurate phases, and superlattices. Additionally, they review the vibrational properties of metal dichalconides, metal dihalides, and certain intercalated materials.

G. Fogarasi and P. Pulay review recent developments in ab initio force field calculations of small polyatomic molecules. Many of the examples are taken from the author's own research and given critical analysis. Both theoretical and experimental data are combined in deducing optimal sets of force constants. The article is not only loaded with constructive guidelines and recommendations for those engaged in ab initio calculations but it also contains much information for the experimental spectroscopist. V. T. Aleksanyan and S. Kh. Samvelyan advance two models (one where the basic unit is the atomic charge and the other the bond dipole) for calculating infrared absorption intensities of fundamental bands and apply the atomic charge model to metal carbonyl complexes and metallocenes. The authors consider aspects of dipole moment additivity and transferability of intensity theory parameters.

E. Hirota reviews a variety of IR laser spectroscopies, including laser Stark spectroscopy and laser magnetic resonance spectroscopy, and convincingly demonstrates their advantages in studying small polyatomic molecules. Sub-doppler spectroscopies (i.e., saturation methods, double resonance methods, or molecules beams) nicely show the utility of high-resolution IR laser techniques. The author brings the reader up to date on advances in the detection of free radicals and transient species using tunable diode lasers and IR gas lasers.

D. A. Ramsay reviews the electronic spectra of polyatomic free radicals. His stated objective is to supplement the classic publication of Herzberg, "Molecular Spectra and Molecular Structure", Volume III. Approximately 50 free radicals are discussed and systematized according to the number of atoms and valence electrons. Finally, J. E. Bertie presents a pedagogical review on the essential features and the implementation of an FT-IR spectrometer. It is primarily intended for those who are about to utilize FT-IR spectroscopy or simply curious about the technique.

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Mass Spectrometry of Heterocyclic Compounds. Second edition. By Q. N. Porter (University of Melbourne). John Wiley & Sons: New York. 1985. xxi + 966 pp. $250.00. ISBN 0471-09901-5.

The fact that this book was snatched away upon its arrival and put to immediate use attests to its usefulness. It is a great expansion of the original work of 1971. The author's main thrust is to rationalize the fragmentations observed, in order to serve the chemist whose primary interest lies in identifying compounds.

The organization is according to type of ring, beginning with oxiranes and oxetanes and proceeding systematically to larger rings and multiple hetero atoms. Fragmentation schemes are immediately and prominently displayed, with m/z values and intensities shown for each fragment. The accompanying text is succinct and points out useful generalizations. There are no tables. The index is extensive, as are the lists of references, but unfortunately, references more recent than 1980 appear to be absent. Although that fact reduces the value of the book, it is nevertheless a work of reference for which very many organic chemists will be thankful.