Book Reviews*

Ion-Selective Reviews. Volume 4. Edited by J. D. R. Thomas. Pergamon Press, Oxford and New York. 1983. 286 pp. $84.00.

This is a hard-bound edition of No. 1 and 2 of the periodical of the same name, Vol. 4, 1982, and includes six reviews reproduced from typescript, plus book reviews, an obituary for Ronald Belcher, and a subject index.

Formaldehyde and Other Aldehydes. By the Committee on Aldehydes, National Research Council. National Academy Press, Washington. 1981. ix + 340 pp. $11.50.

This book is a report prepared at the request of the Environmental Protection Agency to help it assess the need for criteria in evaluating aldehydes as pollutants. A short introductory chapter summarizes the position of aldehydes as industrial chemicals, the analytical methods for them, and health effects of them, with heavy emphasis on formaldehyde. This is followed by a chapter on recommendations, which is noteworthy for the many times that the strength of recommendations must be moderated because of the lack of sufficient reliable data. The remaining eight chapters take up in a more detailed way the commercial side of aldehyde production and use, analytical chemistry, and effects of aldehydes on people, vegetation, and aquatic organisms. There is an appendix of substantial proportions in which are tabulated properties, uses, and synonyms for a large selection of aldehydes. There are extensive lists of references, but no index.

Progress in Analytical Atomic Spectroscopy. Volumes 4 and 5. Edited by C. L. Chakrabarti. Pergamon Press, Oxford and New York. 1982 and 1983. Volume 4: v + 456 pp. $106.00. Volume 5: v + 478 pp. $114.00.

These two books reproduce in hard-bound form the contents of Volumes 4 (1981) and 5 (1982) of the periodical of the same name, and consist respectively of eight and nine review articles, and subject indexes.

Maleic Anhydride. By B. C. Trivedi and B. M. Culbertson (Ashland Chemical Co.). Plenum Press, London and New York. 1982. xvi + 871 pp. $89.50.

This is a comprehensive technical reference work, apparently the first of its kind about the compound, which has become a major industrial chemical since about 1940. It has, of course, been a useful starting material for all sorts of syntheses, but its major use is now in the polymer field, with other significant demands in pharmaceuticals, agricultural chemicals, detergents, etc. It fully merits a book of this sort.

Five of the twelve chapters are devoted to reactions of maleic anhydride. Another five cover different types of polymerization based on it. The remaining two consist of a general introduction, in which physical and biological properties, analytical detection, and uses are treated, and a survey of the methods of production. An appendix lists the numerous patents, arranged in seven tables. The references then take up no less than 114 pages (there exist, the editors claim, over 30 000 references if one counts patents). Although the lists of references are arranged by chapter, they are all grouped at the end of the book, a curious and unexpected feature. Finally, there is a really thorough index of 53 pages. Compiling this book was a remarkable feat.

Survey of Progress in Chemistry. Volume 10. Edited by G. G. Wubbels. Academic Press, New York. 1983. xiii + 266 pp. $47.50.

It is appropriate that this volume should be dedicated to the late Archer F. Scott, who originated the series. A biography and appreciation, written by Joseph Bunnett, precedes the four reviews that make up this volume.

The reviews in this series are intended to enlighten those who are not specialists in the field; they thus have an educational purpose, to bring significant developments to a wider audience. The subjects for this volume are Catalysis from the Point of View of Surface Chemistry (by W. H. Weinberg); Metal Clusters and Metal Surfaces (by E. L. Muetterties and R. M. Wexler); The Belousov-Zhabotinsky Reaction: Dynamical Surfaces as Models for an Oscillating System (by F. D. Tabbutt); and Recent Advances in the Chemistry of Ylides (by D. G. Morris). The first review emphasizes hydrocarbon–hydrogen reactions at metal surfaces. The second is also much concerned with catalysis, and takes up the application of concepts developed in coordination chemistry for the chemistry of metal surfaces. The Belousov–Zhabotinsky reaction about which the third review is centered is the oxidative bromination of malonic acid by bromate catalyzed by ceric salts and is noteworthy because the concentrations of the species present oscillate with time, and under some circumstances with space. This extraordinary phenomenon, originally greeted with great skepticism, is now nearer to an explanation. The last review gathers together advances since the 1960's on the many reactions and different types of ylides, defined as components in which "the structure, or at least one canonical form, contains positive and negative charges in adjacent atoms". Although this does embrace those compounds commonly considered as ylides, it may be dangerously broad, for alkenes appear to fit the requirements, too.

There is a good index.

Handbook of Metal Ligand Heats and Related Thermodynamic Quantities. Third Edition. By J. J. Christensen and R. M. Izatt. Marcel Dekker, Inc., New York. 1983. 800 pp. $95.00.

This book is an enormous table, supplemented by the references from which the data were compiled and several indexes. Ligands, beginning with Acetic Acid, are listed alphabetically, and the various metal ions with which it has been coordinated follow. For each entry are given the heat of interaction in kJ/mol, log K, entropy, conditions, and reference. The compilation is intended to be complete through 1980; the previous edition stopped at the end of 1973. The intervening seven years have contributed 464 more entries. This work is a unique compilation, and should be of much value not only to chemists but also to biochemists and many biologists, physicists, and chemical engineers.

Supplement to Rodd's Chemistry of Carbon Compounds. Second Edition. Volume 1. Part FG. Edited by M. F. Ansell. Elsevier Science Publishers, Amsterdam and New York. 1983. xvi + 404 pp. $115.00.

This supplement starts with pentahydric alcohols and proceeds through larger polyhydric alcohols to their oxidation products, including saccharides. After this come tetrahydric alcohols and their derivatives, a curious order. The four chapters are the work of five contributors: R. J. Ferrier, R. A. Hill, R. Khan, B. S. Paulsen, and J. K. Wold. They build upon the original chapters of the Second Edition, and presumably bring them up to date, although neither the preface nor the individual chapters give any indication of when the literature coverage ends.

The value of this work is that it is more useful to the non-specialist than are the many excellent but narrow monographs. One finds a treatment with sufficient detail and sophistication to give a sound picture of the breadth and much of the depth of recent activity in the areas covered. The style remains succinct but readable. Tables of data are rare, but that fact may be a result of the subject matter. Structural formulas abound, although it would be a distinct improvement if they were drawn in uniform style; as it is, they vary disturbingly from one chapter to another. A great improvement over previous Supplements is the adoption of a uniform type style; earlier volumes had the jarring appearance of a cheaply produced set of conference proceedings.

This is a useful work, and one that will have a special appeal to chemists concerned with carbohydrates. This volume can stand by itself in that respect, and it is appropriate that it has its own index, and a thorough one. Now if only the publishers would provide running headings at the tops of the pages, the utility of these supplements would be greatly increased.

Trichothecenes—Chemical, Biological and Toxicological Aspects. By Yoshio Ueno (Tokyo University of Science). Copublished by Kodansha Ltd., Tokyo, and Elsevier Science Publishers, Amsterdam and New York. 1983. xiii + 313 pp. $85.00.

This timely monograph comprises Volume 4 of the Kodansha–Elsevier "Developments in Food Science" series and should be of interest to investigators within an unusually broad range of scientific disciplines. About 55 naturally occurring trichothecenes, which may be chemically classified as sesquiterpenoids, are covered in this work. They are produced by a number of taxonomically unrelated fungi (but most notably by the ubiquitous *Fusarium* genus) which infect feedstock and exhibit toxic effects on animals and humans. Contemporary concern regarding the possible implication of some of these compounds as biological warfare agents is largely unaddressed in this book.

After a brief but informative chapter presenting the historical background of trichothecene studies, the next four chapters deal successively with chemistry, mycology, analysis, and toxicology. The subject matter of the final chapter, which occupies about one-third of the book and is

*Unsigned book reviews are by the Book Review Editor.

entitled Toxicoses, Natural Occurrence and Control, is dealt with in an interesting manner, consisting of 14 subsections, each concerned with a different national geographic region. Since space is afforded such relatively small land areas as, for example, Denmark and Britain ("So far, no unequivocal link has been established between... trichothecene mycotoxins... and disease... in Britain."), the absence of a contribution from Russia, where many of the earliest significant observations were made, must be regarded as a curious and serious omission.

Chemists will probably find the sections on the less familiar areas of toxicology and biology of most interest. The chemistry of the natural trichothecenes occupies 60 pages, but it is presented in an extremely concise manner with a resemblance to "Chemical Abstracts" style and without critical discussion. The synthesis chapter in particular regrettably falls below an acceptable standard for English phraseology and chemical usage, and a total lack of technical editing is here apparent.

Since about 40 authors make contributions to this work, it is perhaps inevitable that there should be some overlap (e.g., nuclear magnetic resonance spectra coverage), but it is not excessive.

Robert Stevenson, *Brandeis University*

Quantitative Structure–Activity Relationships of Drugs. Edited by John G. Topliss (Warner-Lambert/Parke-Davis). Academic Press, New York, NY. 1983. ix + 528 pp. $69.00.

Modern QSAR (quantitative structure–activity relationships) studies on biological systems began in the early 1960's. A lot has happened since then, as this multiauthored text will attest. The descriptors in the QSAR equations or models have become more diverse and sophisticated. Statistical approaches have grown from simple regression analysis to discriminant, factor, and principal component analyses. Various forms of pattern recognition are being employed. The newest techniques are using computer graphics.

Has all of this effort been economically worthwhile in terms of new product development, or is it an exercise that industry can ignore, leaving QSAR research to academia? The answer given by "Quantitative Structure–Activity Relationships of Drugs" is that it is a valuable and valid part of any systematic search for new products.

There are chapters on how QSAR has facilitated research on synthetic antiinfective agents, semisynthetic antibiotics, antitumor agents, cardiovascular agents, antiallergic and antiulcer agents, nonsteroidal antiinflammatory and antiarthritic drugs, agents affecting the central nervous system, steroids and other hormones, chemicals affecting insects and mites, and absorption, distribution, and metabolism of drugs. The book opens with a brief overview of QSAR methodology and closes with a succinct commentary on the individual chapters. Indeed, this reviewer would recommend that the reader study this well-written commentary by the editor before exploring any of the specific topics. It provides the detailed answer to the question asked in the second paragraph of this review. QSAR has defined the role of lipophilicity in drug action, provided information on specific receptor sites, indicated nonproductive approaches to a drug design problem, and shown how standard statistical methods can be used to design a set of congeners yielding maximum information from a minimum number of compounds.

The authors of the several chapters are established medicinal chemists, mostly from industry, who actively employ QSAR in their research. Although suffering from the typical uneveness found in a multiauthored text, this book is attractively produced, nicely illustrated, and well indexed. Each chapter is well referenced. Every medicinal chemist should own and read this book.

John H. Block, *Oregon State University*

Fluoride, The Aging Factor. By John Yiamouyiannis (Safe Water Foundation). Health Action Press, Delaware, OH. 1983. 210 pp. $11.95.

This book, written in popular style for the general public, presents a matrix of evidence about the toxicity of fluoride and concludes that there is no safe level for fluoride in food or drinking water. Fluoride toothpaste and dental treatments are also considered to be hazardous to health in nondental aspects. Extensive references, case histories, as well as an index are included.

M. C. W. Smith, *Ann Arbor*

Making Science Laboratory Equipment. A Manual for Students and Teachers in Developing Countries. By X. F. Carelse (Department of Physics, University of Zimbabwe). John Wiley & Sons, New York. 1983. xiii + 273 pp. $18.95.

This book is directed toward problems encountered by teachers in underpriviledged schools. Although it is primarily designed for use in developing countries, it could be very useful in any high school or college that does not have adequate funding. Dr. Carelse states that, "The primary thesis of this book is that the subject of improvisation has become of such economic importance to the developing world that it is no longer sufficient to treat it with the hit-or-miss amateurism of the past. It must now be approached with a dedicated overall philosophy by which teachers are trained to fend for themselves continuously, mobilizing all the resources available to them."

The first chapter is devoted to the elements of woodworking. This includes hand tools, power tools, materials, fastenings, and basic frames. Techniques and equipment needed for working with metal, glass, plastics, and electricity are described in the next two chapters. This is followed by a discussion of the most efficient use of limited funds. Local artesans, craftsmen, students, and parents should be encouraged to help in the production of equipment. The design and construction of equipment for physics, chemistry, biology, and geography make up the next four chapters. Equipment for a workshop is described in Chapter 8. Useful techniques and information that will be helpful in acquiring material are included in the appendix.

This is an amazing book. A biscuit tin becomes a mousetrap. Ball point pens find places in L-bends, T-tubes, test tube racks, droppers and as jets in bunsen burners. All manner of odds and ends, including toothpaste tubes, are transformed into useful objects. Any agency that sends teachers to developing countries should provide them with copies of this book!

M. C. W. Smith, *Ann Arbor*

General and Synthetic Methods. Volume 6. Edited by G. Pattenden. The Royal Society of Chemistry, London. 1983. xiii + 416 pp. $75.00.

This volume of the "Specialist Periodical Reports" is concerned with organic chemistry and is arranged in chapters according to structural type, from hydrocarbons to heterocyclics. The literature of 1981 is reviewed intensively, in the terse but informative style typical of the series. This volume includes a new chapter, Highlights in Total Synthesis of Natural Products, which is meant to take the place of the chapter in previous volumes that carried the title Strategy and Design in Synthesis.

Although the density of information in these Reports does not make easy reading, it provides an efficient way to review what has been published recently in ones' area of concern, and to see what one missed. Occasionally the frugality with words leaves one feeling a little deprived, such as when, for example, one is told that a method for selective reduction of nitro groups has been reported, without saying with respect to what structural features the selectivity applies. The references are all there, however, and they are especially convenient to use, since they are set at the foot of each page. As usual, the volume closes with a bibliography of reviews, classified according to subject and including the actual titles of the reviews. This is a most helpful feature. A subject index would not be feasible in a book of this sort, but there is an index of authors.

Analytical Profiles of Drug Substances. Volume 11. Edited by Klaus Foley. Academic Press, New York. 1982. x + 665 pp. $39.00.

This volume contains 16 contributed chapters, each on a specific drug, from aminophylline to sulfadiazine. There are also supplements to the treatment in Volume 1 of five other drugs. This is a new feature starting with this volume.

The guiding principle of this series is to cover all drugs of medical value. For each substance, the "profile" includes general descriptive data, such as nomenclature, physical properties (including spectra), methods of preparation, stability, and metabolism and other biomedical properties, in addition to a comprehensive presentation of methods of analysis. Analysis is interpreted to include identification as well as determination, and to include physical, chemical, and biological methods. There is no subject index, but a cumulative index of drugs treated in Volumes 1 to 11 is given.

The Peptides, Analysis, Synthesis, Biology. Volume 4. Modern Techniques of Conformational, Structural, and Configurational Analysis. Edited by E. Gross (N.I.H.) and J. Meienhofer (Hoffmann-LaRoche, Inc.). Academic Press, New York. 1981. xix + 309 pp. $51.50.

The first three volumes in this series described peptide synthesis. The present volume is the first of several ones that concentrates on analysis.

The first chapter, X-Ray Analysis: Conformation of Peptides in the Crystalline State, by I. Karle is an authoritive review of small cyclic (2–15 residues) and linear (2–8 residues) peptides and depsipeptides. The first part gives a comprehensive description of the structural results classifying and comparing various structures (the literature including 1980 is reviewed; it was not until 1983 that the book was received for review). A careful analysis is made of the different types of folding that are observed. Although this field of research is quite active, the review will stand for some time to come.

The second chapter, Crystal Structure Analysis of the Larger Peptide Hormones, by J. Gunning and T. Blundell is a status report (as of 1980)

on the structure determinations and predicted structures, from homology, of these peptide hormones for which crystallization has been possible. Conformational aspects are described in relation to receptor recognition. Additional results have been obtained in the succeeding years.

The longest chapter is titled Determination of the Absolute Configuration of α-Amino Acids and Small Peptides by Chiroptical Means, by V. Toome and M. Weigele. It gives, for instance, a comprehensive review of the ORD and CD spectra of amino acids and their chromophoric derivatives (24 types) besides a more cursory review for metal chelates. The introduction to the chapter emphasizes the analytical application of ORD and CD, but very little is said about those types of applications, and certainly many of the chromophoric derivatives will never by used for analytical purposes. Instead, the derivatives are interesting from a structural or methodological point of view. That seems even more true in the case of the metal chelates. One is left with the desire for more theoretical results to explain the multitude of observations or the extension of the methods into other parts of the EM spectrum.

Ultramicroanalysis of Peptides and Proteins by High-Performance Liquid Chromatography and Fluorescence Detection (by S. Stein) is the title of Chapter 4. The combination of both techniques makes high specificity and great sensitivity possible with detection at picomole level. One would have preferred greater emphasis on the methodology in order to emphasize the analytical aspects of the subject. Instead, a number of interesting examples are given.

The fifth chapter, Amino Acid Analysis of Peptides, by J. R. Benson, P. C. Louie, and R. A. Bradshaw deals exclusively with single-column chromatography as the method for analytical separation. The chapter gives a literature review for the properties of amino acids and commonly encountered derivatives and a choice of a number of protocols for their separation.

The last chapter is titled Solid-Phase Sequencing of Peptides and Proteins, by R. A. Laursen. It describes the chemistry and strategy of the Edman degradation as it is performed on solid support using the equipment designed by the author. The review is very similar, but less detailed, than the one published in 1980 by Laursen and Machleidt in "Methods of Biochemical Analysis".

The different subjects, although all dealing in principle with analysis, will appeal to readers with quite diverse interests, and one might suggest for the future that each volume in the series would contain a set of more closely related topics.

D. van der Helm, *University of Oklahoma*

Stereochemical Applications of NMR Studies in Rigid Bicyclic Systems. Methods in Stereochemical Analysis. Volume 1. By Alan P. Marchand (North Texas State University). Verlag Chemie International, Deerfield Beach, FL. 1982. xiii + 231 pp. $92.50.

This small reference book is an excellent starting point for an experienced chemist beginning a research project in this field. However, the book is not self-contained. For some data, and most of the arguments, the reader is referred to the original journal articles or to other review articles. The author also assumes a considerable familiarity with the field, so this would not be a recommended first choice for a new graduate student. However, it is a compact, non-exhaustive survey of much of the pertinent literature. A 2-page table containing 20 different atomic systems for which an angular dependence of ^3J spin coupling has been demonstrated was one of the most useful pieces of information presented. This summary is then followed by 52 pages of tabular data for a wide variety of vicinal coupling constants. This tabulated material is very briefly discussed in 10 pages of text interspersed among the tables.

The price of this slim volume appears to be clearly above the norm, even in these days of significant inflation. Since several typographical errors were found in the 70 pages of text (including an incorrect page number in the Contents), the reader is cautioned to check the tabular data before quoting it or using it.

George H. Wahl, Jr., *North Carolina State University*

Isolation, Separation and Identification of Volatile Compounds in Aroma Research. By H. Maarse and R. Beltz (Institute CIDO Analysis). D. Reidel Publishing Company, Dordrecht, Holland. 1981. xii + 290 pp. $54.50.

This book consists of six chapters, namely, Isolation and Concentration of Volatiles from Foods, Separation, Introduction, Identification, Coordination of Sensory and Instrumental Analysis, and Applications in Other Fields of Research.

The book is intended for the practioner in aroma research and in allied fields such as food, nutrition and biomedical analysis. The emphasis tends to be on classical chemical analysis and gas and thin layer chromatographic techniques since these are the methods of assay which have stood the test of time. There is a tremendous amount of detail regarding specific treatments, extractions, and conditions of analysis throughout the book. For example, the isolation and concentration chapter contains a large number of exceptionally clear sketches of glassware which may be used for the title processes. Each chapter is well referenced; the entire volume contains 1187 references, each containing not only the author's name and journal but a full title of the paper.

This densely packed source of information is definitely meant for the specialist. One could imagine entering the field of aroma research and obtaining from this volume a very good idea of the state of the art a few years ago. Due to the organization and indexing, it is somewhat easier to find applications of instrumental techniques and particular detectors than it is, for example, to find out something about a particular flavor or odor. Thus, as a handbook it leans toward instrumental analysis. Each chapter contains sufficient introductory material to allow one either to carry out a procedure if it does not involve complicated instrumentation or to understand more advanced treatices on instrumental methods. For example, the use of various extraction devices is made very clear in the second chapter, and a nice introduction to mass spectrometry is included in Chapter 4. For those who are looking for it, this book provides a unique overview of the use of analytical methods in an industrial discipline. All in all then, this is a well edited, densely packed, somewhat dated review for workers in the field.

Stephen G. Weber, *University of Pittsburgh*

Biothermodynamics: The Study of Biochemical Processes at Equilibrium. By J. T. Edsall (Harvard University) and H. Gutfreund (Bristol University). John Wiley & Sons, New York. 1983. x + 248 pp. $34.95.

The network of relationships among the equilibrium properties of a system given by thermodynamics has a wide application to many divisions of science and engineering. It simplifies the quantitative description of complicated systems and amplifies a small amount of observed information to a much larger set of data. Because of the central importance of energy transformations in living systems, thermodynamics should be especially relevant to biology. Most textbooks in biochemistry and physiology now devote a chapter or more to thermodynamics.

Nevertheless, thermodynamics has never had the impact on biology that it has had on chemical and mechanical engineering. A major reason for this is the extreme complexity of biological systems. These systems contain many components and phases. Their behavior is far from that of the ideal models often used in thermodynamic calculations. The phases are not well-defined homogeneous regions, but instead consist of complicated structures at a series of levels ranging from the macroscopic to the molecular. Furthermore, life is a nonequilibrium phenomena controlled and directed by information stored in macromolecules and by a variety of feed-back loops.

The successful mating of thermodynamics with biology requires growth from both ends. The components, phases, and processes that characterize living systems must be identified and described quantitatively in detail. Thermodynamic calculation techniques must be expanded to handle the necessary complexity. Most discussions in biochemistry textbooks are directed toward observations of relatively simple systems.

"Biothermodynamics" is not intended to be a rigorous treatise on thermodynamics but rather an introductory textbook for students of biological sciences. It should be judged on this basis. The first half of the book consists of a survey of thermodynamics with an emphasis on topics applicable to biology. These include mixtures, partial molal quantities, standard states, activities and activity coefficients, electrochemistry, properties of water and aqueous solutions, and membrane equilibria. Brief discussions of equilibria in the ultracentrifuge and of mechanical stress are also included. Methods of experimental measurements are described. The treatment of these topics is similar to those found in undergraduate textbooks in physical chemistry.

The second half describes biochemical processes. Chapter 4 discusses several examples of enzyme-catalyzed metabolic reactions. Chapter 5 describes binding of small molecules and ions to macromolecules, and Chapter 6 reviews the calorimetric investigations of phase transitions in macromolecules. A bibliography of around 300 citations is given. SI units are used throughout. No practice problems are offered.

The second law of thermodynamics and some of its consequences are discussed in Chapter 2. However, no direct statement of the second law or clear definition of entropy is given.

There is a noticeable discontinuity between Chapters 3 and 4. Chapters 4 and 5 are concerned with chemical equilibria. Ideal solution behavior is assumed, and activities are represented by molar concentrations. Little use is made of the more rigorous concepts developed in the first part of the book. Calculations are based on algebraic manipulations of equilibrium constant expressions, as is commonly described in freshman chemistry. The student is not warned that activity coefficients in the examples given may range from 0.001 to 100 or even more. Chapter 3 explains that thermodynamic properties of individual ions cannot be

rigorously defined and gives a correct explanation of pH. However, in Chapter 4 no justification for, or explanation of, the use of ionic concentrations in place of activities is given.

No mention is made anywhere of the more general and powerful approach to chemical and phase equilibria in terms of the minimization of Gibbs energy subject to stoichiometric constraints. No reference to the extensive literature on this subject or of the computational techniques and available computer software is made.

"Biothermodynamics" does present, in a well-organized manner, the major applications of thermodynamics to biochemistry that have been made to date. It treats them more extensively than most biochemistry textbooks. It could serve very well as the basis of a one-semester course in thermodynamics for biochemistry students, provided the instructor remedies deficiencies such as those described above.

R. C. Wilhoit, *Texas A&M University*

A Dictionary of Spectroscopy. Second Edition. By R. C. Denney (Thames Polytechnic). John Wiley and Sons, New York. 1982. xiii + 205 pp. $39.95.

The first edition of this book was designed to provide the student or non-specialist an easy and quick reference to the terms employed in all areas of spectroscopy (atomic, emission, infrared, mass, photoelectron, Raman, UV–visible, ESR, NMR, photoluminescence) by giving short simple explanations of the specialized terms used in the field. The major branch(es) of spectroscopy in which the term is used is given when appropriate.

The second edition has been expanded and updated to include electron spectroscopy and the latest recommendations for symbols and nomenclature. Unfotunately, the author chose to use photoelectron spectroscopy as a main heading rather than the more inclusive heading electron spectroscopy. this creates some errors in defintiions, such as the statement that electron-impact spectroscopy, which involves no photons, is a form of photoelectron spectroscopy.

For the most part, however, the explanations given are clear and concise, and the book contains many references to the origin of the terms. The book should be useful for those who want a quick reference to spectroscopic terms.

F. A. Grimm, *University of Tennessee*

Ab initio Molecular Orbital Calculations for Chemists. By W. G. Richards (Oxford University) and D. L. Cooper (Harvard-Smithsonian Center for Astrophysics). Clarendon Press, Oxford. 1983. 116 pp. $16.95 (paperback).

In the preface to the second edition of this book, the authors correctly point out that today more than ever experimentalists are using quantum mechanical software in their work, making it desirable to have a brief introduction to the theoretical background involved. At this point the reader might hope that with a minimum of complicated mathematics, the necessary theory would be presented followed by a reasonably documented set of examples of output from current quantum mechanical programs illustrating formats and the type of information that is currently available to those who use the many readily available software packages. Unfortunately, what follows is a somewhat too sketchy introduction to quantum mechanics, and a somewhat too involved discussion of self-consistent-field theory which would be better suited to those who wish to understand the theoretical details rather than to those who would simply like to know what the theory can do. There is only one brief display of output (a set of MO coefficients from a calculation on H_2CO) and only three relatively brief tables showing the good degree of agreement today between theory and experiment, at least in certain areas. In this aspect, then, the book is disappointing, since material more appropriate to the non-expert will more readily be found in non-specialist review articles and even in some of the more recent texts.

The book does contain a reasonably good coverage of the self-consistent-field method; one who has not done so before undoubtedly will derive benefit from following the detailed examples worked out by the authors. The nine chapters of the relatively short book range from an introductory summary of quantum mechanics through the working out of some matrix elements of SCF theory illustrating calculations on polyatomic molecules. The last two chapters dealing with electron correlation and applications are perhaps the best in the book in that they convey to the reader the basic ideas on these important subjects without immersing him in the complicated mathematics involved.

A problem in any short presentation of material in a difficult subject area such as quantum mechanics is oversimplifying to the border of being incorrect. The general wave function is introduced as representing a one-electron wave rather than the complete many electron state function. In discussing basis sets, it is mentioned that sometimes d-orbitals are added to bases even for the light atoms, but that "this does not mean that the atomic d-orbitals are necessarily employed in bonding but simply that they are convenient variation functions". Any function in a basis will be involved in the bonding and the nonbonding and the antibonding; it is the degree of participation in these various activities that is important. Finally, for one who has struggled for years to convince beginning graduate students that quantum mechanics is not only true but good for something, I could not help but cringe at the statement that "exchange is purely a quantum mechanical effect with no physical meaning". The exchange term by itself has no classical counterpart, but it is, of course, a perfectly legitimate member of the physical and classically realized Coulomb interaction.

Those who read this book will indeed learn about the self-consistent-field method. It is questionable whether the time would be better spent studying an introductory text on the subject where an effort is made to be pedagogically clearer and more complete.

D. B. Chesnut, *Duke University*

Chemical Thermodynamics. By Hugh Miller Spencer (University of Virginia). Bailey Printing, Inc., and Anderson Brothers Book Stores, Inc., Charlottesville, VA. 1983. ii + 366 pp. $25.00.

This book contains the standard topics that one expects to see in any rigorous discussion of thermodynamics and its applications to areas of interest to chemists and chemical engineers. It could be used as a text for an intermediate level course on chemical thermodynamics or as supplementary material for the beginning course in physical chemistry. If the reader is already familiar with thermodynamics, this book is useful. Chapter 1 is a discourse on the scope of thermodynamics and its mathematical underpinnings. Chapter 2 is a detailed presentation on partial molal properties and solutions. The third chapter is devoted to the empirical equations of state for gases and examples of their use. Chapters 4–7, which follow a historical perspective, rather than a purely logical one, contain material on the first and second laws of thermodynamics. A brief introduction to statistical mechanics and its applications to chemical systems is given in Chapters 8–10; this treatment is better than what is in most introductory texts. Chapters 13, 14, 16, and 18 are devoted to solutions and solute–solute interactions, i.e., deviations from ideality and ionic interactions. There are also chapters on thermochemistry, Gibbs free energy changes, phase equilibria, and the thermodynamics of surfaces and systems in varying gravitational fields.

One can certainly profit from studying this book, if one already has some knowledge of thermodynamics. The historical material on the origins of the first and second laws is entertaining and informative.

Harry P. Hopkins, Jr., *Georgia State University*

Progress in Physical Organic Chemistry. Volume 14. Edited by R. W. Taft (University of California, Irvine). John Wiley & Sons, New York. 1983. ix + 374 pp. $70.00.

The uniformly high quality of contributions to which readers have becomed accustomed in previous volumes of this excellent series continues in the present volume. This volume consists of six chapters, as detailed below.

The first chapter, Substituent Effects on Chemical Shifts in the Sidechains of Aromatic Systems, by D. J. Craik and R. T. C. Brownlee (La Trobe University, Victoria, Australia), presents a critical evaluation of selected literature examples wherein structural and mechanistic information has been derived from NMR chemical shift information. Substituent effects on side chain chemical shifts in styrenes and derivatives, in carbonyl compounds, in other unsaturated side chains, in saturated side chains, and in carbocations are presented and discussed.

The second chapter, Substituent Effects in the Partition Coefficient of Disubstituted Benzene: Bidirectional Hammett-Type Relationships, by T. Fujita (Kyoto University), analyzes linear free energy (LFE) approaches to understanding the solubility-modifying effect of substituents on aromatic systems (and, hence, upon the hydrophobic properties of these systems). The importance of "variations in the extent of hydrogen bonding solvation of substituents" in this regard is stressed. The concepts introduced in this chapter are complex, particularly so when applied toward analyzing substituent effects on partition coefficients of ortho-disubstituted benzenes. The written presentation, unfortunately, is sometimes stilted; one would have hoped for greater editorial involvement in the process of finalizing the manuscript for publication of this chapter.

The third chapter, Treatment of Steric Effects, by R. Gallo (IPSOI, University of Marseilles-St. Jerome), critically examines LFE, topological, geometrical, and force field methods of quantitative analysis of steric effects. The ensuing discussion briefly summarizes the scope and limitations of each of these four methods. In the Conclusions section, some suggestions are forwarded for applying individual methods to specific situations.

The fourth chapter, Polar Substituent Effects, by W. F. Reynolds (University of Toronto), reviews the various mechanisms that have been suggested to account for the propagation of polar substituent effects in

organic molecules (e.g., field, σ-inductive, and π-inductive contributions to the total polar effect of substituents). Areas of controversy concerning the relative importance of the different mechanisms in this regard are reviewed and discussed.

The fifth chapter, Secondary Deuterium Isotope Effects on Reactions Proceeding Through Carbocations, by D. E. Sunko (University of Zagreb) and W. J. Hehre (Univesity of California, Irvine), surveys the origins of secondary deuterium isotope effects and discusses their applications to the study of reactions that proceed via "carbocatio-like transition states or intermediates". The role of hyperconjugation in secondary β-deuterium isotope effects are examined. Models to explain the origin of more remote (i.e., γ and δ) secondary isotope effects on these reactions are presented.

The final chapter, Protonic Acidities and Basicities in the Gas Phase and in Solution: Substituent and Solvent Effects, by Professor Taft, discusses theoretical and experimental approaches to the study of substituent and gas-phase "solvation" effects on gas-phase proton-transfer equilibria. In addition, solvent effects on proton-transfer eqilibria in solution are classified and analyzed according to behavior as belonging to one of six "types".

As part of a continuing series, this volume will undoubtedly find its way into those institutional chemical research libraries whose present budgets permit the luxury of standing orders. This reviewer joins the ranks of those who bemoan the rising costs of technical books andthe consequent limitations upon distribution and readership. After all, the ability of an editor to attract contributions of the highest caliber to a multiauthored treatise depends in large measure upon his ability to ensure that these chapters, once published, will reach the hands of their intended audience!

Alan P. Marchand, *North Texas State University*

Properties of Liquids and Solutions. By J. N. Murrell and E. A. Boucher (The University of Sussex). John Wiley & Sons, Ltd., New York, NY. 1982. x + 288 pp. $45.95.

In view of the importance of water as being fundamental to life processes and that most chemical synthesis is carried out in the liquid state, it is fundamental that the study of aqueous solutions should form a required part of the education of chemists, biologists, and physicists. The authors of this book support this view and have therefore put together the material in this area that should be known by physical scientists. In addition, this book is a valuable source of information for researchers in this field that have not previously studied all of this material. In particular, this extends the list of possible readers to mathematicians and computer scientists who are working in this area and need to know more of the physical background.

Specifically, for a detailed study of the book, knowledge of some very basic thermodynamics, statistical mechanics, and quantum mechanics is expected. Lest the potential reader be put off by this, please note that these prerequisites are not course requirements but are minimal and explicitly described in the Preface. The book, intended for undergraduate instruction, is very clearly written with references to other books and monographs generously provided throughout.

The text immediately lures the reader onward with a discussion of the problem "What is a liquid?" The subsequent topics are presented in order of increasing complexity. This nicely prepares the reader for what is to come in the later chapters. Students, teachers, and researchers are offered a wide spectrum of topics to choose from. Among these one will find illuminating expositions on the following: The various basic theories of liquids; liquid crystals; non-electrolytes; current research on water, including its computer simulation aspects; electrolytes; polymer molecules in solution; and important examples of colloidal systems.

This book is highly recommended to both beginners and advanced readers in the study of liquids and solutions.

Louis V. Quintas, *Pace University*

The Interpretation of Analytical Chemical Data by the Use of Cluster Analysis. By D. Luc Massart and Leonard Kaufman (Vrije Universiteit Brussel). John Wiley & Sons, New York. 1983. x + 237 pp. $45.00.

This monograph is directed toward familiarizing chemists with the use of cluster analysis in the interpretation of multidimensional analytical chemical data. The book is written on two levels. The first is largely non-mathematical and stresses correct use and applications of cluster analysis, whereas the second level (sections 1.6 and 4.8) provides a more detailed mathematical description of clustering techniques. This arrangement enables practically oriented researchers to gain an understanding of the use of clustering methods without having to digest lengthy mathematical derivations. Frequent critical comparisons of methods are welcome features. The book is clearly written and avoids much, but not all, of the nearly incomprehensible jargon often found in manuscripts dealing with such topics. Literature is selectively covered up to about 1982.

Chapter 1 provides introductory examples, outlines fundamental concepts, and discusses the relation of cluster analysis to other multivariate techniques. Chapter 2 explores methods for graphical display of multivariate (multidimensional) data in ways comprehensible to three-dimensional humans, while Chapter 3 describes hierarchical clustering methods. In Chapter 4, the authors discuss non-hierarchical methods, which they claim are more versatile. Problems that can be encountered when using cluster analysis, along with their solutions, are outlined in Chapter 5, and various applications in analytical chemistry are discussed in Chapter 6. Chapter 7 provides a short but useful list of the characteristics of various computer programs available for doing cluster analyses. A problem involving classification of branched chain fatty acids in milk in order to differentiate between biosynthetic pathways is explored in detail in Chapter 8. This last chapter gives the reader a picture of how cluster analysis is used to solve a real problem.

In summary, this short book is an excellent introduction to the practice and potential uses of cluster analysis. It should serve as a good reference even for those more knowledgeable in such techniques. It is a welcome and needed addition to the growing literature of Chemometrics.

James F. Rusling, *University of Connecticut*

Electrical Double Layer at a Metal-Dilute Electrolyte Solution Interface. No. 33. Lecture Notes in Chemistry. By G. A. Martynov (USSR Academy of Sciences) and R. R. Salem (Mendeleev Chemical and Technological Institute). Springer-Verlag, Berlin-Heidelberg-New York. 1983. vi + 170 pp. $15.60.

This monograph presents a highly theoretical and coherent treatment of the subject with enough reference made to experimental data to buttress the theory. It is organized into two sections, one dealing with the "ionic" part of the double layer, i.e., charges due to ions in solution, and the other dealing with the "electronic" part, i.e., charges due to electrons in the metal.

The book is admittedly biased toward the authors' work and viewpoint. It is interesting and valuable because it presents the Russian school of thought which otherwise does not seem to be available in comprehensive form. Western readers will be unfamiliar with large parts of the theory presented, such as, the model of the electronic capacitor, which is treated in detail. There are 186 references, mostly from the Russian literature. In keeping with the professed bias of the book, Western literature is not well represented and some of the Russian work is ignored as well. At times, the English text is a bit lumpy, but the book is nevertheless quite readable.

G. M. Schmid, *University of Florida*

Introduction to Polymer Viscoelasticity. 2nd Edition. By John J. Aklonis (University of Southern California) and William J. MacKnight (University of Massachusetts). John Wiley & Sons, New York. 1983. 295 pp. $49.95.

This book serves as a fine example to the neophyte wishing to be introduced to the topic of polymer viscoelasticity. This volume, which is based on the first edition that was also co-authored with the late Professor Mitchel Shen, has had some revamping, but overall it principally contains the material of the first edition. The newer material consists of a separate chapter on dielectric relaxation as well as a short section on the topic of reptation, the latter of which is included in chapter seven focusing on viscoelastic models. This reviewer finds it somewhat disappointing that a greater emphasis has not been placed on the topic of reptation, since it has become so useful in terms of helping to understand the viscoelastic properties of polymers. The chapter on dielectric relaxation is a very positive input. The authors have done a very nice job of interrelating the discussion of the dielectric properties of polymers to those of the dynamic mechanical and general viscoelastic character of polymeric systems. The book is viewed as a highly recommended introductory text to both undergraduates and graduate students in the area of viscoelasticity. In fact this reviewer has utilized the first edition several times in this respect. The book is very readable with clear figures and equations. In addition, problems have been provided. Many of these have answers provided at the end of the text along with an explanation on the details of achieving their solution. In summary this book is viewed as a highly recommended text or reference for those having an interest in polymer viscoelasticity.

Garth L. Wilkes, *Virginia Polytechnic Institute and State University*