

Book Reviews

Advances in Chemical Physics. Volume LXVII. Ab Initio Methods in Quantum Chemistry. Part I. Edited by K. P. Lawley (Edinburgh University). Series editors: I. Prigogine and S. A. Rice. John Wiley and Sons: New York. 1987. x + 556 pp. \$118.00. ISBN 0-471-90900-9

This volume is the first of a two-part collection of in-depth reviews of selected areas of modern quantum chemistry, written by active participants in the recent development of the topics covered. Although there is some variation in the level of the reviews, in general they are not directed toward complete beginners, but they can be read with pleasure by anyone familiar with the elements of quantum chemistry at the level of, for example, A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry* (Macmillan, London, 1982). The separate reviews should be especially valuable to practicing theoretical chemists who wish to learn the current state of research areas in which they have not yet been active or for students who are entering research in quantum chemistry.

The first volume in this set consists of the following reviews: "Excited State Potentials" by P. J. Bruna and S. D. Peyerimhoff, "Molecular Property Derivatives" by R. D. Amos, "Transition Structure Computations and Their Analysis" by F. Bernardi and M. A. Robb, "Optimization of Equilibrium Geometries and Transition Structures" by H. B. Schlegel, "Relativistic Quantum Chemistry" by K. Balasubramanian and K. S. Pitzer, "Effective Hamiltonians and Pseudo-Operators as Tools for Rigorous Modelling" by P. Durand and J.-P. Malrieu, "Molecular Calculations with the Density Functional Formalism" by R. O. Jones, "Basis Sets" by S. Wilson, and "The Coupled Pair Approximation" by R. Ahlrichs and P. Scharf. Each review has an extensive reference list, averaging about 150 entries, and at the end of the volume there is a complete author index of all workers to whom reference has been made and also a somewhat brief general subject index.

Many of the reviews are extremely thorough, covering not only methods and ideas that are now most commonly in use but also techniques that have been proposed but dropped or not seriously explored. For this reason, they should serve as a useful stimulus to additional innovation and be of special interest to researchers in the field. This set of reviews will be read with much interest by most quantum chemists and, considering the rapidly expanding impact that quantum chemistry is having on all fields of chemistry, should be a part of all major academic library collections.

James E. Boggs, *The University of Texas*

Advances in Chemical Physics. Volume LXIX. Ab Initio Methods in Quantum Chemistry. Part II. Edited by K. P. Lawley (Edinburgh University). Series editors: I. Prigogine and S. A. Rice. John Wiley & Sons: New York. 1987. x + 588 pp. \$125.00. ISBN 0-471-90901-7

The second volume of this two part collection of reviews of modern areas in quantum chemistry is similar in style to Part I, and the general comments made there are also applicable here. Part II contains the following reviews: "Matrix-Formulated Direct Multiconfiguration Self-Consistent Field and Multiconfiguration Reference Configuration-Interaction Methods" by H.-J. Werner, "The Multiconfiguration Self-Consistent Field Method" by R. Shepard, "Propagator Methods" by J. Oddershede, "Analytical Derivative Methods in Quantum Chemistry" by Peter Pulay, "Symmetry and Degeneracy in X_α and Density Functional Theory" by B. I. Dunlap, "Modern Valence Bond Theory" by D. L. Cooper, J. Gerratt, and M. Raimondi, "The Complete Active Space Self-Consistent Field Method and its Applications in Electronic Structure Calculations" by B. O. Roos, "Transition-Metal Atoms and Dimers" by D. R. Salahub, and "Weakly Bonded Systems" by J. H. van Lenthe, J. G. C. M. van Duijneveldt-van de Rijdt, and F. B. van Duijneveldt.

It should be noted that the reviews in both volumes are mainly concerned with methods, as the title indicates, rather than with applications or results. In only a few cases where applications have been relatively few, as for the transition-metal atoms and dimers in Part II, is there any effort to give a reasonably complete survey of chemical problems that have been treated. As reviews of methodology, however, the separate sections of these two volumes are invaluable.

James E. Boggs, *The University of Texas*

Thermodynamic Properties of Helium. Volume 1. By V. V. Sychev, A. A. Wasserman, A. D. Kozlov, G. A. Spiridonov, and V. A. Tsymarny (National Standard Reference Data Service of the USSR). T. B. Sel-

lover, Jr., English Edition Editor. Hemisphere Publishing Corporation: New York. 1987. XVI + 316 pp. \$120.00. ISBN 089116-613-0

This book is the first volume of a series of books dealing with the properties of technologically important fluids. It represents an extensive and valuable contribution to the already widely publicized properties of helium. The first part of the book (125 pp) deals with the experimental data, with the method of constructing a reliable equation of state, with the methods of evaluating the thermodynamic properties, and with the reliability of the calculated data. Tables of thermodynamic properties are given in the second part of the book (177 pp). The book is clearly written and the data are well organized. Theoretical as well as experimental scientists, interested in studying and using this second most common substance in the universe, will find this publication of great help in their work. Unfortunately, the 175 references by no means cover the entire literature dealing with helium. The only (minor) fault I have found with this compilation is the unusual designation of helium-4 as He⁴ instead of the widely accepted designation of ⁴He. Every scientific library should have this valuable book on its shelves.

Vojtech Fried, *Brooklyn College of the City University of New York*

Thermodynamic Properties of Oxygen. Volume 5. By V. V. Sychev, A. A. Wasserman, A. D. Kozlov, G. A. Spiridonov, and V. A. Tsymarny (National Standard Reference Data Service of the USSR). T. B. Selover, Jr., English Edition Editor. Hemisphere Publishing Corporation: New York. 1987. XIV + 307 pp. \$120.00. ISBN 0-89116-616-5

This book represents a thorough compilation of the thermodynamic properties of oxygen. The organization of the material is similar to that used in Volume 1. The experimental data, the method of developing a reliable equation of state, and the methods of evaluating the thermodynamic properties occupy 90 pp of the text, while the tables listing the evaluated thermodynamic properties occupy 210 pp of the text. The book is a very useful compilation. The 96 references at the end of the book cover the subject matter adequately. The book should be on the shelves of all scientific libraries.

Vojtech Fried, *Brooklyn College of the City University of New York*

Thermodynamic Properties of Ethylene. Volume 7. By V. V. Sychev, A. A. Wasserman, E. A. Golovsky, A. D. Kozlov, G. A. Spiridonov, and V. A. Tsymarny (National Standard Reference Data Service of the USSR). T. B. Selover, Jr., English Edition Editor. Hemisphere Publishing Corporation: New York. 1987. XIV + 278 pp. \$120.00. ISBN 0-89116-612-2

The organization of the book is the same as in the other volumes of the series. The book is an excellent compilation of the thermodynamic properties of ethylene. Part one, dealing with the experimental data, with the method of deriving a reliable equation of state and with the methods evaluating the thermodynamic properties occupies 73 pp, while the tables listing the evaluated thermodynamic properties occupy 160 pp. The 132 references given at the end of the book cover the subject matter reasonably well. The book is a must for everyone working with ethylene and should be on the shelves of every science library.

Vojtech Fried, *Brooklyn College of the City University of New York*

Thermophysical Properties of Freons. Volume 9. Methane Series, Part 2. By V. V. Altunin, V. Z. Geller, E. A. Kremenevskaya, I. I. Perelshtein, and E. K. Petrov (National Standard Reference Data Service of the USSR). T. B. Selover, Jr., English Edition Editor. Hemisphere Publishing Corporation: New York. 1987. XVII + 243 pp. \$120.00. ISBN 089116-601-7 (Part 2)

This ninth volume of the series deals with the thermophysical properties of methane-based freons: CCl₄ (freon 10), CFCl₃ (freon 11), CF₂Cl₂ (freon 12), CF₃Cl (freon 13), and CF₄ (freon 14). The organization of this volume is somewhat different from that used in the other volumes of the series. A very thorough introduction to the properties of freon is followed by five chapters, each dealing with one particular freon. In addition to the properties discussed in the other volumes of the series, this volume also covers transport properties extensively. The book is well written and very effectively organized. In 223 pages the authors managed to cover much very important information about this industrially very significant group of chemicals. The 463 references given at the end of

the book provide a more than adequate coverage of the subject matter. No science library should be without this very important source.

Vojtech Fried, *Brooklyn College of the City University of New York*

Topics in Current Chemistry. Volume 137: Organic Synthesis, Reactions and Mechanisms. Editorial Board: M. J. S. Dewar, J. D. Dunitz, K. Hafner, E. Heilbronner, S. Ito, J. M. Lehn, K. Nödenzu, K. N. Raymond, C. W. Rees, F. Vögtle, and G. Wittig. Springer-Verlag: New York, Heidelberg, Berlin. 1987. 260 pp. \$83.50. ISBN 0-387-16904-0

Volume 137 of *Topics in Current Chemistry* is a useful addition to the series, which is designed to provide critical reviews of the present position and future trends in chemical research for research and industrial chemists.

The first of three chapters is a review of propellane and spiran synthesis. The focus of the article is on product prediction. In addition to being informative, this chapter conveys the excitement and beauty that underlies the synthesis of these visually appealing molecules. The second chapter concerns the development of the computer program system, EROS (Elaboration of Reactions for Organic Synthesis). EROS is an expert system for the design of syntheses and for the prediction of organic reactions. The article is clearly presented and provides valuable insights for the use of this system by organic chemists. The third chapter, on transition-metal-catalyzed decomposition of diazo compounds, is an extensive survey of the literature between 1978 and August 1985. This article constitutes more than half of the entire volume. A wide range of topics is covered in depth with clear tables and illustrations. It is an extremely informative chapter for chemists interested in the synthetic applications (e.g., cyclopropanation) of diazo compounds.

Alfons L. Baumstark, *Georgia State University*

Carbohydrates. Edited by P. M. Collins (Birkbeck College, University of London). Chapman and Hall: London and New York. 1987. xi + 720 pp. \$175.00. ISBN 0-412-26960-0

This book is part of the series *Chapman and Hall Chemistry Sourcebooks*, which aims to provide carefully tailored information to individuals working in particular areas of chemistry and biochemistry.

The presentation follows the general format of the *Dictionary of Organic Compounds* and much of the information is derived from that publication, but each such entry has been reviewed and updated. In addition a large number of new entries have been added. The latest references noted were to the 1986 literature.

Monosaccharides constitute the major entry type and include examples of thiosugars, aminosugars, halogenosugars, unsaturated sugars, etc. Within each of the above types of monosaccharides, available derivatives are cited with physical constants noted so that the book provides great assistance to synthetically oriented carbohydrate chemists. Similar information is supplied for a large number of disaccharides and, to a much smaller extent, for oligo- and polysaccharides. There is an extensive coverage of information for glycosides and nucleoside antibiotics and for important nucleosides and derivatives. Many entries are concerned with complex natural glycosides. In addition to physical constants, entries often include information about sources, medicinal or other uses, and succinct statements of biological activity data. The literature references for each entry often note where synthetic information, NMR data, etc., can be found.

The volume is arranged alphabetically by entry name and each entry is assigned a number that also applies to the derivatives. There are four indexes each one of which refers to the entry numbers noted above so that a superb system of cross-referencing exists. A Name Index lists every compound name or synonym in alphabetical order. A Molecular Formula Index follows and, in turn, is followed by a CAS Registry Number Index, listed in serial order. Finally a Type of Compound Index is supplied which has 102 headings, e.g., *lyxo*-Pentoses, *gluco*-Hexoses, 2,3-Anhydrosugars, 4-Amino-4-deoxysugars, Unsaturated sugars; 3-enes, Glycuronic acids, Cyclitols, Antibiotics, Nucleosides, etc.

This Sourcebook contains an enormous amount of information that will be helpful to researchers who deal with any of the types of molecules enumerated above. Certainly every library that is used by such researchers should have a copy. I think it might be made more accessible to individual ownership if it were divided into two volumes. One with the mono-, di-, oligo-, and polysaccharide entries that have more relevance to the synthetic chemists, and a second one containing the natural product glycosides, antibiotics, and nucleosides. Perhaps a further condensation could be possible by a more rigorous definition of "carbohydrate". I noted a number of entries, e.g., succinic acid, 1,2-ethanediol, 1,3-propanediol, 1,4- and 1,5-pentanediol, 2,2-diphenyl-1,3-dioxane, nitroglycerine, brevicomin, 3,4-dihydropyran, etc., which, I think, have less significance for carbohydrate chemists. Finally, it must be noted, as the Editor indicates in the Preface, that this book represents

a first, but very useful, scan of the literature. There are necessarily many omissions of carbohydrate molecules, and the fact that a given compound cannot be found in the Sourcebook is not an indication that it does not exist in the literature.

Leon Goodman, *University of Rhode Island*

Samples and Standards. By Brian W. Woodget (Hatfield Polytechnic, U.K.) and Derek Cooper (North Staffordshire Polytechnic). John Wiley & Sons: New York. 1987. xvii + 299 pp. \$21.95. ISBN 0471-91290-5

This is the first volume in a series of 29 "open learning" books on analytical chemistry. The book is designed to be used for self-instruction or instruction with a tutor. It contains numerous self-assessment questions scattered through the text, and the final quarter of the book consists of detailed answers to these questions. The book seems to be intended for technicians in industrial laboratories.

The book contains three main parts. A somewhat pedantic introductory chapter discusses the analyst's approach. This is followed by three chapters on sampling. (For example, how should one go about determining the composition of material filling an entire coal car?) This is the best part of the book, because it addresses a subject often omitted in the training of analytical chemists. Readers will gain an understanding of why sampling protocols are sometimes elaborate and why the quality of sampling often controls the quality of the result reported by an analyst. The final part consists of 7 chapters on standardization and calibration. These chapters deal in considerable detail with such topics as fitting a straight line to data by the least-squares method, calibrating with standard additions, using internal standards, and so forth. An attempt is made to discuss these topics in a completely general way, without reference to specific analytical methods. The wisdom of including this material is questionable. Other books in this series, dealing with specific methods, will almost certainly need to cover these topics as well.

George R. Helz, *University of Maryland*

Photochemistry in Organic Synthesis. Edited by John D. Coyle. Royal Society of Chemistry: London. 1986. vii + 333 pp. \$71.00. ISBN 0-851-86656-5

The appearance of a second book on the application of photochemistry to organic synthesis within two years of the publication of *Synthetic Organic Photochemistry* (Plenum Press, 1984; reviewed in *J. Am. Chem. Soc.* 1985, 107, 7237) attests to continued interest in the technique. *Photochemistry in Organic Synthesis* shares a number of authors and overlaps with the earlier book. In spite of its smaller size, however, the present book is a more complete overview of classical organic photochemistry than the earlier book, which examines more limited areas, including the newer field of photoinduced electron transfer reactions, in greater depth.

Several chapters in *Photochemistry in Organic Synthesis* are devoted to practical aspects of photochemistry, including an unusual chapter titled "Practical Photochemistry: Scale-up" by K. H. Pfoertner, a discussion of the experimental and economic considerations involved in choosing photoreactions that are suitable for production on an industrial scale, and light sources and reactor design for such reactions. The chapter "Photoinitiated Free-radical Chain Reactions" by J. Hutchison also has a practical bent. Other chapters (sixteen in all) are "Basic Principles" and "Alkaloids" by J. D. Coyle; "Practical Photochemistry: General Considerations" by J. Hutchison; "Carbonyl Compounds: α -Cleavage" by R. F. Newton; "Carbonyl Compounds: Hydrogen Abstraction" and "Terpenoids" by W. M. Horspool; "Carbonyl Compounds: Cycloaddition" and "Enone and Dienone Rearrangements" by H. A. J. Carless; "Steroids", "Alkenes: Isomerization and Rearrangement", and "Aromatic Compounds: Substitution and Cyclization" by A. Gilbert; "Alkenes: Cycloaddition" by P. A. Wender; "Alkenes: Photo-oxidation" by K. H. Pfoertner; and "Aromatic Compounds: Isomerization and Cycloaddition" by P. A. Wender and T. W. von Geldern.

Each chapter gives a brief introduction to the type of reactions covered and then examples of the application of the reactions to synthetic goals. Some mechanisms are shown. Some of the chapters are more comprehensive than others in the survey of the relevant literature, but all provide chemists who may not be familiar with the technique adequate leads into the different areas of photochemistry.

The book suffers from the lack of an index. The table of contents, which could have compensated partly for this lack by being more detailed, consists only of the title of the chapters. The book is not typeset, so it also suffers from an uneven quality in type and structural formulas. My copy also included badly smudged pages. On the other hand, this method of production makes it possible to include references to the 1986 literature in a book published that year.

Seyhan N. Ege, *University of Michigan*