

Computer Software Reviews

ENTVAPOR, A Retrieval and Computation System. Blackwell Scientific Publications Ltd. (for the International Union of Pure and Applied Chemistry—IUPAC): Osney Mead, Oxford OX2 0EL, United Kingdom. Standard Price: US \$150.00. IUPAC Affiliate and Committee Members: US \$112.50.

ENTVAPOR is an interactive menu-driven program for computation of the enthalpy and entropy of vaporization at 298.15 K of over 600 organic compounds. Published for IUPAC by Blackwell Scientific Publications, the program comes on a single 3.5 in. low density floppy disk and occupies about 438 K of disk space when loaded (a 5.25 in. version is available). PC-DOS or MS-DOS 2.0 or higher is required, along with 512 K or more of RAM. The program is not copy protected and can be run on either a floppy disk or copied to a hard drive.

The data contained in ENTVAPOR are derived from a project of the IUPAC Subcommittee on Thermodynamic Tables at the Institute for Chemical Technology in Prague. All values are from calorimetric data; no data derived from vapor pressure measurements for from chromatography are included. The database is available in manuscript form in the IUPAC publication *Enthalpies of Vaporization of Organic Compounds, Critical Review and Data Compilation*, by V. Majer and V. Svoboda (Blackwell Publishing, 1985).

ENTVAPOR calculates the enthalpy and entropy of vaporization and the standard enthalpy of vaporization at 298.15 K for the compounds in its data base, and extrapolates for other temperatures where the original data justify such extrapolation. Extrapolation and interpolation is accomplished by fitting the temperature and critical temperature of the compound of interest to a 3-parameter fitting equation. Quoting from the manual, "A special algorithm was developed to determine temperature limits of reasonable extrapolation and to establish the expected accuracy of the experimental data. The following factors were taken into account; accuracy of the experimental data, chemical type of a substance, width of temperature range where experimental data were available, location of this range on the vapor pressure curve". Extrapolation is not

permitted for compounds whose critical temperatures were not available.

Operation of the program is on a menu-driven text system. The user is prompted for a Property Option (choice of Enthalpy and Entropy of Vaporization, Standard Enthalpy of Vaporization, or a Help file). Next, the user is prompted for the units, the choices being either kJ/mol or kJ/kg, and either Kelvin or Celsius for temperature. Searching for the compound of interest is accomplished by CAS registry number, official IUPAC chemical name, empirical formula, or compound class. When searching by name, a maximum of 30 characters is used for the search. If the search is unsuccessful, the user is returned to the search menu to try again. When a compound is selected, the following information is given: IUPAC name, empirical formula, CAS registry number, code in the IUPAC publication, molar mass, normal boiling point and critical temperatures (if available), temperature range of experimental data, and the temperature intervals over which the data can be computed with a given uncertainty. The user is given 5 computation options depending on the data available for the compound. Enthalpies and entropies are then listed with expected maximum absolute and percent errors. When computations are performed outside the temperature interval of the experimental data, an "E" is displayed.

ENTVAPOR is not a universal program for all chemists. However, when needed, it is a handy program for retrieving basic thermodynamic data, and for calculating values. The thoroughness of the IUPAC committee on critically evaluating the database, and on conservatively extrapolating the values along with the error limits, gives one considerable confidence when using the program. The use of a menu-driven data entry system is adequate, but a little archaic. Likewise, some difficulties could be encountered when searching for compounds when the CAS number is not handy, or the IUPAC name is long or confusing. However, the availability of a solid reference text, and the care with which the data were selected and evaluated, make this a solid program.

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Book Reviews*

A Specialist Periodical Report. Volume 20. Nuclear Magnetic Resonance. By G. A. Webb (University of Surrey). The Royal Society of Chemistry: Cambridge, England, 1991. xxii + 601 pp. \$230.00. ISBN 0-85186-432-5.

This is the 20th anniversary volume of the *Specialist Periodical Reports on Nuclear Magnetic Resonance*. One should congratulate the Editor, G. A. Webb, for his efforts which make the life of many NMR researchers easier in times of explosive growth of all literature. In the age of electronic literature retrieval, one may ask whether it is really worthwhile to continue this series, but after looking over this volume, the answer is a resounding yes. The reason for the success of this series lies in the excellent organization of each volume which covers specialized subfields of NMR. This series is valuable both for seasoned practitioners in NMR and researchers who are contemplating entering a specific subfield or want to use NMR in their studies.

After a list of symbols and abbreviations, this volume starts with G. A. Webb's compilation of books and reviews on NMR, and in particular, this chapter illustrates in an impressive way the progress and continued expansion of the field of NMR spectroscopy. Chapters 2–5, which deal with different aspects of nuclear shielding and spin–spin couplings, include C. J. Jameson's article on theoretical and physical aspects of nuclear shielding, and I. P. Gerathanassis addresses their applications. In a similar vein, theoretical aspects and applications of spin–spin couplings are covered by J. Oddershede and K. Kamienska-Trela and Z. Biedrzycka, respectively. The chapter by H. Weingartner discusses NMR relaxation phenomena in liquids and gases, and the increasing popularity of solid-state NMR spectroscopy is illustrated by the impressive number of references (632) given in Chapter 7 by C. J. Groombridge. The

chapter on multiple pulse NMR spectroscopy by L. Y. Lian is followed by a discussion of NMR studies of biopolymers (Chapter 9 by H. G. Parkes) and of synthetic macromolecules (Chapter 10 by A. H. Fawcett).

In view of a personal interest of the referee, Chapter 9 dealing with NMR studies of natural macromolecules will be discussed in more detail. This chapter was written by H. G. Parkes. This specific review is limited to NMR studies of polypeptides, proteins, polynucleotides, and polysaccharides, as including studies of lipids, membranes, biosynthesis, and metabolic studies would have made this review essentially unmanageable. As in the other chapters, the centrality of NMR in a specific study provided the selection criterion for its inclusion.

This review has four main sections dealing with linear and cyclic peptides, polypeptides and proteins, oligo- and polynucleotides, and saccharides. In each section, the author reviews the NMR techniques focusing on new approaches used to solve a specific problem. Tables 1–4 are particularly useful, since in addition to the literature reference and the labelling of the systems and nuclei studied, one finds for each entry a comment which specifies the main object of the study, e.g., conformational equilibrium from NOESY assignment, the role of salt bridges in β turn, protein folding intermediates, etc. This type of review is of great value when one considers the overwhelming number of publications, particularly in the field of NMR spectroscopy applied to biopolymers. There are 527 literature references in Chapter 9.

The wide spectrum of problems where NMR experiments play an important and/or decisive role documented by Chapters 11 (C. Jones), 14 (P.-O. Westlund), and 15 (A. Khan), which discuss conformational analysis, NMR studies of paramagnetic systems, and NMR studies of liquid crystals and micellar solutions.

The rapid expansion in the biomedical applications of NMR spectroscopy is well documented in Chapter 12 by P. G. Morris, which is devoted to NMR spectroscopy of living systems, and Chapter 13 on

*Unsigned book reviews are by the Book Review Editor.

NMR imaging of living systems by S. C. R. Williams. In the introduction to Chapter 13, S. C. R. Williams points out that due to the limited length of the article and the vast number of literature references of NMR imaging (>4000), it was necessary to omit many specialized clinical case studies.

By including references in Chapter 1 dealing with books and reviews, the total number of references cited is 5006, covering the period from June 1989 through May 1990.

In summary, this monograph will be particularly valuable to those who want to get rapidly familiar with a specific subfield of NMR spectroscopy and who do not get discouraged by the relative high price of £140 (US \$230.00).

Jiri Jonas, *University of Illinois*

Stereochemistry of Organic Compounds. Principles and Applications. By D. Nasipuri (Formerly Professor of Chemistry, Indian Institute of Technology, Kharagpur, India). John Wiley and Sons: New York. 1991. xx + 527 pp. \$41.95. ISBN 0-470-21639-5.

In a detailed preface, the author indicates that this 15-chapter book is intended "to fill up the void in the stereochemical literature" which has existed since Professor E. L. Eliel's comprehensive textbook on stereochemistry was published in 1962. The author attempts to cover all major areas of fundamental organic stereochemistry at a level appropriate to an audience composed of advanced undergraduate and beginning graduate students. The author provides a summary of important concepts at the end of each chapter. However, "for reasons of space", no illustrative problems have been included, a regrettable omission in view of the fact that this book is intended for use as a textbook.

The first chapter presents basic concepts of molecular geometry and chemical bonding. Molecular symmetry and chirality are covered in the second chapter. Point group classifications are introduced in Chapter 2 along with sample molecular structures, which are used to illustrate symmetry concepts. Basic definitions and classifications of stereoisomers are presented in Chapter 4. Chapter 5 provides additional examples of stereoisomerism with primary focus upon concepts that relate to axial chirality, planar chirality, and helicity.

The sixth chapter deals with topicity and prostereoisomerism. Systems of nomenclature of stereoheterotropic ligands and faces are introduced, and the use of NMR spectroscopy as a method for the study of stereoheterotropic ligands is presented and discussed. Chapter 7 deals with racemization and methods of resolution. This chapter includes a discussion of physical methods by which optical purity and enantiomeric excess can be assessed. Methods used to determine absolute configuration of enantiomers and relative configuration of diastereoisomers are presented and discussed in Chapter 8.

Chapter 9 deals with conformational analysis of acyclic molecules. Particular attention is given to the use of physical methods in this regard. Conformations of cyclic systems are covered in the next two chapters (monocyclic compounds in Chapter 10 and fused ring and bridged ring compounds in Chapter 11).

Dynamic Stereochemistry is discussed in Chapters 12–14. The Curtin–Hammett Principle is introduced in Chapter 12, and conformational effects on reactivity are discussed. Several examples of stereoselective reactions are presented in Chapter 13, including a brief (13 pp) exposition of enantioselective synthesis. Pericyclic reactions are covered in Chapter 14.

Finally, molecular dissymmetry and chiroptical properties are discussed in Chapter 15. The principles of circular birefringence, circular dichroism, and optical rotatory dispersion are introduced. Empirical and semiempirical rules are presented by which the sign of the Cotton effect can be correlated with chiral environment.

The major strengths of this book lie in its comprehensive approach to the complex and far-reaching subject of organic stereochemistry and the level at which the subject matter is presented (which is appropriate to its intended audience). Of particular value is the fact that the author has stressed the importance of the role that conformational and configurational analysis plays in promoting improved understanding of reaction mechanisms.

However, some important weaknesses are also apparent. It appears that the book developed slowly over a number of years, and no real attempt has been made to render the subject matter current for a student in the 1990s. This failing is evidenced by the fact that there are relatively few references to primary literature at the end of each chapter, a very small percentage of which cite primary literature published since 1988. At the end of the list of references in Chapter 13, the author notes that "references 91 to 98 are later addition". Since these references to 1989–1990 chemical literature are not discussed in the body of the text of Chapter 13, their inclusion must be regarded as gratuitous.

Similarly, some of the more recent secondary literature sources (i.e., monographs and/or multiauthored treatises that deal with various aspects

of organic stereochemistry and have appeared since 1988) were overlooked in the lists of references. In addition, the vast majority of the examples used to illustrate pericyclic reactions in Chapter 14 have appeared in earlier treatments of this subject. No fresh insights into this topic are provided by the present author.

This book was produced inexpensively (the review copy was printed in India on very thin paper and was published by Wiley Eastern Limited: New Delhi) and is priced affordably. It is likely that it will find extensive use as a textbook in a graduate-level special topics course on organic stereochemistry. Eventually, it will face major competition from a second edition of Professor Eliel's stereochemistry book, which is now being prepared in collaboration with S. H. Wilen and L. Mander (Professor Eliel refers to this forthcoming book in his Foreword which appears in the present book).

While neophytes will find this book useful and informative, it is unlikely that more experienced students of organic stereochemistry will encounter many surprises therein. Nevertheless, professors of organic chemistry may want to keep a copy on hand, as they are likely to find numerous examples in this book which will greatly assist them in the task of preparing examination questions for organic chemistry courses and graduate-level "cumes".

Alan P. Marchand, *University of North Texas*

Handbook of Petrochemicals and Processes. By G. Margaret Wells (FRPI). Gow Publishing Company: Brookfield, VT. 1991. xii + 400 pp. \$120.00. ISBN 0-566-02775-5.

This book is a collection of data on organic compounds that are produced industrially in large quantities. Each compound has its own section which includes the following: synonyms; processes for production (with reaction schemes and flow charts); less significant processes; properties; applications; health and hazards; major production facilities; and licensors. This book will serve as an excellent source of information on industrially important organic compounds. It should prove to be especially valuable to academic chemists as it will serve as a convenient source of information on industrial processes. The text is at once clear, concisely written, and readable; it appears to be quite up to date.

Cyclobutrenes. The Chemistry of Benzocyclobutene, Biphenylene, and Related Compounds. By Michael K. Shepherd (School of Applied Chemistry, Polytechnic of North London). Elsevier: New York and Amsterdam. 1991. XIV + 332 pp. \$183.00. ISBN 0-444-88171-9.

This book is the latest member of the Elsevier series entitled *Studies in Organic Chemistry*, 44 of which have now appeared.

In 1967, this reviewer and M. J. Mitchell published the monograph "Cyclobutadiene and Related Compounds", in which we attempted to collect all that was known through 1964 on the subject of cyclobutadiene, as well as the known condensed aromatic cyclobutadienes. Since 1965, no further comprehensive review has appeared. Dr. Shepherd has now partially filled this gap with the present volume, in which the chemistry of the condensed aromatic cyclobutadienes (cyclobutrenes) has once more been reviewed, with emphasis upon the considerable developments of the last two decades. The author has omitted the chemistry of cyclobutadiene itself which, as he suggests, merits a future volume of its own.

A word to the wary is in order at this point. The author has chosen to employ the name *benzocyclobutene* for the totally unsaturated hydrocarbon usually referred to as *benzocyclobutadiene*, and *1,2-dihydrobenzocyclobutene* for the compound commonly referred to in the literature as *benzocyclobutene*. Without debating the intrinsic merits of one system of nomenclature over the other, I fear that the author's chosen usage may confuse many organic chemists who will expect to find the chemistry of 1,2-dihydrobenzocyclobutene discussed in this book.

Having dealt with this minor problem, Dr. Shepherd must be commended for collecting together in a well-organized manner a great deal of fascinating chemistry, most of which will be a revelation to the general reader, and an invaluable compendium for those with a special interest in condensed cyclobutadienes. There is no doubt that this work will attract new converts to this theoretically interesting and experimentally challenging area of aromatic chemistry.

The book consists of seven chapters, divided as follows: 1. Electronic Configurations and Physical Properties of the Cyclobutrenes. 2. Methods of Generation of Benzocyclobutene and Related Compounds. 3. The Chemistry of Benzocyclobutene and Related Compounds. 4. Methods of Preparation of Biphenylene and Related Compounds. 5. The Chemistry of Biphenylene and its Derivatives. 6. Substituted Derivatives of Biphenylene. 7. Annulated Derivatives of Biphenylene. 8. Heterocyclic Biphenylenes and Their Derivatives. In addition to a good subject index, appendices of NMR data are included. The largest portion of the book concerns the biphenylenes, and much useful unpublished work in this area is reported.

This volume is not only useful as fascinating browsing material, but it will stand for some years to come as the essential reference work in the field. Although its high price will exclude it from most private collections, it is an essential work for any serious chemistry library.

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Chemistry of Organosulfur Compounds. General Problems. Edited by L. I. Belen'kii. Ellis Horwood Ltd.: Chichester, U.K. 1990. 378 pp. \$129.95. ISBN 0-13-132051-3.

For those who are curious about the contribution of chemists in the "old" Soviet Union to organic sulfur chemistry, this book will be a good introduction. Of the 1225 references, approximately 35%, or over 400, are to work published by Soviet authors, sometimes in theses. This compilation is intended as an overview rather than a detailed review of the subjects included. The English is good and the typography is excellent (clear typeface, numerous well-drawn schemes, structures, and figures); but the book is rife with annoying errors, some of which could be misleading to a neophyte in sulfur chemistry.

There are 15 chapters, each by a Soviet scientist, covering topics in various categories: (1) uses of sulfur compounds in synthesis (anions, cations, desulfurization, thermal and radiochemical syntheses, introduction of sulfur into organic compounds, catalytic and photochemical methods); (2) physical methods (sulfur NMR, UV-IR, X-ray fluorescence, MS); (3) mechanism (free radical, uses of radioactive sulfur, photo-, thermo-, and radiochemistry); and (4) theoretical. The sections on the uses of sulfur stabilized carbanions (267 references), sulfur-containing electrophiles (99 references), and desulfurization (189 references) are of the most general interest. The bonding in sulfur compounds as revealed by X-ray fluorescence spectroscopy is covered in much detail (199 references).

Overall, the book is a mixed bag, comprising several useful and detailed reviews alongside briefer contributions on topics of more limited interest. Many of the topics also have been reviewed elsewhere, but are brought relatively up-to-date (and with an emphasis on work done in the Soviet Union) in this collection. Literature references as late as 1985-86 are included with a smattering of more recent ones including a 1990 "in press" citation.

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NMR and Biomolecular Structure. Edited by I. Bertini, H. Molinari, and N. Niccolai. VCH Publishers: New York. 1991. 209 pp. \$89.00. ISBN 1-56081-116-1.

The awarding of the 1991 Nobel Prize in Chemistry to Richard Ernst recognized not only the achievements of an extraordinary scientist but also the now-central role of NMR spectroscopy in modern chemistry and biochemistry. The editors of this well-produced multiauthored volume set as their goal the presentation of a "didactical (treatment) providing an introduction to...frontier NMR techniques while...(providing examples) of applications to macromolecular systems". The level is intended for graduate students in chemistry and biophysics.

The first chapter attempts a review of many technical considerations that arise in the collection and processing of NMR spectra in one and more dimensions. The chapter is ambitious in its breadth, is written in a breathless style, and is not always idiomatic. Tyros entering the field will not find the chapter useful, except as a catalog of things they should become familiar with, and more experienced practitioners will be able to skip it. The second chapter provides an admirable discussion of Overhauser effects in paramagnetic macromolecules and suffers only from an almost complete neglect of rotating frame experiments. Griesinger provides an introduction to three-dimensional experiments in Chapter 3 that will be useful to those already experienced with two-dimensional NMR. The focus is mostly on homonuclear experiments; recent heteronuclear experiments emerging from other labs, especially those at the NIH, are not included. Techniques for fitting observed Overhauser effects to structural models are discussed in Chapters 4 and 5, with Chapter 5 also summarizing nicely results from Kaptein's studies of the *lac* repressor headpiece-operator complex. A long chapter by Gorenstein and his co-workers reviews studies of oligonucleotides by proton and phosphorus-31 NMR. The last chapter in the volume summarizes observations made with the enzyme dihydrofolate reductase by Feeney and his collaborators that provide indications of the presence of multiple conformations of the enzyme and ligands bound to it. NMR is unique in being able to furnish information of this nature about biomolecular systems, and this chapter is an appropriate closing to the volume.

In nearly all chapters the most recent references cited are from 1988; the evident long publication delay in fields that move as rapidly as these is disadvantageous to everyone involved.

The applications of NMR spectroscopy to investigations of biological structures are many, and it may be that no one volume can survey the

field adequately. The present volume contains no mention of structural studies of polysaccharides or membranes, for example. Nonetheless, because of the high quality of many of the presentations the book deserves a place on the library shelf. For reasons of limited scope, dated references, and steep price, students could probably more profitably invest in other works.

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Lipid Biochemistry, An Introduction. Fourth Edition. By M. I. Gurr (University of Reading and Oxford Polytechnic) and J. L. Harwood (University of Wales). Chapman and Hall: London. 1991. viii + 406 pp. \$89.95 (cloth); \$42.00 (paper). ISBN 0-412-26610-5 (cloth); ISBN 0-412-26620-2 (paper).

This newly re-written introductory text to lipid biochemistry does an admirable job of integrating a traditional treatment of the lipid biochemical pathways of microorganisms, plants, and animals with a number of contemporary topics of interest and relevance, including lipids in health and disease, protein biochemistry and molecular genetics of lipid metabolizing enzymes, and laboratory techniques in lipid biochemistry. Intended primarily as a text for undergraduate courses in lipid biochemistry, this book will not only superbly serve this audience but, because of the depth of treatment of many topics, will also serve as an excellent general text for the graduate student or practicing researcher.

The arrangement of the material is perhaps one of the most notable features of the revised text, and an introductory chapter helps to provide overall perspective on this arrangement as well as introduce basic concepts and definitions. The second chapter gives a brief summary of the techniques used in studying the molecular structure of lipids with emphasis on their separation by chromatographic methods. Chapter three focusses further on the structures of lipids and then provides a comprehensive treatment of the biosynthesis and catabolism of fatty acids. A final section of Chapter 3 gives an overview of essential fatty acids and briefly describes their metabolites, the eicosanoids. The biosynthesis, storage, and catabolism of energy storing triacylglycerols is covered in depth in Chapter 4. Chapter 5 breaks the flow of presentation somewhat but provides a well written, fascinating, and up to date account of dietary lipids in human health and disease, focussing special attention on essential fatty acids and lipoprotein mobilization of lipids in the body. Additionally, this chapter contains a number of extremely useful summary tables on the compositions of lipid oils in nature and human diets. This is followed by a nicely detailed discussion of current thoughts on membrane structure and then a description of the biosynthesis of various classes of complex lipids (phospholipids, sphingolipids, and cholesterol). A final chapter discusses a wide variety of lipid functions not discussed elsewhere in the text, from a number of additional functional features of membranes and their receptors to the role of lipids in pulmonary surfactant, immunity, cancer, skin diseases, and lipid storage diseases. The text finishes with an adequate although not extensive index (18 pp). This is in part ameliorated by cross referencing of relevant sections within the text. This is particularly helpful in this "functional approach" to the text construction which results in the treatment of different dimensions of some topics (e.g., essential fatty acids) occurring in 3 or 4 different locations in the book.

The style of writing is clear and concise in a consistent manner throughout the text. Each chapter is followed by a rather extensive set of references to book reviews and primary literature. The narrative is frequently punctuated with meaningful tables of data, chemical structures, and biochemical flow diagrams. While these black on white diagrams are clear and well composed, there is just no substitute for color for making complex metabolic pathways easily comprehensible. A fairly normal number of typographical errors, such as the redoubtable penta-valent carbon atom, are present in these graphical materials. A few factual errors exist in the brief treatment of the eicosanoids and the sphingolipidoses, perhaps in part due to rapid developments in the understanding of these fields. Further, the rather dense construction of the page format (6" x 9"), absence of marginal notes, and frugal use of bolding of text items combine to force the reader to introduce his/her own marginal notes and highlighting in order to derive and retain the essence of these detailed discussions.

Altogether, this is a well-written, well-conceived account of lipid biochemistry that nicely integrates health and molecular biological features of lipid biochemistry with the classical treatment of the pathways. Comprehension of this inherently complex and detailed material will demand the reader "actively participate" in the reading and outlining of the text. Its up-to-date and multifaceted treatment of lipid biochemistry, and referencing to the primary literature, will be well appreciated by the student and researcher alike.

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