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 or 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. Gerothanassis 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.