COMPUTER SOFTWARE REVIEWS

Desktop Molecular Modeller

C. J. H. SCHUTTE
Chemistry Department, University of South Africa, P.O. Box 392, Pretoria, South Africa

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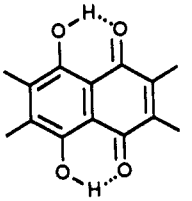
The *Desktop Molecular Modeller*,[1] written by M. James, C. Crabbe, and John R. Appleyard and published by Oxford University Press, is a very handy molecular graphics program which is primarily intended to teach and to make the student familiar with the procedures of molecular graphics and with the energy minimizations of molecular mechanics programs. The program is designed for IBM-compatible PC computers, as well as PS/2 computers, and can thus be used by practically every student.

The required background theory to understand the energy minimization procedure is to be found in Vinter et al.,[2] and Appendix D gives a short list of references for the inquiring reader which introduces him to the most important literature on computer graphics, structural data bases, structural analysis, etc. This appendix also contains a list of all the references cited in the manual.

The *Desktop Molecular Modeller* (DTMM) has a structural data file (similar to those of the *Cambridge Data File*) from which can be loaded molecular fragments or even whole molecules which can then be used to build up other molecules in three dimensions. The displays on the screen can easily be changed from line models to ball-and-stick models to space-filling models. The molecules can be easily rotated to be viewed from different orientations to make the student familiar with habitually thinking in three dimensions. I have found the procedures to construct these molecules and to rotate them very easy to grasp and to use. The program can handle quite large molecules (1500 atoms and bonds, or 1800 atoms and bonds for the mathematical coprocessor version).

The energy minimization routine works very smoothly, and I was quite pleased with the results I obtained for a wide range of molecules. One of the tests which I applied was to rotate one of the OH-bonds of the intramolecularly H-bonded molecule naphthazarin or 5-8-dihydroxy-1-4-naphthoquinone (I) out-of-plane of the molecule. The program had no difficulty in rotating the OH-bond back into the plane of the molecule again within a very reasonable period of time. I must admit that the process is a bit slow on an XT PC without a mathematical coprocessor, but I had no complaints on a 10-MHz AT equipped with a coprocessor. The larger the molecule, the longer the convergence time; the reader is adequately warned about this in the manual.



(I)

The program works with very clear pull-down menus, and the average reader should be able to grasp the manual without any trouble and to venture designing molecules without any trouble. The manual is very lucidly written, and the drawings, done with the data of DTMM pulled into *Ventura Publisher*, show the power of this little program. I had some trouble, however, in deciding how to produce my own drawings. I found that they produce quite easily with *PC-paintbrush*, which is within the reach of the budget of most students.

The program contains some examples which can be worked through by the user to teach, to enlighten, and to delight. I found them very instructive.

To summarize: I find that this program can be recommended to both the professional chemist who wants to work away from his mainframe, as well as to the student who desires to educate himself in molecular geometry and in the complex calculations involving energy minimization techniques.

REFERENCES AND NOTES

(1) Crabbe, M. J. C.; Appleyard, J. *Desktop Molecular Modeller*; Oxford University Press: 1989. The list price is $95.00, except in the EEC, where it is £295 (ISBN: 0198552734; Oxford Electronic Publishing, Walton St., Oxford OX2 6DP, U.K.; Phone: 44-865-567-67; FAX: 44-865-566-46).
(2) Vinter, J. G.; Davis, A.; Saunders, M. R. *J. Comput.-Aided Mol. Des.* **1987**, *1*, 31.

ENTVAPOR—A Retrieval and Computation System[1]

KENNETH N. MARSH
Thermodynamics Research Center, Texas A&M University, College Station, Texas 77843-3111

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This product was developed for the International Union of Pure and Applied Chemistry (IUPAC) Committee on Chemical Databases. This Committee was established in 1985 to advise IUPAC on all aspects of computerized databases involving chemical properties on the standardization of database formats and chemical structure records and policies concerning database dissemination. Another aim of this Committee is to promote within IUPAC, as well as the chemistry commu-

nity, a greater awareness of the potential application of computers in the management, dissemination, and use of chemical data.

One responsibility of this Committee is to encourage the development of computerized databases within the various IUPAC Commissions and Subcommittees. ENTVAPOR is the first database product released by this Committee. Other products are under development.

This product was developed by Drs. Vladimir Majer and William E. Davis at the University of Delaware and is based upon recommended values of enthalpies of vaporization presented in the IUPAC publication *Enthalpies of Vaporization of Organic Compounds, Critical Review and Data Compilation* by V. Majer and S. Svoboda of the Institute of Chemical Technology in Prague, Czechoslovakia (Chemical Data Series No. 32, Blackwell Scientific, Oxford, 1985). This publication and the software resulted from a project sponsored by the Subcommittee on Thermodynamic Tables of the IUPAC Commission on Thermodynamics.

The recommended values are based on calorimetrically measured enthalpies of vaporization of organic compounds. ENTVAPOR allows for the search, retrieval, and computation of enthalpies of vaporization over an extended temperature range.

The system comes on either a single $3^1/_2$ in. disk or two 360 K $5^1/_4$ in. disks. The instructions for either running the system directly from the disks provided or installing the system on the hard disk are not clear. For example, instructions should be given on how to make an appropriate directory on a hard disk. The system requires an IBM or equivalent PC running under MS DOS 2.0 or later with at least 512K of RAM. The system runs considerably faster from a hard disk.

The program runs and works without any problems. One disappointment is that the results of searches and calculations are not saved in a temporary file for printing. Results can only be printed using the print screen function. This is annoying.

The menu system is awkward, and the wording is archaic. The initial screen after the introduction and copyright screens asks if the user wishes to obtain enthalpy and entropy of vaporization or standard enthalpy of vaporization. This option seems to be in the wrong order. Once one has found a compound, one would wish to obtain either or both the enthalpy and standard enthalpy of vaporization. At present, one has to backtrack to the beginning of the program and repeat the selections.

The next two screens are the Units option. Despite the fact that this is a IUPAC product, the user should have a wider choice of units. The only choices here are kJ mol^{-1} or kJ kg^{-1} for the enthalpy and K or °C for the temperature.

Compounds can be searched by chemical name, formula, or Chemical Abstracts Service (CAS) Registry Number. The chemical name is restricted to the official IUPAC name, and there is only one name for each compound. This is annoying since if a matching name is not found (which occurs often), the system returns you to the property selection menu and two menus must be answered before an alternative name can be entered. The formula index search is equally awkward. For example: $C_2Br_2F_4$ has to be entered as C2.BR2.F4. A redeeming feature is that the entry c2.br2.f4, or entries with mixed upper and lower case can be used, but this is not stated in the help screens. However, the system cannot locate a formula such as C1.CL4.

The search by compound class is useful. However, working through only five compounds at a time is tedious, and it is unclear how and when you do the calculations after the selection as there are no online help screens to assist the user if he gets lost. The help file is useful, but the user has to discard his selections to go into that file.

The computation section is straightforward. For each compound, the molar mass, normal boiling temperature, and critical temperature are given. The authenticity of the last two values is not documented. An estimate of the accuracy of the data in various temperature ranges is given, and the calculations give the temperature, enthalpy value, and the expected error as both an absolute value and a percentage. It is unclear if the error refers to the accuracy of the measurement or the precision of the correlation.

After selecting a calculation for a compound at one temperature (say 298.15 K), the program takes you back three steps rather than allowing a calculation at a different temperature (such as the boiling point). This is annoying and time-consuming. Calculations can also be made at selected set temperatures, or at specific intervals over a selected temperature range. The parameters of the correlating equation can be displayed.

The system appears robust. However, I had problems a number of times when it did not recognize a number entered as requested. The system comes with a concise manual, which has annoying spelling and other mistakes.

For those requiring enthalpy of vaporization data for the limited range of compounds in this database, this is an adequate product.

REFERENCES AND NOTES

(1) Available from Blackwell Scientific Publishing. The price is $150.00 ($112.50 for IUPAC affiliates or committee members).