COMPUTER SOFTWARE REVIEWS

Desktop Molecular Modeller

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

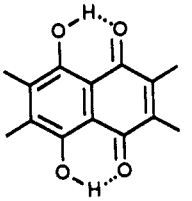
Received September 6, 1990

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

Received September 14, 1990

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-