Quantum Mechanics on a Microcomputer

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The Quantum Chemistry Program Exchange (QPCE, Creative Arts Buikding 181, Indiana University, Bloomington, IN 47405) has recently announced the availability of a compiled version of the Fortran-77 MOPAC Version 6.0 quantum chemistry package that will run on IBM/clone 386 and 486 microcomputers with math coprocessors. The price is only $125 for the compressed program on two 750KB 3 1/2-inch diskettes. Additional requirements for running the compiled version of MOPAC include 8MB of RAM, 10MB of disk space and the Phar Lap Dos Extender (Par Lap Software, Inc, 60 Aberdeen Avenue, Cambridge, MA 12138, $495). As delivered, the executable file will handle structures with up to 25 heavy (non hydrogen) atoms and 25 light atoms. (The normal workstation version of MOPAC is set for 40 heavy and 40 light atoms.) If the source files have to be recompiled for use with larger molecules, the NDP-Fortran compiler (MicroWay, Inc., P. O. Box 79, Kingston, MA, 02364, the 386 version is $695.; the 486 version is $995.) is required. Compilation for forty light atoms and forty heavy atoms will require 20MB of RAM.

In order to make the best use of MOPAC 6.0 a front-end program is uselful to prepare MOPAC input files by drawing on the computer screen, and to view and manipulate MOPAC output. PCMODEL Version 4.0 (Serena Software, Box 3076, Bloomington, IN 47402-3076) can be used to prepare MOPAC input files easily. MOBY Version 1.5 (Springer-Verlag NY, Inc., 175 Fifth Ave., New York, NY 10010), which will be available soon, will prepare input files for MOPAC, and also allow stereo viewing of the resulting structure with the ability to rotate the stereo view in real time. With the companion program, QC4MOBY, MOBY will display graphically (in motion) each vibration from the infrared spectra predicted by MOPAC and will also show graphical representations of the calculated molecular orbitals. (MOBY alone will run AM1 and MNDO calculations of molecules up to the size of glucose.)

Don't plan to do quantum chemistry on a microcomputer if you expect very fast calculations. A small molecule which can be run in less than a minute on an IBM RISC/6000 can take upwards of a half hour (using the AM1 PRECISE calculations).

I used a beta test copy of MOBY Version 1.5 this past summer in Organic Chemistry I, II. I found that students really enjoyed being able to construct and rotate stereoviews and to view infrared vibrations. After trhis experience, I am convinced that at least half of the students who currently pass organic chemistry do it without much of a sense of what an organic molecule looks like in three dimensions. This may explain why many students find organic chemistry so dfficult.

BOOK REVIEW COLUMN

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Many chemistry instructors are discovering that it's possible to do rather complex computer applications in their classes without expensive hardware or complicated software. A popular way of accomplishing this is to adapt commonly available spreadsheet programs for chemical problems. Most of the popular spreadsheets, like Lotus, Quattro, and Excel, include not only excellent graphing capabilities but also the mathematical functions that are needed for most types of chemical calculations. In addition, these programs are often available in inexpensive student editions and are relatively easy to learn.

Those who wish to pursue this approach need a textbook that teaches spreadsheet fundamentals using chemical examples. Such a book can both serve as a source of homework problems and also minimize the lecture time which an instructor must spend discussing how to use