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COMPUTER SOFTWARE REVIEWS

PCMODEL 9.2. Serena Software, Box 3076, Bloomington, IN 47402-3076. www.serenasoft.com. See Web site for pricing information.

PCMODEL is characterized by its developers as "a modeling program for organic chemists as opposed to quantum chemists", reflecting its root use of molecular mechanics for optimizations. It is touted for its ability to create high-quality graphics and movies and as an interface to quantum chemistry programs, listing several for which it can create input files or run automatically. It can also read and write many types of chemical information files. Developed for the Windows platform, it has recently been ported to the Macintosh OS X and Linux platforms. We tested the program on a PC running Windows Vista and on several Macintosh PowerPC computers running OS X 10.3.9 or OS X 10.4.11. We did not install it on Macintoshes containing Intel CPUs, so we do not know if the program runs natively or under Rosetta mode or at all on these. We also did not install the program on systems running OS X 10.5, as the developers indicated that problems occur when running PCMODEL under this release.

General Comments. We did not test the molecular mechanics or semiempirical implementations extensively. However, the tests we did perform finished quickly, requiring only seconds to minimize large molecules on the slowest CPU. We found that minimizations routinely located reasonable structures, even when the starting structures were fairly distorted. The modules for rotational energy barriers and dihedral drivers proved especially user-friendly, giving a relatively straightforward and fast way to calculate and present related energy values. Thus, PCMODEL can provide useful starting structures for quantum chemistry suites. That said, although the program generated correct input files for several such suites (including ones for Gaussian 03 ONIOM jobs, impressively), we found it impossible to use it as a graphical interface to Gaussian 03 M on the Macintosh. PCMODEL could not initiate the G03 executable on our machine in several tests.

The manual provides step-by-step tutorials for learning the program. PCMODEL is sufficiently nonintuitive that we recommend new users run these while taking notes. In this respect, we cannot recommend PCMODEL as a teaching tool for beginners. For example, building molecules from scratch is challenging; e.g., one cannot just click on the drawing window to generate atoms—one must enter Draw or Build mode first. The use of commands to push atoms figuratively into and out of the plane of the monitor screen requires patience and often several reorientations during the process. To allay this somewhat, PCMODEL provides templates for a number of organic, organometallic, and biomolecules. Once the molecule has been drawn, it can be manipulated, rotated, and displayed in a variety of ways, including Pluto and CPK renditions for small molecules and ribbon and backbone renditions for proteins. Enantiomers and epimers are easily generated; fusing of rings proved more straightforward than in other programs. PCMODEL accurately assigned point groups to molecules built reasonably symmetrically. The movie creation module worked very well, and the resulting movies showed no jerkiness, even when the molecules were rendered with high resolution.

Macintosh Version. Macintosh users will find PCMODEL to be a "work in progress", reflecting its infancy on the platform. We found that certain features consistently caused the program to crash. The PC-oriented manual rarely reflects unique features of the Macintosh GUI. The interface is insufficiently "Mac-like" to allow immediate, efficient use of the program.

The main drawing window layout is simple and clean, using the standard Aqua brushed-metal theme. Once a molecule has been drawn, interface behavior is fairly straightforward, following the comments made above. Generally, we found that, with the knowledge from the tutorials and the manual as background, we were able to accomplish the desired tasks of minimization, modification, printing, and creating movies. However, we found several frustrating quirks in the interface. Foremost among these were inadequate responses to input. For example, buttons on the Tools menu, which appears to the left of the drawing window, flash blue when pressed, but they do not hold that color or present any other sign that the item was selected. Since this menu acts as the major controller for interaction between user and program, users will generally be uncertain what menu mode they are in. Atom-labeling options were inflexible, detracting from the otherwise impressive graphics-rendering features.

Windows Version. PCMODEL displays fewer problems on this platform, making its positive points stand out. Graphics output, once a molecule was built, was particularly notable. Compared to the Macintosh version, fewer annoyances were discovered during testing. The only constant source of frustration involved creating and locating files under Vista. We found that files generated by PCMODEL could be located within the environment of the program but would not appear in that of the operating system. Vista would eventually locate the files (noting a shortcut problem), but this points to a problem in the interaction between PCMODEL and the operating system. This was not resolved when Vista was run in XP Compatibility mode.

PCMODEL has some impressive features and may serve both academic research and industrial institutions as an environment for molecular graphics/creating movies/presentation and as an interface to programs in quantum chemistry. Its molecular modeling implementations are fast and stable. However, owing to the quirks within and decisions made in developing the program, potential users need to evaluate whether PCMODEL's strong abilities for creating graphics outweigh its frustrations. We strongly recommend potential purchasers test a trial version to see if PCMODEL meets their needs.

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