Additions and Corrections

L-Methionine Methyl Is Specifically Incorporated into the C-2 and C-7 Positions of the Porphyrin of Cytochrome c_3 in a Strictly Anaerobic Bacterium, *Desulfovibrio vulgaris* [*J. Am. Chem. Soc.* **1993**, *115*, 12185–12186]. HIDEO AKUTSU,* JANG-SU PARK, AND SEIYO SANO

Page 12186: The source of the IUPAC-IUB atom-numbering scheme for heme *c* (Figure 2A) is a paper by Mei-Hing Chau, Meng Li Cai, and Russell Timkovich [*Biochemistry* **1990**, *29*, 5076–5087]. We regret the omission of this reference. Also, the bond between C5 and C6 of the heme *c* in Figure 2A should be a double bond.

Computer Software Reviews

AMPAC, Version 4.5. Semichem, Inc.: 7128 Summit, Shawnee, Kansas 66216. Voice: (913)268-3271. FAX: (913)268-3445. E-mail: aholder@vax1.umkc.edu. List price: $9995.00; educational discounted price $800.00.

AMPAC 4.5 is the second commercial release of Prof. Michael J. S. Dewar's general purpose semiempirical molecular orbital program. Prof. Michael Dewar has handed over the development responsibilities and commercial rights to Dr. Andrew Holder, President of Semichem (also, a professor at the University of Missouri–Kansas City). Dr. Holder not only is responsible for supporting the AMPAC software but also will continually be adding new capabilities. The distinguishing factor between previous versions of AMPAC and the commercial one is that the commercial version has a graphical user interface (GUI). The GUI enables the user to prepare input structures for computation and to analyze the computational results. Since the GUI was programmed to Motif/X Window System specifications, it will run on any computer which supports X. The real advantage of an X-based GUI is that the program can reside on a main computer (e.g., a Cray supercomputer) and the GUI may be used remotely over ethernet on several different workstations. The GUI is not integrated with the computational module of AMPAC which means that the user cannot directly submit jobs for computation from the GUI and must do so from the command-line interface. Computers which are supported in running the computational module and the GUI include Silicon Graphics, DEC, IBM RS6000, Hewlet-Packard, Convex, and Sun. People who want to know more detailed information about these supported computer systems should contact Semichem.

AMPAC is distributed in two ways: magnetic media (e.g., tape) or electronically (ftp to a host computer at Semichem). The actual installation of the software is straightforward. A software key-license file must be installed in the appropriate directory for running the GUI and the computational module. This key-license file will notify the user of the expiration of the license. Scripts are provided for running the computational module and may need some minor editing, depending on the particular computer environment. For example, on a Silicon Graphics Indigo computer, no script modifications were necessary; however, the scripts needed some minor modifications to take into account the batch environment of a Cray supercomputer with the Unicos operating system. Another consideration in installing the program is choosing the particular computational module executable which depends on the amount of memory (RAM) and the particular computer. For example, the executable, amp100.exe, will run fine in 32 Mbytes of memory on most computer systems (the Cray is an exception) and is limited to a molecule with no more than 100 heavy atoms and 100 hydrogens.

Some of the capabilities of AMPAC 4.5 computational module are: SAM1, AM1, PM3, MNDO, MNDOC, and MINDO/3 Hamiltonians; RHF, UHF, and CI (useful for predicting UV–visible spectra) methods; geometry optimization to local minima or transition states: reaction coordinate path calculation; intrinsic reaction coordinate calculation; simulated annealing for multiple minima searches; force constants and vibrational frequency analysis; solvation properties of molecules in aqueous solution; electrostatic potential surface and derived atom charges; and polarizability (nonlinear optical) properties.

The SAM1 method is the new, improved successor to the AM1 procedure and is available for H, C, N, O, F, Si, P, S, Cl, Br, and I. This new theoretical model computes the two-center two-electron repulsion integrals in a manner different from the previous methods which should allow the study of molecules containing elements with d orbitals. In fact, it is planned that future releases of AMPAC will include metals from the first transition series. For geometry optimizations of minima or transition-state structures, the eigenvalue following (EF) algorithm is available. Methods are available for studying reactions paths: (1) drive a particular reaction (internal) coordinate of interest, (2) determine a transition-state structure between two minima, and (3) given the transition-state structure, calculate the properties at points along the reaction pathway from reactants to products. Simulated annealing is one of the newer capabilities and is used to collect a variety of possible conformational structures for a particular molecular system. This technique uses a Monte Carlo approach with explicit boundaries defined by the user for the changing coordinates. In my work, this method has been especially useful in finding most, if not all, of the minima structures of a 14-membered ring and its acyclic counterpart. One note of caution is that this capability requires significant computer time (e.g., the 14-membered ring required almost 10 h of Cray YMP time).

The remainder of this review will focus on the GUI since this is the part of the software package with which users will interact the most. As noted above, the GUI provides the means of setting up the input file for submission to the computational module. Molecules may be constructed an atom at a time, each selected with a particular coordination geometry, or from fragments which have been pre–minimized at the AM1 level. Bond distances, angles, and dihedral angles may be readily modified. For better viewing, the molecular structure may be rotated about or translated along the *x*, *y*, or *z* axes, using the three-button mouse. The molecule may be displayed and manipulated in wireframe or ball-and-stick mode. After the molecule has been built, its internal coordinates may be modified by bringing up the z-matrix editor window. Selecting a row in the z-matrix for modification highlights the corresponding atom on the screen. Atom ordering, optimization flags, and connectivity may all be changed within this editor. Although I found this feature to be a useful visual aid in fine-tuning the internal coordinate representation of a molecule, it could be greatly improved by clearly displaying the atom numbers next to the atoms at all times and by highlighting all the atoms involved in the internal coordinate representation of an atom when it is selected/changed in the editor. Finally, some of the computation keywords and associated values may be selected/set through a combination of dialog windows. Not all of the computational capabilities and input parameters are accessible through the GUI, and it will be necessary to edit the saved input file for certain types of computation. However, for geometry optimizations and vibrational frequency analyses, the GUI is quite satisfactory.

The GUI may also be used to analyze computational results. For a reaction coordinate path calculation in which an internal coordinate is varied incrementally, the energy as a function of the reaction coordinate may be displayed in a two-dimensional plot. The actual reaction coordinate may be animated as well in which the molecular structure changes as the program cycles through the reaction coordinates. The vibrational frequencies may be displayed in line format with a rough idea of what the relative intensities might be. A particular vibrational mode may be animated based on the corresponding Cartesian displacements in order to identify the normal mode. A graphical representation of the simulated annealing results may be displayed in which the conformer energies are sorted (lowest to highest) and plotted relative to the lowest energy structure. The user may view any of the minima structures by cycling through the points on the graph or by directly selecting a point on the graph.

The manual does a very good job of explaining the setup of an input file for the computational module. All the keywords are briefly defined,