AMPAC 4.5[1]

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AMPAC 4.5 is the latest commercial version of software originally developed in the Dewar group for general purpose semiempirical calculations. It is currently supported on Unix and VMS platforms, including Silicon Graphics, DEC (VAX/VMS, Alpha (VMS and OSF/1), DECStation), IBM RS6000, Convex, Cray, Hewlett-Packard, and Sun. A PC version is available which includes the computational modules only. Use of the graphical interface requires the Motif/X-Windows protocol, which should pose no problem as virtually every platform presently available supports Motif graphics. The software includes most, if not all, of the semiempirical Hamiltonians in widespread use. SAM1, AM1, PM3, MNDO, MNDOC, and MINDO/3 parameters are available for use in both RHF and UHF (restricted and unrestricted Hartree–Fock, respectively) calculations. A variety of configuration interaction (CI) methods are also implemented, as are the property calculations users have come to expect in any computational chemistry program (e.g. transition-state location, force constants, and normal mode analysis). In addition, the program provides options for reaction path following, including calculation of the intrinsic reaction coordinate. Inclusion of the AMSOL model of Cramer and Truhlar[2] provides the user with insight into the energetics of solvation.

Several new features are to be found in this version of AMPAC, as well as updates to older features, improved documentation, and some bug fixes. In particular, I found the comprehensive listing of references helpful. It can be very annoying to try to track down the basic references to unfamiliar algorithms; the plethora of references sprinkled throughout the documentation goes a long way toward making this task bearable. The tables found in the second chapter are also a help. My students typically wallpaper the laboratory with photocopies of "useful pages" from various manuals. Most of that sort of information for AMPAC can easily be found in the second chapter of the documentation, which will hopefully improve the state of the walls in many labs and offices. SAM1 parameters for the halogens up to iodine are now available, as are polarizabilies calculated by a finite field method.

The graphical user interface (GUI) has been substantially expanded. It now provides display of vibrational models and line spectra. The latter is a special boon to those of us who were using home grown and, therefore usually, external code for visualizing line spectra from ab initio or semiempirical calculations. The integrated code is certainly more convenient. Reaction coordinate profiles can also be displayed; again, this means more accessible visualizing of these data. Several molecules can now be displayed simultaneously. Perhaps most useful to those using more than one computational chemistry package, and especially to users needing z-matrices, is a graphically based z-matrix editor. It should be noted here that the AMPAC GUI does not provide a seamless interface to the computational module, as do GUIs in some competing programs. It does greatly simplify the task of preparing input to AMPAC.

I installed AMPAC 4.5 on a Silicon Graphics Indigo from tape over a network. The instructions for installation are simple and clear. The only glitch I encountered was that I could not directly install the program over the network, using NFS, but needed to unpack the tape onto the machine with the tape drive and then move the files over to the machine on which I intended to actually run AMPAC. The customer support line at Semichem responded quickly to my question, and the problem was resolved that afternoon. Semichem accepts input by telephone, FAX, and e-mail. The last is particularly convenient.

I encountered no particular problems when using AMPAC 4.5. The code seems particularly robust in comparison to other semiempirical codes I have used recently. I tested the GUI, single point calculations, and optimizations using several of the available models for a variety of organic and organometallic molecules. When building molecules, the AMPAC GUI uses slightly different cues than the interface I usually work with, but after a bit of practice I had no trouble switching back and forth between the two programs. The only major lack I see in the GUI is not in the implementation but in the documentation. Most of the other major tasks in AMPAC are documented and include a worked example. The GUI is well documented, but a worked example of tutorial would be of great assistance in getting a new user up and running. Since I use these programs regularly in my graduate and advanced undergraduate courses, I find it helpful to have a ready made example to show the students, rather than having to write my own. Semichem tells me that a tutorial is in the works which should be available, along with the release of version 5.0 in May of this year.

In closing, I would highly recommend AMPAC 4.5 to both experienced computational chemists and the occasional user. Computational chemists will find up-to-date, robust code with most of the bells and whistles they are accustomed to having. Experimentalists looking for well tested methodologies will also find the code very usable. I would particularly like to recommend the code for teaching purposes. The availability of the GUI enhances the utility of this program for teaching. Many students these days are very comfortable with GUIs of all sorts and quickly adapt to using them for scientific input. The utility of AMPAC for teaching goes beyond the GUI; it is the only code that I am aware of that has a GUI and gives access to several semiempirical models for molecules that range from simple organic molecules to transition metal complexes. The speed of semiempirical theory, in particular, lends itself to teaching. One can show the principles of CI, solvation modeling, reaction path following, etc., without significantly compromising the time available for "real work". At academic prices, AMPAC and a suitable platform are affordable even for the junior level physical chemistry course. I look forward to seeing future versions of AMPAC from Semichem.

REFERENCES AND NOTES

(1) AMPAC 4.5. Semichem, 12715 W. 66th Terrace, Shawnee, KS 66216. List price: academic users, $800; industrial users, $10 000.
(2) Cramer, C. J.; Truhlar, D. J. *J. Am. Chem. Soc.* **1991**, *113*, 8305; 9901.