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COMPUTER SOFTWARE
REVIEWS

AMPAC 8 with AGUI (AMPAC GUI) for Mac OSX.
SemiChem, Inc., P.O. Box 1649, Shawnee Mission, KS
66222. http://www.semichem.com. Single-user commercial
pricing $4000 with customer support, $1200 without.
Single-user educational pricing $975 with customer sup-
port, $300 without. A special educational site license is
available for $2000.

SemiChem recently ported the AMPAC semiempirical com-
putational modeling program with its AGUI graphical user
interface to the Macintosh OS X platform. Although the UNIX
version has been reviewed previously (Bachrach, S. M. *J. Am.
Chem. Soc.* **2000**, *122*, 12411, Compaq TRU64 platform), given
the sizable Macintosh user base in chemistry and the many
improvements made to the software since this review, it is
appropriate to revisit AMPAC/AGUI and review its Macintosh
implementation. We reviewed version 8.16.5; updates up to
version 8.16.7 have been distributed as of March 2006. The
program requires at least Mac OS 10.2. We tested it on several
systems, including an iBook G3/667 MHz (OS 10.2.8), a Beige
G3/233 MHz (OS 10.2.8), a Mac Mini G4/1.4 MHz (OS 10.4.3),
and a Duo Core Power Mac G5/2.0 MHz (OS 10.4.4). The
program was impressively stable under all these conditions, even
though OS 10.4.4 and the Duo Core machine were released after
we received the software, so it had not been updated for these.
AGUI ran rather slowly on the G3/233 MHz machine, some-
times to the point of frustration; we do not recommend using it
with a CPU running at less than 500 MHz.

AMPAC/AGUI installation is not very Mac-like. The software
comes as a UNIX tar/gzip file rather than as a disk image (dmg)
file, and one installs it using the Terminal program rather than
through an OSX installer. Although an included text file gave
explicit and accurate instructions for installation, doing so still
required knowledge of the UNIX underpinnings and commands.
The license key file was sent separately by e-mail and arrived
corrupted. This is evidently common, so SemiChem makes the
application "keycleaner" available. This is a command line
executable with required options; unfortunately, finding the
documentation indicating the proper syntax was difficult (it is
available in a README file in the AMPAC folder and also on
the SemiChem Web site).

Once installed, the package behaves in a more Mac-like way.
Although one can run AMPAC from the Terminal command
line, we initiated jobs solely through the AGUI application.
Bachrach's review covered the model-building aspects of AGUI
extensively, and we recommend that readers interested in
AMPAC/AGUI read that review as well as this one. Listed
below are the improvements, strengths, and weaknesses we
noted during testing.

Improvements and strengths in AGUI:

(1) SemiChem has implemented the Aqua interface well.
Installations of XWindows or variants (X11, XDarwin, etc.) are
not required. Menus and windows display the brushed metal
frames of OS X and have properly organized buttons and

commands. Contextual menus are available through right-button
or control-button clicking.

(2) AGUI supports creating and submitting Gaussian03 jobs
as well as AMPAC jobs. An impressive, though incomplete,
number of Gaussian keywords are available from menus, and
most users of AGUI will find it an adequate interface to G03.

(3) The Atom List Editor has been improved, although we
consider it somewhat clunky. We would have preferred drag-
and-drop reorganization of the z-matrix/atom numbering, for
example. The Editor supports point group symmetry and will
force it on coordinate changes if requested. This sped up editing
the Atom List and subsequent AMPAC jobs. Particularly handy
was the menu system that allows the user to set a tolerance for
error in defining what symmetry a molecule should have.
Tolerances can be set to arbitrarily large values, although this
is *not* recommended, so AGUI can make molecules symmetrical
from atomic positions quite far from the symmetrically ideal
ones.

(4) AGUI allows the user to export graphics in TIFF, JPEG,
EPS, BMP, and PNG formats, allowing their use in publications
and Web pages. We examined TIFF files in detail and found
their color matching and resolution very good. Users will need
to choose their atom colors carefully, though, because there
appears to be no way to accentuate the atom spheres—by putting
borders around them, for example—so white and gray atoms
tend to blend into the white background.

(5) The slider bars in the distance/angle/dihedral windows
allow one to change the values and see the effect of the change
in real time. This makes orienting side chains to desired
conformations wonderfully easy.

Weaknesses in AGUI:

(1) The implementation of windows in AGUI could be
improved. We disliked the "builder window + working
window" approach to model building that AGUI uses. With
practice, working in the two-window mode becomes straight-
forward, but there is a learning curve associated with this. Those
used to the Macintosh interface will probably struggle most with
the fact that clicking in the working window to bring it from
background to foreground will also transfer the fragment from
the builder window. One must learn to click a background
working window only in the border area to avoid this.
Fortunately, AGUI allows multiple undos; the novice user will
often require these.

In general, foregrounding and backgrounding of windows
rarely worked correctly. This was particularly annoying when
calling up a Help window from another window. Interface
guidelines dictate that the requested window should appear in
the foreground, but this rarely happened. Moreover, in many
cases clicking the top bar of the Help window did not bring it
to the front; it had to be moved away from covering windows
to be accessed.

(2) The Help Viewer documentation is frustrating in that it
uses Windows graphics to illustrate command menus and screen

pictures, so some of the graphics do not illustrate what they should, and commands are Windows-type (e.g., Alt-C vs Command (Apple)-C to copy). Multiplatform users will not find this a problem, but Mac-only users will. Some important commands are undocumented. In particular, as is typical for Macintosh graphics programs, the shift-drag process moves the molecule around in the working window, while Command-drag resizes it. Novice users might be unaware of this.

(3) Some buttons and pop-up menus were too small to contain all the text they should. This is generally annoying rather than problematic but did occasionally mislead us as to what the pop-up menu contained.

(4) It is possible to rearrange the atoms in the Atom List to create a z-matrix that contains bond angles of 180°. This should be proscribed. To the program's credit, an error message appears when such a file is saved. However, we found this often pointed to a problem engendered by the error rather than the error itself, making resolution of the error challenging. For example, when the atoms of 1,2-diethynylbenzene were sorted so that the ethynyl hydrogen was atom1, the adjacent sp carbon was atom2, the triply bonded carbon was atom3, and the ring carbon was atom4, the Atom List showed the $3-2-1$ angle as 180°. When the z-matrix was saved, the error message indicated a problem with the dihedral angle for atom4, which in the z-matrix was an acceptable value of 180°. This will certainly prove confusing to a novice user or one unfamiliar with z-matrix rules.

(5) The AMPAC Help files, which are in html format and thus open in a browser, are unavailable in AGUI despite the fact that a menu command for accessing them appears, albeit grayed out, in the Help menu.

We note that SemiChem has promised to address all these criticisms in future revisions of AMPAC/AGUI. We believe them, as inspection of the revisions page of their Web site shows that the package is regularly and extensively upgraded.

Most of the changes to the AMPAC program are "under the hood" and so are invisible to the typical user. According to the documentation, the program now uses memory more efficiently and has an enhanced SCF engine, so that jobs run more quickly. Though we could not test this directly, since no older versions of the program exist, we found that all types of jobs ran quickly, even on slower machines. Configuration Interaction calculations, which predict excitation energies, ran impressively rapidly, given their computational intensity.

The publishers have devoted considerable effort to improve location and identification of transition states. Toward this end, AMPAC includes two new features. The LFORCE command generates a partial force matrix, providing a direction quickly for an eigenvalue-following optimization. The CHAIN algorithm links structures the user believes represent points on the potential surface between starting material and products. Despite these improvements, we found that locating transition states was a $50-50$ proposition, with the program unable to find or settle on several "standard" transition states, such as the six-membered cyclic array for the Diels−Alder reaction. This may speak more to the semiempirical methodology of the program rather than these modules.

Overall, SemiChem has implemented AMPAC/AGUI well on OSX, and the program will prove useful for those who employ semiempirical computational approaches. The program runs at an impressive speed, and it contains features for including configuration interaction and locating transition states that extend its capabilities significantly. The AGUI interface creates an ease-of-use level appropriate for undergraduate instruction, and the visualization modules for orbitals, surfaces, and vibrational modes provide concrete graphics and insight for students and researchers.

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