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COMPUTER SOFTWARE REVIEWS

AMPAC 9. Semichem, 12456 W, 62nd Terrace, Suite D, Shawnee, KS 66216. www.semichem.com. See Web site for pricing information.

AMPAC continues to be *the* complete semiempirical quantum-mechanical program. The AMPAC program development project was started by Dewar in the late 1960s and has been continued and expanded since 1992 by Holder and colleagues. The release of AMPAC 9 occurs four decades after Dewar published his seminal book *The Molecular Orbital Theory of Organic Chemistry*, and today AMPAC is the "flagship product" of Semichem, Inc., with AMPAC 9 its fourth major new release. The long history of AMPAC is described in exemplary fashion in the user manual, and the intellectual tradition is also reflected by the fact that Dewar continues to lead the author list that includes Holder, Dennington, Liotard, Truhlar, Keith, Millam, and Harris.

The installation of AMPAC 9 is very easy to perform; it is fully automated by an installation wizard and requires no more than a few minutes and basic computer literacy skills, i.e., directory trees, file extension assignments. We installed and tested AMPAC 9.1.3 on a PC. The semiempirical quantum-mechanical program AMPAC comes bundled with AGUI, the AMPAC graphical user interface, and the documentation for both programs is excellent. AMPAC comes with an extensive user manual, which is provided as a PDF file (738 pages) as well as a suite of locally stored HTML pages.

The most important and distinguishing new features of this release are the popular solvation models developed by the groups of Truhlar and Cramer, which we tested fully by studying solvation effects on the homolysis reactions of *N*-methyl-γ-picolinium ions and large annulated analogues. We are delighted to report that the software performed as advertised in all of these cases and that even the computation of solvated polyannulated radicals proceeded effectively. The new release also features important improvements in its configuration interaction (CI) module, and CI computations could be performed with or without solvation.

AMPAC 9 includes two new semiempirical methods developed by Stewart. The RM1 (Recife Model 1) presents a reparameterization of AM1 for H, C, N, O, P, S, F, Cl, Br, and I (*J. Comput. Chem.* **2006**, *27*, 1101−1111). The PM6 parameter set (*J. Mol. Mod.* **2007**, *13*, 1173−1213) is based on well-established experimental data and reliable results from *ab initio* and density functional computations. Most notably, PM6 provides higher accuracy in the modeling of intermolecular interactions.

Many years of experience and feedback from the growing community of computational scientists have contributed to the evolution of AGUI, and the latest version is simply outstanding. There are too many new features to discuss here—the developments include major improvements of 3D surface plots, improvements of the PBC editor and redundant coordinate editor, expanded fragment libraries, and much more—but I do want to highlight one feature that will be quite welcome by practitioners of the art. The analysis of "tricky" potential energy surfaces can be challenging, and to solve such problems usually requires the graphical inspections of many trial geometries along search paths. This inspection will be greatly facilitated with the new "multiview" feature of AGUI.

The licensing policy has been restructured to adapt to the needs of the modern computing landscape. The most significant innovation in this regard concerns the offering of a single-user site license category for academic institutions, which is designed to encourage the use of AMPAC in educational settings. Computation and simulation are integral to modern research in all of the life sciences as well as the materials-related engineering disciplines, and this reality should be reflected more fully in curricula for undergraduate education in the STEM disciplines. Although AMPAC clearly has been designed as a research tool, it also presents a powerful tool for authentic instruction of the next generation of interdisciplinary scientists and engineers.

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