Computer Software Reviews

AMPAC 6.6 with AMPAC 6.0 Graphic Interface. Semichem, Inc., P.O. Box 1649, Shawnee Mission, KS 66222. http://www.semichem.com. List price: $11,000. Educational price: $900

The AMPAC software package is, in fact, two separate programs that can be used individually or as a team. The first piece is the graphical user interface (GUI), called AMPAC 6.0 Graphical Interface. The second component is AMPAC 6.6, the computational engine. Codes are available for a variety of workstation platforms and Windows. This review is based on the version for the Compaq DEC Alpha platform. The code was delivered by FTP off of the Semichem server. Full and clearly defined instructions (along with a license key) are easily implemented, and this reviewer was performing calculations within five minutes of accessing the FTP site. Obtaining the program in this manner is certainly fast and efficient (and avoids the dreaded shrinkwrap and superfluous oversized box of most software packages), but the manual is then only available online, or must be printed by the user. Fortunately, a great deal can be accomplished with AMPAC without ever referring to the manual.

The main computing engine is the AMPAC program, which provides a superlative semiempirical quantum chemistry package. A full description of the package is really dependent on a scientific evaluation of the semiempirical models, which is well beyond the scope of this review. If the questions being asked and the molecules of interest are appropriate for analysis by the semiempirical method, AMPAC is more than capable of handling the situation. All of the standard semiempirical methods are available: AM1, MNDO, MNDO/c, MINDO/3, AM1, PM3, SAM1, and MNDO/d. Structures can be optimized to local minima or transition states, with a variety of optimization procedures. Effects of solvation can be assessed using the AMSOL or COSMO approach. Simple test cases including calixarenes, small poly amino acids, and DNA sequences all optimized quite rapidly.

The aim of any interface for a computational chemistry package is to streamline the creation of an input structure and the visualization and interpretation of the output. The AIMPAC GUI is generally successful in achieving this aim. It allows one to sketch a molecule, select the computational methodology and options, and submit the job for execution. The completed job can then be brought back into the same interface for the purposes of examining the structure, molecular orbitals, and electrostatic surfaces and animating vibrational modes. One nice extension of the GUI is that it is completely compatible with GAUSSIAN-98, allowing users to create input, launch the computation, and visualize output for this widely utilized ab initio program. (Although it is a bit outside the scope of this review, the AMPAC GUI did work seamlessly with G-98 and offers a nice builder for creating ONIOM calculations that can be awkward to prepare from scratch.)

To judge this GUI, I utilized it extensively over two months along with six undergraduate students who had no prior experience with any computational chemistry GUI. As an experienced practitioner in the field, I found the AMPAC GUI easy to learn and use for most applications. The graphical molecular builder allows one to construct a molecule one atom at a time or to add predefined groups, such as rings, amino acids, and organic functional groups. Altering a structure is accomplished by modifying distances, angles, or torsions by selecting the atoms involved and then using a slider (or typing in a value) to adjust the parameter. Unfortunately, these tools do not always accomplish the desired effect. For example, altering the distance between two atoms may change the relationship between other atoms in unanticipated ways; one cannot lengthen a bond by just moving one atom, because both atoms will move. In altering torsion angles, the user has the option of having the atom or the whole attached group respond to the change. Sometimes, it can be difficult to get the correct atom or group to move. A trick I discovered was to disconnect some atoms prior to adjusting the parameters; this offered finer control of the larger structure. Fortunately, the program has an effective multiple undo/redo option so one can experiment without fear of total loss.

Once the structure has been implemented, it can be “cleaned” to give a better initial guess. In my experience, the clean function works well for simple systems, particularly acyclic molecules, but can produce quite unreasonable structures for more unusual molecules. Again, the undo/redo function can bail one out.

With geometry optimization performed using the Z-matrix molecular definition, AMPAC provides the ability to edit the Z-matrix. The user can change the atoms used to define the connectivity, reorder the atoms, redefine the atom type (change a carbon to a nitrogen, for example), and select which parameters should be frozen and which optimized. I found these features particularly useful for taking one optimized structure and modifying it to create a related molecule. The program will forcefully keep one from making a critical mistake, such as using the same atom to define a distance and angle. My only serious complaint is that the interface does not recognize and utilize symmetry, so that symmetry-related parameters are not defined with the same variable. If one wishes to invoke the symmetry in this way, hand-editing of the Z-matrix must be done by invoking an editor outside of the interface.

With an initial guess in hand, the user can set up the job type by using drop-down menus and buttons to select the computational method, optimize to ground or transition state, calculate frequencies, incorporate solvents, etc. (Similar type options are available for setting up GAUSSIAN jobs as well, such as selection of basis set, computational method, etc.) The calculation can then be directly submitted from the interface, invoking AMPAC and directing the just-defined molecule as input. The status of submitted jobs can be monitored within the interface.

Once completed, the output file can be loaded into the GUI and analyzed. Distances, angles, and torsion angles can be obtained using the inquire button followed by selecting the atoms of interest. If vibrational frequencies have been calculated, the GUI can animate each vibration, an especially useful feature for interpreting IR and Raman spectra and for analyzing transition states. Unlike some other visualization tools that require external generation of the orbital density, total density, or electrostatic potential, these are readily generated by the GUI itself and then imaged. Manipulation of these surface plots is seamless and without flicker or hesitation.

The undergraduate students in my group who have utilized the AMPAC GUI have been universally pleased. They have found it to be easy to learn (without even knowing that a manual exists!) and critical for evaluating the results of their computations. Particularly useful has been the creation of input, where the interplay between the text input file and the three-dimensional representation lead to rapid development of accurate input files and visualization of vibrational frequencies, particularly the imaginary vibration in transition states. While not positioned as an educational tool, the AMPAC suite clearly has pedagogical value that can be readily exploited.

Overall, the AMPAC suite is well-designed and easy to use. It deserves very serious consideration by any serious user of semiempirical methods or GAUSSIAN-98.

Steven M. Bachrach, *Trinity University*

JA004755H

10.1021/ja004755h

Book Reviews *

Solid-Phase Extraction: Principles, Techniques and Applications. Edited by Nigel J. K. Simpson (Varian Associates). Dekker: New York and Basel. 2000. xi + 514 pp. $195.00. ISBN 0-8247-09021-X.

This book represents a joint effort by 19 contributing authors. After five introductory chapters, there is an excellent chapter on the theoretical aspects of solid-phrase extraction (SPE). The next chapters cover specialized applications such as drug screening in toxicology, veterinary drug abuse, biological samples, applications of immobilized phenyl-

---

*Unsigned book reviews are by the Book Review Editor.

boronic acid, immuno-affinity extraction, matrix solid-phase dispersion, and automation of SPE. The book is well edited and attractively produced.

A very strong emphasis is placed on SPE that is performed with commercial cartridges containing various types of silica particles. The rationale is that these are the most widely used materials. The rich history, present applications, and advantages of polymeric and carbonaceous sorbents are largely ignored. Only cursory mention is made of particle-loaded membranes that offer distinct advantages for use in SPE. The many enthusiastic users of SPME will be disappointed that almost nothing is included on this exciting technique.

James S. Fritz, *Iowa State University*

JA0047976

10.1021/ja0047976

Handbook of Antioxidants. Bond Dissociation Energies, Rate Constants, Activation Energies and Enthalpies of Reactions. 2nd Edition. By E. T. Denisov and T. G. Denisova (Institute of Problems in Chemical Physics, Russia). CRC Press: Boca Raton. 1999. xxii + 290 pp. $99.00. ISBN 0-8493-9004-4.

This handbook, written by two well-respected chemical kineticists from Russia, is comprised of 10 chapters that deal with most aspects of liquid-phase autoxidation of organic compounds with particular emphasis on inhibition. The book begins with a chapter outlining the semiempirical model of intersecting parabolas for estimating activation energies of the free radical–molecule reactions and free radical-generating reactions of autoxidation. The second chapter discusses the kinetics of autoxidation and provides rate constants for reactions of alkyls with oxygen, the solubilities of oxygen in organic solvents, bond dissociation energies in solution, kinetic data for all the elementary reactions of peroxyls in uninhibited autoxidation, and rate constants for the homolysis of hydroperoxides. The kinetics of the little understood radical-generating reaction of oxygen with organic compounds are also presented in this chapter.

The mechanisms of inhibition by the major groups of antioxidants, phenols, aromatic amines, hydroxylamines, and thiophenols are discussed in the next few chapters. These include bond dissociation energies, kinetic parameters for reaction with alkylperoxyls, stoichiometric factors, and reactions with alkyl hydroperoxides, oxygen, ozone, and nitrogen dioxide. In Chapter 6 the reactions of the radicals derived from antioxidants, such as phenoxyls, aminyls, and nitroxides, are discussed. A great deal of kinetic data are gathered in 41 tables. The commercially important phosphorus- and sulfur-containing antioxidants are discussed in Chapter 7. The chemistry involved in autoxidation in the presence of these compounds is complex and has only been covered superficially in this book for trialkyl phosphites, triphenyl phosphine, and sulfur dioxide.

The subject of antioxidant regeneration (Chapter 8) is a popular one with the authors, but they have omitted one of the more important mechanisms, namely that involving aromatic amine formation by disproportionation of an alkoxydiarylamine produced by reaction of a nitroxyl with an alkyl during inhibited autoxidation. In Chapter 9, the important and complex process of the oxidation and inhibition of polymer oxidation is covered in 20 pages, including 10 tables and 4 pages of references. The chapter on biological oxidation is very brief, indeed, but might prove to be a starting point for anyone who is unfamiliar with the literature. There are extensive lists of references after each chapter that are reasonably up-to-date. In conclusion, although the book is heavy on numbers and light on words, it might be a useful reference book for scientists concerned with the chemistry of antioxidants.

James A. Howard, *Laurentian University*

JA004759M

10.1021/ja004759m

Theilheimer's Synthetic Methods of Organic Chemisty. Vol. 57. Edited by Alan F. Finch (Cambridge). Karger: Basel. 2000. xxiv + 304 pp. $474.00. ISBN 3-8055-7077-5

Abstracts of new synthetic methods in organic chemistry and supplementary data from papers published from April 1999 to September 1999 are presented in this latest volume of Theilheimer. A listing of reviews in synthetic organic chemistry for the period from October 1999 to March 2000 is also included, as is a "trends" section discussing recent advances in synthetic organic chemistry up to and including March 2000.

JA004808V

10.1021/ja004808v

Fluorine Calorimetry: History, Applications, Results. Second Augmented and Revised Edition. By V. Ya. Leonidov (Russian Academy of Sciences) and P. A. G. O'Hare (formerly of the National Institutes of Standards and Technology). Begell House, Inc.: New York. 2000. xxii + 240 pp. $94.50. ISBN 1-56700-146-7

This book is an updated, English version of *Ftornaya Kalorimetriya*, which was published in Russian in 1978. New surveys and analyses of results obtained by fluorine combustion calorimetry have been added to this revised edition. The chapters are organized into two sections: Part One: Problems Associated with the Development of Fluorine Calorimetry; and Part Two: Determination of Enthalpies of Formation of Substances by Fluorine Calorimetry. The references do not extend beyond 1996.

JA004816B

10.1021/ja004816b

Silicones and Silicone-Modified Materials. Edited by Stephen J. Clarson (University of Cincinnati), John J. Fitzgerald (General Electric Co. Silicones), Michael J. Owen (Dow Corning Corp.), and Steven D. Smith (Procter and Gamble Corp.). American Chemical Society: Washington, DC (distributed by Oxford University Press). 2000. xii + 602 pp. $150.00. ISBN 0-8412-3613-5

This book brings together the papers presented at the ACS Silicones and Silicone-Modified Materials symposium held in the Spring of 1998. There is no unifying organization to its 37 short chapters. Following two introductory overviews—on siloxane polymers and the chemistry of silicones—the remaining chapters cover a variety of more specific topics on the characterization and chemistry of silicones.

JA004806A

10.1021/ja004806a

Houben-Weyl. Methods of Organic Chemistry. Additional and Supplementary Volumes to the Fourth Edition. Volume E23k. Substance Index. Cyclic Compounds VII. Tricyclic Compounds I. Georg Thieme Verlag: Stuttgart. 2000. viii + 552 pp. DM 3300. ISBN 3-13-111714-1

JA0048174

10.1021/ja0048174

Houben-Weyl. Methods of Organic Chemistry. Additional and Supplementary Volumes to the Fourth Edition. Vol. E23l. Substance Index Cyclic Compounds VIII. Tricyclic Compounds II. Georg Thieme Verlag: Stuttgart. 2000. viii + 558 pp. DM 3300. ISBN 3-13-126854-9

These two index volumes list all of the tricyclic chemical compounds containing three-membered ring systems that were covered in the supplementary volumes E1–E21. These compounds include carbocyclic, heterocyclic, and organometallic systems. The indices are based on chemical formulas, and no full systematic names are given.

JA004818W

10.1021/ja004818w