Computer Software Reviews

MacSpartan Plus. Wavefunction, Inc., 18401 Von Karman, Suite 370, Irvine, CA 92612. Phone: (714) 995-2120. E-mail: sales@wavefun.com, http://www.wavefun.com. Pricing: academic $449, government $749, commercial $999

MacSpartan Plus is a molecular modeling program designed to give chemists the ability to perform molecular mechanics and molecular orbital calculations on a desktop computer. The software requires a MacOS computer having a PowerPC processor running System 7.5 or later, at least 16 Mbyte of RAM, and a CD-ROM. The 68K Macintoshes are not supported. MacSpartan Plus software consists of a program called MacSpartan Plus, which serves as its main graphical user interface, and five other compute modules. In the likely event that it is necessary to run MacSpartan Plus at the same time as one of its modules (i.e., with the Ab Initio Engine), an additional 16 Mbyte of RAM will be required. The additional RAM over the required amount need not be physical RAM, but can be virtual RAM. A version installed (without the numerous example files) occupies 10.1 Mbyte of disk space. With all the provided supporting information, an additional 18.5 Mbyte is needed. New users can quickly master the fundamentals of building molecules and running calculations through its easily understood graphical interface. A demonstration version of the software can be ordered from the Wavefunction web site: http://www.wavefun.com/software/multiplex/demoform.html.

As with MacSpartan, the real strength of this program is the increased accessibility of powerful molecular modeling to the desktop computer user. In addition to basic mechanics (SYBYL force field), MacSpartan Plus is capable of semiempirical calculation of orbitals (AM1, AM1-SM2, PM3) and ab initio calculation of molecular wave functions (3-21G, 3-21G*, 6-31G*). The maximum number of atoms and basis functions are 50 and 500, respectively, for an ab initio calculation and 100 atoms for a semiempirical module. Thus, calculations that in the recent past required UNIX-based workstations are now completed with a desktop Mac. The graphical output of MacSpartan and MacSpartan Plus are also far ahead of what was produced only a few years ago with computations performed using Cray supercomputers. The program is also capable of exporting high-resolution pictures (PICT format) that are suitable for the creation of journal quality illustrations.

Even the purist of experimental chemists can be enticed by the program's graphical interface, which makes building molecules, measuring bond lengths and angles, creating 3-D images of charge distribution and other properties, and animating vibrational modes extremely easy. Planes and central points can be defined by a few clicks of the mouse. The graphical interface is one of MacSpartan's and MacSpartan Plus's outstanding features. However, unlike most other Macintosh applications, MacSpartan Plus (like MacSpartan) possesses an inconvenient help system that must be implemented separately from the main program. With the easy understandable graphical interface, however, references to this unconventional help system will most likely be minimal for most users. Other features of the program follow normal Macintosh application protocols; text and graphics, for example, from MacSpartan Plus can be simply incorporated into other applications by cutting and pasting. Moreover, molecules do not have to be entirely built in the graphical interface as MacSpartan Plus is capable of importing and exporting SPARTAN (Wavefunction's UNIX workstation software version), PDB, and SYBYL Mol2 files.

MacSpartan Plus's graphical interface possesses added functionality over MacSpartan by inclusion of an interactive molecule builder that is used for the assembly of inorganic and organometallic reagents. This important addition to MacSpartan's organic and peptide builders allows the inorganic chemist to more readily participate in meaningful ways in desktop computer modeling projects. The builder for inorganic and organometallic molecules makes changing the bond type and adding a variety of ligands extremely easy. Thus, molecules such as $[Cp_2Ta(CH_3)({=}CH_2)]$ are easily built. In MacSpartan Plus, optimization using PM3 parameters and newly developed PM3 semiempirical parameters for the transition metals are available now.

While MacSpartan Plus is truly a powerful modeling program, some limitations are recognized. For example, while the measurement of atom distances and angles within a single molecule is easily performed, the measurement of intermolecular angles and distances between two or more molecules is not possible. This limitation could prove frustrating, for example, to those chemists interested in exploring molecular assemblies. Moreover, crystal building is also not possible with this software. Other commercially available desktop molecular modeling programs for MacOS computers allow the building of crystals. Likewise, a few parameters, such as the PM3 parameters for bismuth that do exist, are not available on MacSpartan Plus. However, most elements are available and calculations for organic or organometallic applications can be performed painlessly.

In summary, the MacSpartan Plus is a good package for desktop computer modeling that can be effectively used within minutes of installation. However, the software is still working within the bounds of the modern desktop machine and should not be expected to have the speed of the UNIX-based workstation modeling software packages. Although any PowerPC can run the calculations, some processors will run unbearably slow. For example, a 90 MHz machine took approximately 6 CPU hours to ab initio optimize a four-carbon amine chain. Doing computations on a large system demands at least a 200 MHz or faster PowerPC. Generally speaking, in the hands of one of the newer, faster MacOS computers, this modeling package gives the inquisitive chemist the power to tackle a wide variety of computational problems.

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Book Reviews *

Growth of Crystals. Volume 20. Edited by E. I. Givargizov and A. M. Melnikova (Russian Academy of Sciences, Moscow). Plenum: New York and London. 1996. vii + 169 pp. $95.00. ISBN 0-306-18120-7.

The first volume of this series on crystal growth was translated from Russian into English and was published in 1958. The papers which appeared in that and subsequent volumes were for the most part originally delivered at the crystal growth conferences convened at various locations in the former Soviet Union. As the language of future volumes is planned to be English, Volume 20 is likely to be the last to appear first in Russian.

In Volume 20, Givargizov and Melnikova have solicited original papers and self-reviews from some of the best crystal growth groups currently active in Russia and Ukraine. In the Preface, they explain that, in keeping with tradition, these papers cover the subjects of vapor growth, solution growth, and melt growth of crystals.

The first section of Volume 20 deals with vapor growth and contains five papers covering, respectively, molecular beam epitaxy of Ge−Si, heterostructures and strained superlattices in Ge−Si, long-range stresses in epitaxial films, defect formation in Cd_xHg_{1-x} films, and the structure of niobium oxide films.

The second section, which covers solution growth, contains two papers addressing, respectively, the morphological stability of a step and the $KOH-ZrO_2-SiO_2-H_2O$ hydrothermal system, and two papers on the growth of crystals of KH_2PO_4.

The third section, which is devoted to melt growth, contains a total of five papers covering, respectively, growth of $YBa_2Cu_3O_x$ and $TmBa_2Cu_3O_x$ superconductors, the theory of centrifuge and microgravity growth, the theory of convection effects in the Stockbarger growth of

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[*] Unsigned book reviews are by the Book Review Editor.

CaF_2, growth front structure in the crystallization of $CBr_4 + C_2Cl_6$, and methods for determining the compositions of congruently melting three-component solid solutions. This last paper is typical of the impressive advances in phase diagram theory and applications of the phase rule which have appeared over the last 30 years or so in the *Russian Journal of Physical Chemistry*.

Volume 20 is appropriate reading for crystal growth specialists and those interested in keeping up with Russian and Ukrainian advances in the field. Unfortunately, readers will have to write the editors directly for more information, since nowhere do the addresses of the individual authors appear. The publishers, however, have promised to include both conventional addresses and e-mail addresses in the next volume. In keeping with Russian practice, Volume 20 does not contain an index, although since the longest paper extends over only 16 pages, this omission is of little consequence.

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Solvent Effects and Chemical Reactivity. Edited by O. Tapia (University of Uppsala, Sweden) and J. Bertrán (Universitat Autònoma de Barcelona). Kluwer Academic Publishers: Dordrecht, The Netherlands. 1996. X + 377 pp. ISBN O-7923-3995-9.

This book contains seven review chapters dealing with various aspects of the theoretical treatments of solvent effects with a special emphasis on chemical reactivity.

The first chapter by Cramer and Truhlar, entitled Continuum Solvation Models, is an excellent introduction to the various quantum chemical methods in which the solvent is treated as a dielectric continuum. It starts with a clear theoretical introduction in which the electrostatic bases of the models and their introduction into the quantum chemical treatments are reviewed. The role of nonelectrostatic contributions to the solvation free energy is then analyzed. The various implementations of these models in computer codes is then thoroughly reviewed, with a remarkable modest presentation of the authors' increasingly popular SMx approaches. The treatment of equilibrium properties in solution takes a large place in this chapter. The problem of computing solvation free energies is first addressed, and then several illustrative examples are reviewed. They are focused on intra- and intermolecular proton transfers, tautomeric equilibria, and lactolization. The chapter ends with a short review of dynamic effects in chemical kinetics and spectroscopy. An extensive bibliography (385 references) makes this contribution a basic text to anyone who intends to enter the very active field of solvent effects by means of the simple and very effective continuum models.

The second chapter by Contreras, Pérez, and Aizman deals with the use of density functional theory. It is a rather technical chapter in which the authors mainly develop their own approach which is based on a reaction field (i.e., continuum) model.

The use of Monte Carlo techniques to compute the thermodynamic quantities which enter the transition state theory of chemical reactivity when the solvent molecules are considered explicitly is developed in the third chapter by González-Lafont, Lluch, and Bertrán. A large part of the text is devoted to the methodologies derived from the Monte Carlo method, with some illustrative reference examples.

The next chapter, entitled Computer simulations for chemical systems: from vacuum to solution, by Corongiu, Estrin, and Paglieri mainly deals with aqueous solutions studied at different levels of theory. The chapter starts with a methodological review of density functional theory and its use in molecular dynamics simulations and of the self-consistent reaction field models. A series of illustrative examples is analyzed, starting with the ammonia–hydrochloric acid reaction. The solvation of Li^+, the structure of water clusters, and finally the stability and vibrational spectra of DNA base pairs are the other examples considered in the review.

The basic aspects of chemical reaction dynamics in solution are analyzed in a short (27 pages) but very clear chapter by Hynes entitled Crossing the transition state in solution. The author develops the so-called "stochastic" theoretical approach of the reaction rates in solution and the molecular dynamics simulations designed to test the theoretical conclusions. The paper is based on the Grote–Hynes theory of reaction rate constants which is developed first. The author then considers the case of charge transfer reactions involving a quantum particle. The part devoted to simulation studies briefly relates some simulation results on S_N2 and S_N1 reactions and ion pair combinations in aqueous solutions and some examples of nonadiabatic solvation effects. In the second half of this part, transfer reactions of light particles (proton, electron) are analyzed, mainly from a theoretical point of view.

Bianco and Hynes develop, in the sixth chapter, a combination of valence bond treatment of the solute with a dielectric continuum description of the solvent. The nonequilibrium solvation effects are approached by considering the time dependent molecular reorientation contribution to the electric polarization of the solvent. The method is applied to the authors' favorite reactions ($I_2^- \rightarrow I + I^-$; S_N1 and S_N2).

The last chapter, by Tapia, Andres, and Stamato, entitled Quantum Theory of Solvent Effects and Chemical Reactions, develops some rather formal views on the various phenomena expected to influence chemical reactions in solution, and their theoretical consequences. The chemically interesting examples are just mentioned without great detail. Nevertheless, a long and useful bibliography (more than 300 references) makes the chapter interesting to consider.

In conclusion, this book contains some very useful reviews on various aspects of solvent effects, and although it appears as a simple collection of contributions, without any visible editorial effort, it is highly recommendable to all the theoretical or computational chemists having some concern with solution chemistry.

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Annual Review of Physical Chemistry, Vol. 48. Edited by Herbert L. Strauss (University of California–Berkeley), Gerald T. Babcock (Michigan State University), and Stephen R. Leone (University of Colorado). Annual Reviews, Inc.: Palo Alto, CA. 1997. x + 875 pp. $64.00. ISBN 0-8243-1048-9.

The field of physical chemistry continues to progress in many surprising directions. The applications reviewed in this volume involve systems that range from new views of traditional physical chemistry problems (e.g., hydrogen bonding) to new techniques that have just started to contribute to physical chemistry (e.g., subfemtosecond kinetics, single-molecule spectroscopy). There is an author index, subject index, cumulative index of contributing authors, Volumes 44–48, and cumulative index of chapter titles, Volumes 44–48.

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Kirk-Othmer Encyclopedia of Chemical Technology, Volume 23, Sugar to Thin Films. Edited by Jacqueline I. Kroschwitz and Mary Howe-Grant. Wiley/VCH: New York. 1997. xxviii + 1118 pp. $325.00. ISBN 0-471-52692-4.

This is the 23rd volume of a 25-volume encyclopedia set, four volumes being published each year. The fourth edition is similar in format to the earlier editions with updates to the entries as necessary and the addition of several new subjects. This volume contains 36 entries ranging from Sugar to Thin Films. This volume does not contain an index; however, paperback indexes are published every four volumes, and the supplement and index volumes are scheduled for publication in 1998.

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