BIOVIA MATERIALS STUDIO VAMP
DATASHEET

BIOVIA Materials Studio VAMP is a semi-empirical molecular orbital package for molecular organic and inorganic systems. BIOVIA Materials Studio VAMP is an ideal intermediate module between force-field and first principles methods and is capable of rapidly calculating many physical and chemical molecular properties. BIOVIA Materials Studio VAMP is optimized to be numerically stable and fast, enabling most calculations to be run interactively on a PC.

OVERVIEW

BIOVIA Materials Studio VAMP provides fast and reliable predictions of structural and electronic properties of molecules. BIOVIA Materials Studio VAMP is an ideal choice when making trade-offs between the speed of force-field methods and the accuracy of first-principles methods. BIOVIA Materials Studio VAMP is optimized to be numerically stable and fast, enabling users to perform high throughput calculations using even a PC.

Semiempirical molecular orbital (MO) theory was developed as an everyday tool for answering questions related to standard problems in the laboratory. BIOVIA Materials Studio VAMP provides an efficient way of obtaining these results, including a simple graphical interface to make these powerful methods easily accessible. The tasks that can be performed by BIOVIA Materials Studio VAMP include geometry optimization, transition state search and optimization, and the evaluation of many chemical and physical properties.

The breadth of BIOVIA Materials Studio VAMP encompasses organic, inorganic, and organometallic molecules, polymers, oligomers, and peptides. Because of its speed, BIOVIA Materials Studio VAMP can be used to perform scans over wide areas of a potential energy surface or reaction pathway; or it can be used to perform high-throughput calculations on hundreds or even thousands of molecules. Such results can be used in conjunction with Quantitative Structure-Activity Relationships (QSAR) to create a formidable predictive tool for areas such as drug design.

BIOVIA Materials Studio VAMP contains other truly unique features that make it a powerful tool for any researcher in the chemical, pharmaceutical, or materials industry who needs to predict properties of new compounds.

For example, BIOVIA Materials Studio VAMP contains three methods designed explicitly to handle transition elements, an area very challenging for semiempirical methods MNDO/d[1], AM1*[2] and PM6[3]. The AM1* method predicts accurate geometries and energies for metals such as Ti, Zr, and Mo. The method, in addition, increases the accuracy of results for non-transition elements such as Al, Si, and P. The new PM6 method provides parameters for 70 elements include transition metals.
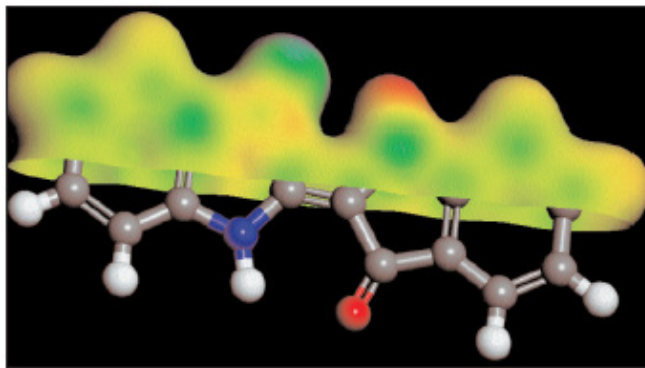
The dye indigo showing a section of isosurface with the electrostatic potential mapped onto the electron density. Molecular electrostatic potential and total electronic density calculated using BIOVIA Materials Studio VAMP. Image generated using BIOVIA Materials Studios volumetric analysis tools.

BIOVIA Materials Studio VAMP is the only program that calculates both ESR hydrogen hyperfine coupling constants and ^{13}C chemical shifts. Current accuracy (standard deviations from experiment) is about 0.5 Gauss for ESR coupling constants and 6-8 ppm for ^{13}C chemical shifts[4].

Solvent effects must be considered when determining the properties of molecules in almost all real situations, yet these are often ignored by calculations. Solvent effects are simulated in integrals via a multipole approximation, rather than an exact calculation.

BIOVIA Materials Studio VAMP uses two different models for solvation: numerical Self-Consistent Reaction Field (SCRF)[5] calculations, and COnductor-like Screening MOdel (COSMO)[5]. Such models are essential for understanding the properties of molecules in solution and are easily included in BIOVIA Materials Studio VAMP calculations.

BIOVIA Materials Studio VAMP computes optical excitation spectra (UV/vis) using the ZINDO Hamiltonians which were parameterized for this very purpose. ZINDO provides a number of different model Hamiltonians[7,8] that can be selected according to the desired property, accuracy, and available elements. The parameterization includes a wide number of transition metals, allowing the prediction of UV spectra for organometallic compounds as well as for organic molecules.

Electrostatic potential maps are often essential for understanding the activity of a molecule. BIOVIA Materials Studio VAMP includes routines for a rapid an accurate evaluation of the potential. The Natural Atomic Orbital-Point Charge (NAO-PC)[9] model is used for molecular electrostatic properties. The type of analysis obtained using NAO-PC provides a more exact picture of the molecular electronics than the normal population analysis—a picture that rivals the accuracy of ab initio methods hundreds of times slower.

Finally, BIOVIA Materials Studio VAMP provides a number of molecular properties such as ionization potential, multipole moments, accurate molecular polarizabilities, atomic polarizabilites, and optical spectra.

THE BIOVIA MATERIALS STUDIO ADVANTAGE

BIOVIA Materials Studio VAMP is operated from within the BIOVIA Materials Studio® software environment that provides a user-friendly interface, complying with Windows® standards. BIOVIA Materials Studio Visualizer offers a wide range of model building and visualization tools that allow you to rapidly construct models of the system of interest, select the BIOVIA Materials Studio VAMP module with two mouse clicks, and run a semi-empirical calculation. BIOVIA Materials Studio VAMP can, of course, be used to compute molecular properties as described above; or it can be used in conjunction with other modules in the BIOVIA Materials Studio suite of programs. BIOVIA Materials Studio VAMP predictions provide good starting points for refinement with more accurate calculations such as density functional theory (DFT). Alternatively, BIOVIA Materials Studio VAMP can compute optical & IR spectra, 13C NMR shifts, or optical polarizability on molecular structures predicted by other modules of BIOVIA Materials Studio.

HOW DOES BIOVIA MATERIALS STUDIO VAMP WORK?

BIOVIA Materials Studio VAMP uses semi-empirical techniques in which many of the more complex terms are ignored or replaced using approximations. Empirical parameters and functions are used to compensate for the errors introduced by these approximations. These empirical parameters are fitted to reproduce experimental data. Suitable methods for the evaluation of energetic data are MINDO/3[10], MNDO[11], AM1[12], and PM3[13]. Accurate optical spectra can be obtained using the INDO[7] and CNDO[8] methods.

BIOVIA Materials Studio VAMP uses semi-empirical calculations to determine a molecular wavefunction which can then be used to derive molecular properties such as energy and dipole moments. The molecular wavefunction is constructed according to the LCAO method in which molecular orbitals are obtained as a linear combination of Slater-type atomic orbitals. Semi-empirical methods can use Slater functions by evaluating the two-electron integrals via a multipole approximation, rather than an exact calculation.

By default, BIOVIA Materials Studio VAMP performs a MNDO Hamiltonian calculation. However, you can use controls on the BIOVIA Materials Studio VAMP setup dialog to select AM1, PM3, MNDO/C or MINDO/3 Hamiltonians. The elements for which each of these methods is parameterized are given in the 'Features and Capabilities' section of this document.

Geometry may be optimized in BIOVIA Materials Studio VAMP by several different schemes. The default optimizer is Jon Baker's Eigenvector Following (EF) routine[14] which was chosen for its reliability and excellent general performance. A typical geometry optimization starts either by calculating all or part of the Hessian matrix, or by estimating its diagonal values. BIOVIA Materials Studio VAMP also offers two different and very effective transition state optimizers: EF and Powell's transition state optimizer.

You can access BIOVIA Materials Studio VAMP through the MaterialsScript API. Scripting allows you to automate repetitive task and customize workflows.

FEATURES AND CAPABILITIES

Features marked with an asterisk (*) can not be accessed via the user interface, but are available by modifying the input file.

Calculation Tasks

- Open- and closed-shell Hartee-Fock methods: Restricted (RHF), Unrestricted (UHF) and spin-Annihilated Unrestricted Hartee-Fock, (A-UHF)
- Geometry optimization
- Transition state optimization
- Vibrational frequency calculation
- Solvent effects: Self-Consistent Reaction Field (SCRF) and
- COnductor-like Screening MOdel (COSMO) (available solvents are acetone, acetonitrile, benzene, carbon tetrachloride, chloroform, diethyl ether, dimethyl sulfoxide, ethanol, methanol, methylene chloride, n-hexane, n-hexadecane, nitrobenzene, pyridine, water)
- CI calculations : Full, CIS, CISD and PECI

Hamiltonians

- PM6 [H through Bi, with the exception of trans-Lanthanides]
- MNDO [H, He, Li, Be, B, C, N, O, F, Mg, Al, Si, P, S, Cl, K, Ca, Zn, Ge, Br, Sn, I, Hg, Pb]
- MNDO/C is an MNDO method designed to be used with a perturbational theory correction for electron correlation. It is only parameterized for C, H, N and O
- AM1 [H, B, C, N, O, F, Mg, Al, Si, P, S, Cl, Zn, Ge, Br, Sn, I, Hg]
- PM3 [H, Li, Be, B, C, N, O, F, Na, Mg, Al, Si, P, S, Cl, Ca, Zn, Ga, Ge, As, Se, Br, Cd, In, Sn, Sb, Te, I, Hg, Tl, Pb, Bi]
- MNDO/d : standard MNDO parameters for : H, He, Li, Be, B, C, N, O, F, and MNDO/d parameters for: Na, Mg, Al, Si, P, S, Cl, Zn, Br, Cd, I, Hg
- AM1*: Standard AM1 parameters for H, C, N, O, F, and parameter sets with d-orbitals for elements Al-Cl, Ti-Zn, Br, Zr Mo, I, and Au.
- CNDO/1 [H, Li, Be, B, C, N, O, F, Na, Mg, Al, Si, P S, Cl, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, As Se, Br, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, I, Lu, La, Ce Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb]
- CNDO/2 [H, Li, Be, B, C, N, O, F, Na, Mg, Al, Si, P, S, Cl, K, Ca, Sc , Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, As Se, Br, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag]
- INDO/1 [H, Li, Be, B, C, N, O, F, Na, Mg, Al, Si, P, S Cl, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Se Br, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, I]
- INDO/2 [H, Li, Be, B, C, N, O, F, Na, Mg, Al, Si, P, S Cl, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Se, Br]

Job Control Options

- BIOVIA Materials Studio VAMP jobs can be run as background processes on a server or as synchronous (interactive) jobs on your PC.

Properties

- Electron density
- Molecular orbitals (canonical), or localized orbitals
- Electrostatic potentials
- Atomic charges : NAO-PC, Coulson, and Mulliken
- Molecular and atomic multipoles
- Static first-order polarizabilities(*)
- ESR hyperfine coupling constants to hydrogen(*)
- 13C chemical shifts
- Optical spectra
- Heat of formation, entropy, and heat capacity.

Analysis of BIOVIA Materials Studio VAMP results

- Volumetric display of: total electronic density, spin density, electrostatic potential, molecular orbitals, and localized orbitals
- Thermodynamic properties (enthalpy, entropy, and heat capacity)
- Atomic charges and bond orders.

To learn more about BIOVIA Materials Studio, go to **accelrys.com/materials-studio**

REFERENCES:

1. Thiel, W; Voityuk, A. A., J. Phys. Chem. 1996, 100(2), 616-626; Thiel, W.; Voityuk, A. A., THEOCHEM 1994, 119(1), 141-154; Thiel, .; Voityuk, A. A.,Theoretica Chimica Acta 1992, 81(6), 391-404 (with an erratum in Theoretica Chimica Acta 1996, 93(5), 315).

2. Voityuk, A. A.; Roesch, N., J. Phys. Chem. A 2000, 104(17), 4089-4094.

3. J.J.P. Stewart, J. Mol. Model. 2007, 13, 1173-1213.

4. Clark, T.; Breindl, A.; Rauhut, G., J. Mol. Model. 1995, 1, 22.

5. Rauhut, G.; Clark, T.; Steinke, T., J. Am. Chem. Soc. 1993, 115, 9174.

6. Klamt, A.; Schüürmann, G., J. Chem. Soc., Perkin Trans. 2, 1993, 799.

7. Ridley, J.; Zerner, M., Theor. Chim. Acta (Berlin) 1972, 32, 111.

8. Pople, J. A.; Santry, D. F.; Segal,G. A., J. Chem. Phys. 1965, 43, S129.7.

9. Rauhut,G.; Clark, T., J. Comput. Chem. 1993, 14, 503.

10. Bingham, R.C.; Dewar, M.J.S.; Lo, D.H., J. Am. Chem. Soc. 1975, 97, 285; 1294; 1302; 1307; Dewar, M.J.S.; Lo, D.H.; Ramsden, C.A., J. Am. Chem. Soc. 1975, 97, 1311.

11. Dewar, M.J.S.; Thiel, W., J. Am. Chem. Soc. 1977, 99, 4899.

12. Dewar, M.J.S.; Zoebisch, E.G.; Healy, E.F.; Stewart, J.J.P., J. Am. Chem. Soc. 1985, 107, 3902.

13. Stewart, J.J.P ., J. Am. Chem. Soc. 1989, 103, 1413.

14. Baker, J., J. Comput. Chem. 1986, 7, 385.

Our **3D**EXPERIENCE Platform powers our brand applications, serving 12 industries, and provides a rich portfolio of industry solution experiences.

Dassault Systèmes, the **3D**EXPERIENCE Company, provides business and people with virtual universes to imagine sustainable innovations. Its world-leading solutions transform the way products are designed, produced, and supported. Dassault Systèmes' collaborative solutions foster social innovation, expanding possibilities for the virtual world to improve the real world. The group brings value to over 170,000 customers of all sizes in all industries in more than 140 countries. For more information, visit **www.3ds.com**.

3DEXPERIENCE®

Dassault Systèmes Corporate
Dassault Systèmes
175 Wyman Street
Waltham, Massachusetts
02451-1223
USA

BIOVIA Corporate Americas
BIOVIA
5005 Wateridge Vista Drive,
San Diego, CA
92121
USA

BIOVIA Corporate Europe
BIOVIA
334 Cambridge Science Park,
Cambridge CB4 0WN
England

DASSAULT SYSTEMES | The **3D**EXPERIENCE® Company

DS-8024-1014