



The Spartan Computational Methods. *Spartan'14* provides a full range of computational methods, addressing the needs of educators, bench chemists, and professional modelers. All methods are easily accessed via Spartan's seamless graphical interface.

Methods: (Items in *Italics and underlined* are available in Parallel with the Spartan'14 Parallel Suite)

Molecular Mechanics Molecular mechanics is presently the only practical method for calculations on very large molecules or for conformational searching on highly flexible molecules. MMFF94, in particular, has proven to be a reliable and fast tool for conformational analysis. There are no atom limits for molecular mechanics calculations.

Both the SYBYL and MMFF94 force fields are supported. SYBYL extends throughout the entire Periodic Table while MMFF94 has been specifically parameterized to reproduce geometries and conformations of organic molecules and biopolymers. Additionally, an MMFFaq option applies an aqueous solvent energy correction to energy data, of special utility in ranking conformers.

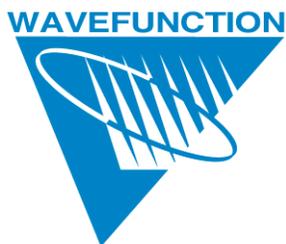
**Semi-Empirical
Molecular Orbital** Semi-empirical models are the simplest of the quantum chemical schemes, and are useful for equilibrium and transition-state structure calculations. PM3, in particular, has proven to be a reliable tool for geometry calculations on transition metal inorganic and organometallic compounds.

MNDO, AM1, RM1, PM3, and PM6 methods are supported. MNDO/d extensions for heavy main-group elements have been implemented and PM3 parameters for most transition metals are available.

The RM1 (Recife Model 1) reparameterization of AM1 is new in Spartan'06. In most cases RM1 yields superior results to both AM1 and PM3 (for organic molecules).

Hartree-Fock
Molecular Orbital

Hartree-Fock models useful for predicting structure,
energy and property calculations, in particular for



organic molecules.

A variety of standard basis sets are supported: STO-3G, 3-21G, 6-31G*, 6-311G*, cc-pVDZ, cc-pVTZ and cc-pVQZ, with extensions including (d), (d,p), (2d), (2d,2p), (2df, 2dp), (3d, 3p), (3df, 3dp) and diffuse functions and/or additional polarization functions. Also supported are a variety of pseudopotentials for calculations on molecules incorporating heavy elements. Spartan allows for the import of additional basis sets, and for the construction of user-created basis sets. Additionally, a new dual basis set procedure is available, allowing the approximation of basis set extension using perturbation theory (for improved precision and performance).

Methods:

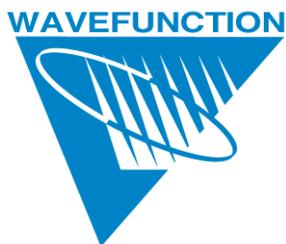
Density Functional

Density functional models typically provide results of a quality comparable to conventional correlated models such as MP2, but at a cost only slightly greater than that of Hartree-Fock models. As such, they are particularly useful for high-quality structure, energy and property calculations, including calculations on transition-metal inorganic and organometallic compounds.

Local density models and BP, BLYP, EDF1, EDF2, and B3LYP models are supported with the same basis sets and pseudopotentials as available for Hartree-Fock models. The non-empirical GGA functional PBE has been implemented. Five Minnesota hybrid meta-GGA functionals from Zhao and Truhlar have also been implemented, in particular, M05, M05-2X, M06, M06-2X, and M06-HF; and the local meta-GGA from that group, namely M06-L, is also available. Additionally, a wider range of functionals is available as calculation options with the ability to specify model and percentages for exchange and correlation (these include Slater-Dirac), Vokso-Wilk-Nusair, Perdew-Zunger, Wigner, Becke88, Gill96, Gilbert-Gill99, Lee-Yang-Parr, Perdew86, GGA91, BMK, EDF1 and EDF2).

Møller-Plesset

MP2 is perhaps the simplest model to take reasonable account of electron correlation, and generally provides



accurate descriptions of equilibrium structure, conformation and energetics of a variety of chemical reactions, including reactions where chemical bonds are broken. MP methods are supported for the same basis sets and pseudopotentials available for Hartree-Fock and density functional models.

The RI-MP2 model, providing nearly identical results to MP2 but with significant performance improvements: energy calculations an order of magnitude faster and structure calculations a factor of 3 times faster than conventional MP2.

MP3 and MP4 models are available for single-point energy calculations only, as is a fast localized orbital variant of MP2. The same basis sets and pseudopotentials supported for Hartree-Fock are available.

Thermochemical Recipes Several recipes for obtaining highly accurate heats of formation are available, including the [*T1 recipe*](#) that provides results within 2 kJ/mol of the (also available) G3(MP2) approach, but with performance several orders of magnitude faster than G3(MP2). Additional recipes include G2, G3.

Advanced Correlated A number of high-order correlated models are available for energy calculations only. These include CCSD, CCSD(T), OD, OD(T), QCISD, QCISD(T), QCCD, and QCCD(T) models, with the same basis sets and pseudopotentials available for Hartree-Fock, density functional and Møller-Plesset calculations.

Excited-State Methods Calculations on excited states may be performed using CIS, CIS(D), RI-CIS(D) and TDDFT models in addition to the entire range of density functional models. The same basis sets and pseudopotentials supported for ground-state calculations are available.