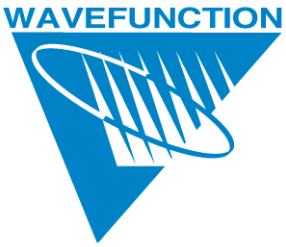

Spartan Molecular Properties: In addition to energies, equilibrium and transition-state geometries and frequencies, Spartan'14 provides a number of valuable properties**.**

Atomic Charges	Mulliken and Natural Bond Orbital Charges are available as are charges based on fits to electrostatic potentials.
Thermodynamics	Enthalpies, entropies and free energies as well as isotope effects, based on calculated geometries and IR vibrational frequencies.
Electrical	Dipole, quadrapole and higher moments, polarizabilities (including alpha, beta, and gamma terms).
Acidity and Basicity	A new feature in ***Spartan'14***, calculated acidities and basicities are available for common carboxylic acids and amines.
Additional Properties	Weight, Area, Volume, Symmetry Group, HOMO and LUMO Energies, Polar Surface Area, LogP, Ovality, Q-Minus, Q-Plus, Electronegativity and Hardness
IR Spectra	Vibrational spectra available from IR calculations including plotting and animation of vibrational modes.
Solvation	Aqueous solvation energies from SM6, SM5.4 or SM50R models. An additional continuum solvation model is also included.
NMR Calculations	Chemical shift calculations for Hartree-Fock and DFT models, and, new in Spartan'10, a correction scheme for the EDF2 model for chemical shifts with accuracy of 1.7-1.8 ppm.
UV/vis Spectra	Vertical excitation spectra based using either CIS/CIS(D) or Time Dependent DFT models is provided.