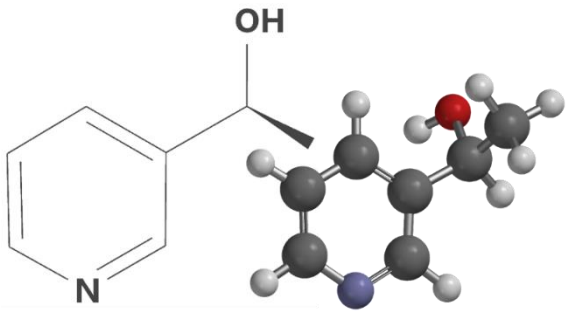
New in ***Spartan Student 8*** (for program brochure click here):

Parallel Processing.

Spartan Student 8 will take advantage of *up to 16 cores* in parallel, ***significantly*** improving performance (speed) of energies, geometry optimizations and transition state optimizations from Hartree-Fock, density functional, and Møller-Plesset models. The individual steps of the T1 thermochemical recipe have also been parallelized.

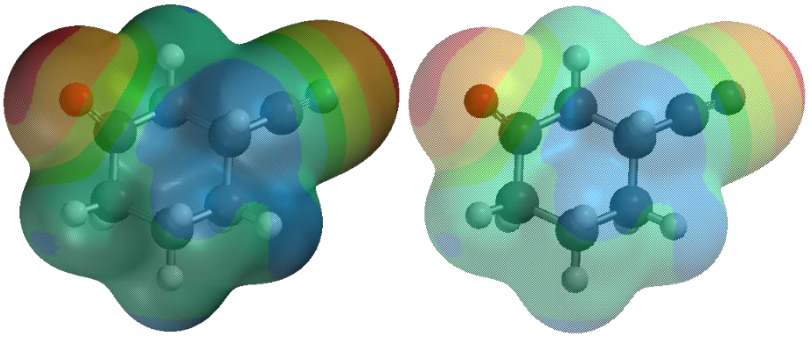
Graphical Interface.



2D Drawings. Spartan derived 2D drawings (from the Sketch builder) replace the library of 2D drawings previously used and also provides 2D drawings for whatever (organic molecules) the user s. The intention is to be able to add drawings to plots, spectra and spreadsheets (among other places). In principle, everything the user builds in 3D should have a corresponding 2D drawing.

Output Summary. This is now a tabbed dialogue and has been revamped to include a Summary output as an HTML pane that can be saved as a PDF file and/or printed. These include tabular presentations of molecular orbitals, atomic charges, calculated bond orders, and optionally proton and carbon spectra as typically appear in experimental papers (shifts, coupling constants, and HMBC correlations) as well tables of HH, CH and CC coupling constants. There is also an IR table of frequencies, intensities and symmetry labels as well as a thermodynamic properties table. All tables can be copied to the clipboard for utilization in other programs (MS Excel for example). This is a significant improvement over text output files from previous versions (which also remain available).

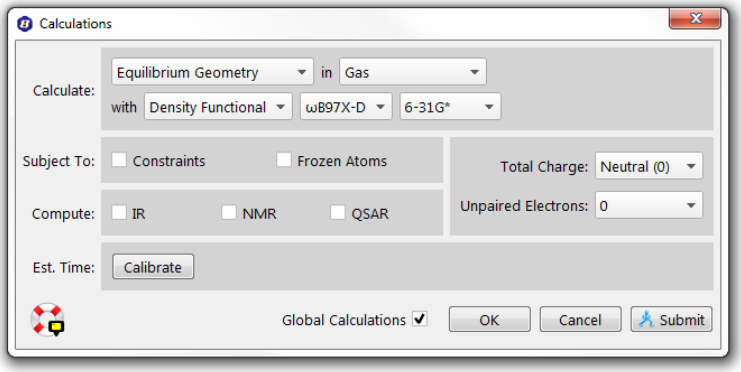
Graphical Surfaces. Background bleeding has been addressed to improve visualization of transparent surfaces. This rendering, called "Silhouette" can be enabled for any non-solid surface to improve display of the interior boundary of the surface (silhouette is turned on for the left-most image at right), and is available from the Surface Properties dialogue.



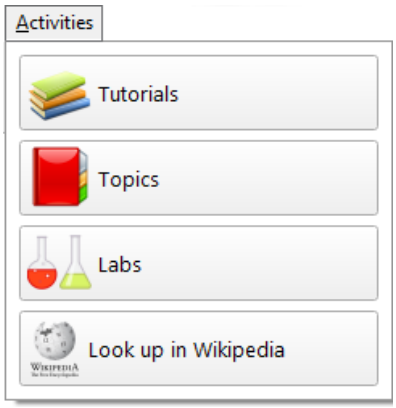
Spectroscopy.

NMR. A 3rd generation empirical correction scheme for ^{13}C chemical shifts has been implemented and is available for ωB97X-D/6-31G* and B3LYP/6-31G* (the EDF2/6-31G* utilizes an earlier correction scheme), offering increased accuracy with fewer parameters than in previous versions.

IR. ωB97X-D/6-31G*, B3LYP/6-31G* and EDF2/6-31G* frequencies are automatically scaled to account for systematic errors associated with the underlying harmonic approximation.



Calculations.
The ωB97X-D functional and the T1 thermochemical recipe have been added as new computational options. The former provides superior results to B3LYP and EDF2 (available in previous versions) and the latter follows a multi-step recipe providing for a highly accurate heat of formation, previously only available from the SSPD database or from the research version of ***Spartan***.



Integrated Lab Activities. In addition to the Topics and Tutorials sections, the Activities menu has been extended to include a set of molecular modeling lab activities covering topics in general, organic, physical, and inorganic chemistry.

Computational Models.
Molecular Mechanics (MMFF) with no atom limits.
Semi-empirical (PM3) up to 75 atoms.
Hartree-Fock molecular orbital up to 30 atoms.
Density functional theory (ωB97X-D, B3LYP and EDF2) up to 30 atoms.
Møller-Plesset (MP2) up to 20 atoms.
T1 thermochemical recipe up to 20 atoms.
Solvation Models. Hartree-Fock and density functional models include the option of using the **C-PCM** solvent model (polar, non-polar, and water) for energy calculations and for geometry or transition state geometry optimizations. Aqueous Solvent models are also available for MMFF (SM5.0R) and PM3 (SM5.4).

Spartan Spectra & Properties Database. The SSPD has been expanded to include ωB97X-D/6-31G* structures, properties and NMR data. Additionally, highly accurate ωB97X-V/6-311+G(2df,2p) energies are available (as a property) for ωB97X-D/6-31G* structures. These energies are accessible from the Molecule Properties and Reactions dialogues.

Reactions Calculator Dialogue. The Reactions dialogue has been updated to utilize not only (total) energies or T1 heats of formation, but also enthalpy and Gibbs free energy (ΔH° and ΔG°) data.

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