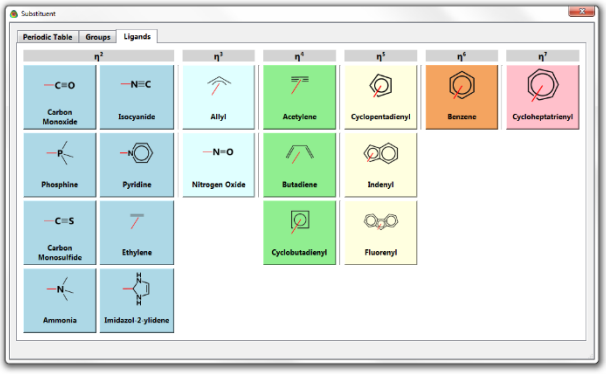
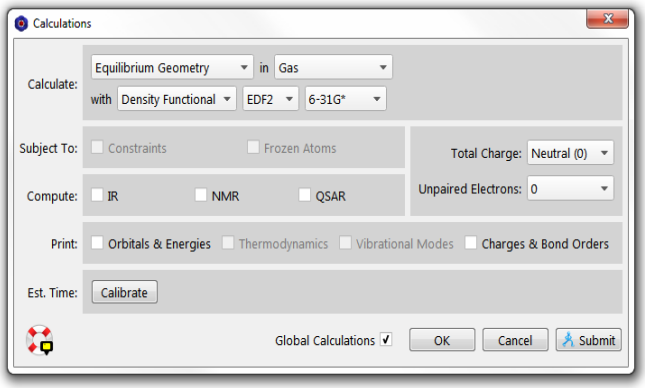
New in ***Spartan Student 7*** (for program brochure click here):

Graphical Interface.



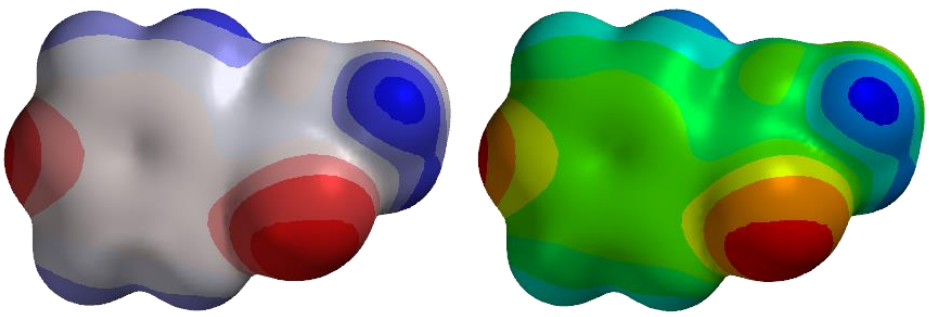
Building. Extensions to the 2D sketching from Spartan Student 6 to accommodate inorganic and organometallic molecules (including new templates for functional groups and ligands). Transition states may also be defined in 2D. All 2D sketches can be automatically converted into 3D structures for analysis. The 3D building functions now include the ability to fuse rings. A single click/tap access to R/S chirality display is available (chiral centers or absolute chirality may be inverted in the Build mode).



Calculations.

The calculations dialogue has been extended to include calculations in solvent. The conformer distribution task has also been added (available using the MMFF model). Enhanced tool tips and an integrated Help function that anticipates setup errors (before submission) and provides advanced help for jobs that have not completed successfully. A new time estimating feature is provided. Upon initial opening, the calibrate button triggers a single background job that is used to provide a time estimate for successive calculations.

Visualization and Data Analysis. Property maps (like the electrostatic potential map) can optionally be viewed with Red-White-Blue color scale. Users can toggle between default property ranges (ideal for comparisons between molecules) and absolute property ranges for individual molecules. Visualization of macromolecules is enhanced with refinements to ribbon displays. An improved Spreadsheet includes direct access to all properties from the Molecule Properties dialogue and the Orbital Energy diagram now offers a direct post of orbital energies to the Spreadsheet. An integrated Formula tool is available for accessing more advanced spreadsheet capabilities.

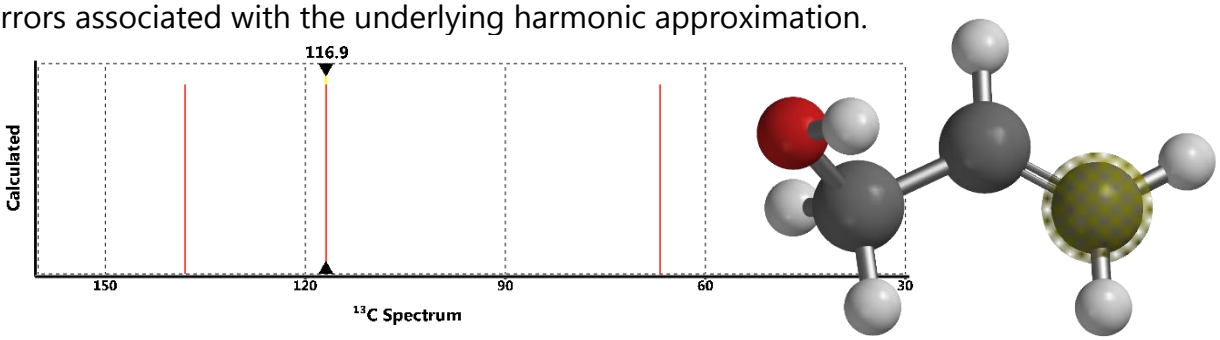


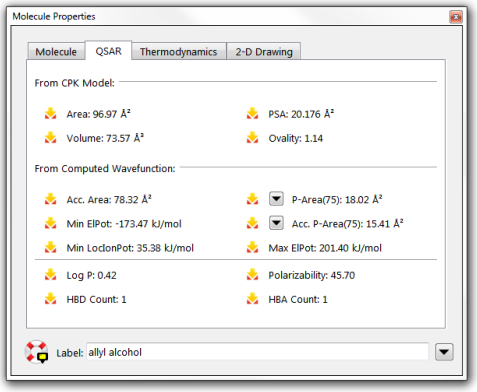
Computational Models.

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 (B3LYP and EDF2) up to 30 atoms.
Møller-Plesset (MP2) up to 20 atoms.
Solvation Models. For Hartree-Fock and Density Functional models, a new solvent model (**C-PCM**) is available for energies, geometry and transition state optimizations. Aqueous Solvent models are also available for MMFF (SM5.0R) and PM3 (SM5.4).

Spectroscopy.

NMR. A 3rd generation empirical correction scheme for ^{13}C chemical shifts has been implemented and is available for B3LYP/6-31G* and EDF2/6-31G* offering increased accuracy with fewer parameters than in previous versions.
IR. B3LYP/6-31G* and EDF2/6-31G* frequencies are automatically scaled to account for systematic errors associated with the underlying harmonic approximation.





Molecular Properties.

Spartan Student 7 now includes additional QSAR and thermodynamic properties, conveniently accessed from the molecule properties dialogue. **QSAR tab.** Access and post area, volume, PSA, ovality, LogP, and polarizability. Wave function-computed QSAR properties such as accessible area, polar area, accessible polar area, min. and max. electrostatic potential and min. local ionization potential are also available. **Thermodynamics tab.** Zero point energy, entropy, enthalpy, Gibbs free energy, and heat capacity are available and may be scaled based on temperature (excluding zero point energy).

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