New in *Spartan'18 Parallel Suite*. Below is a list of new features planned for the 2018 release of ***Spartan Parallel Suite***. Click **HERE** for full program brochure.
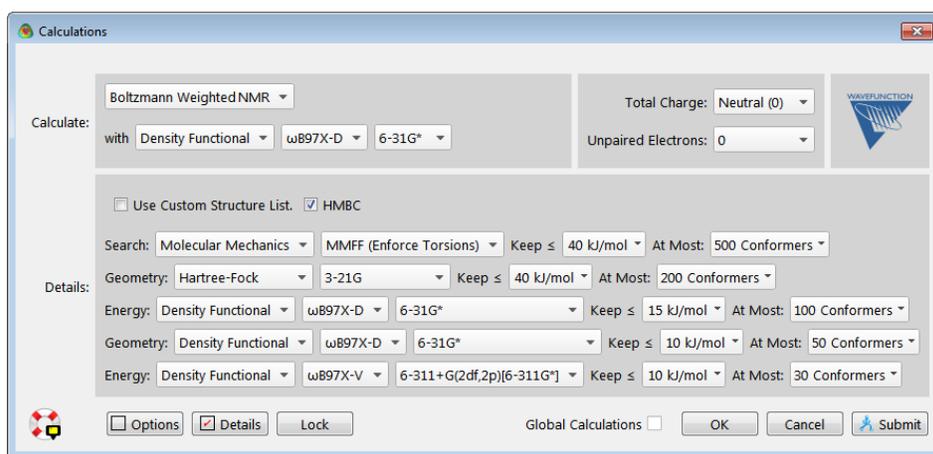
Conformation.

Set Torsions. A new algorithm has been implemented (a significant improvement over previous routines) for molecules that have both rings with >6 members and rotatable bonds (many if not most natural products fit this category). It is perhaps an order of magnitude faster previous versions.

Equilibrium Conformer. Now includes a quantum mechanics entry which leads to a selection of (two) multi-step procedures. Returned is the lowest-energy conformer according to the method used in the last step of the procedure (either B3LYP/6-311+G(2df,2p)[6-311+G*] or ωB97X-V/6-311+G(2df,2p)[6-311+G*]). A wide variety of user-defined procedures are also available.

Conformer Distribution. Like the *Equilibrium Conformer* task, this also now includes a quantum mechanics entry which leads to a selection of (two) multi-step procedures (as well as a wide variety of user-defined procedures. The lowest-energy conformer is returned (according to the method used in the last step of the method chosen, either B3LYP/6-311+G(2df,2p)[6-311+G*] or ωB97X-V/6-311+G(2df,2p)[6-311+G*]. The energy, dipole moment, and charges correspond to a proper Boltzmann weighted average. A supplementary list of the individual conformers (and their Boltzmann weights) is provided.

NMR.

Boltzmann Averaged NMR. A new computational task which utilizes the same automated multi-step procedures as *Conformer Distribution*. The NMR step involves either B3LYP/6-31G* or ωB97X-D/6-31G*. The Boltzmann weights are obtained from B3LYP/6-311+G(2df,2p)[6-311+G*] or ωB97X-V/6-311+G(2df,2p)[6-311+G*]), respectively.

While there are only two computational model options for NMR, alternative procedures may be used to obtain the Boltzmann weights (as in *Conformer Distribution*). Returned are Boltzmann averaged chemical shifts (and coupling constants if requested). A supplementary list of the individual conformers (and their Boltzmann weights) is provided. This is meant for conformationally-flexible molecules but also functions where there is only one conformer. The NMR check-box (and a new Coupling Constant check-box) are available as a Compute: option when either *Energy* or *Equilibrium Geometry* tasks are specified.

DP4 Support. The DP4 measure proposed by Goodman may be applied to find the best match either assuming the conformer provided for each (stereo/regio) isomer or Boltzmann averaging of conformers for each isomers. Both are automatic (starting from a list of one conformer for each isomer) and both may be based on either the B3LYP/6-31G* or ωB97X-D/6-31G* models for chemical shift calculation.

Coupling Constants. Spartan previously employed a Karplus-type approach to estimate 3-bond HH coupling constants (what the textbooks talk about when they draw proton spectra). This has been extended to 2-bond HH coupling constants. 2, 3 and 4-bond (and higher) CH coupling constants which are "almost never" reported as numbers but are essential to the construction of 2D HMBC spectra cannot be obtained empirically. This latest release includes an efficient procedure (involving only the so-called Fermi contact term and using the so-called PCJ-0 basis set) which provides satisfactory results. Spartan can utilize additional terms and use larger basis sets, but neither approach leads to statistically significant improvements. The CH calculations also lead to (provide) HH and CC coupling constants.

2D NMR Spectra. While the main goal of our 2D NMR development has been to produce calculated HMBC spectra, with HH coupling we can also produce COSY spectra. These (in various permutations) are the two most popular experimental 2D spectra. Previous Spartan versions have had this capability, but in the new release we will also be able to overlay the calculated spectra onto experimental spectra. Typically, the experimental data are not reported in digital form (only as PDF's), so we are working to implement a user-friendly means of comparison. At present we have a procedure for bringing in an image of 2D spectra and fitting this range/display to calculated Spectra for comparison. Some manual manipulation is required and we are working to optimize these tools.

Databases. (Parallel Suite only)

Energy Database. The *Spartan Spectra & Properties Database* (SSPD) is presently being expanded to include ωB97X-V/6-311+G(2df,2p) energies (as a property) will be available from existing ωB97X-D/6-31G* structures and NMR spectra. These energies will be accessible from the Reactions dialog.

Parallel Processing. (Parallel Suite only)

The shared memory parallelization routines which first appeared in *Spartan'16* have been extended to include frequencies. Two license options will be available, an *up to 16 cores* (default) and a *greater than 16 cores* for high performance servers (or cluster nodes). Initial benchmarking done with Hartree-Fock and large basis sets reflects a factor of 40 performance increase (over single core frequencies) on a 64 core system. Additional improvements are being worked on by our partners in Q-Chem, Inc.

Graphical Interface.
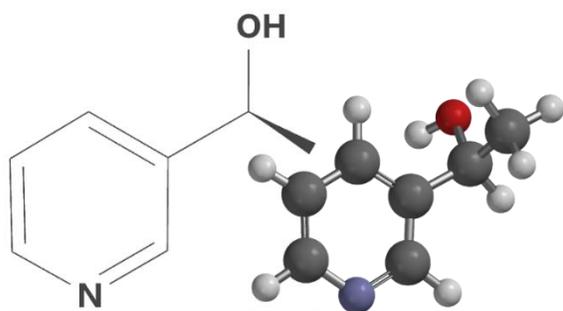
2D Drawings. Spartan derived 2D drawings (from the Sketch builder) will replace the library of 2D drawings we presently use and more importantly allow us to add whatever (organic molecules) the user provides. The intention is to be able to add drawings to plots, spectra and spreadsheets (among other places). In principle, everything the user builds in 3D should have a corresponding 2D drawing.

Output Summary. This has been revamped to include output as an HTML file, which can also be saved as PDF files and (hopefully by release time) can be printed (without explicitly going through Adobe tools). These include presentation of proton and carbon spectra as it typically appears in experimental papers (shifts, coupling constants, and HMBC correlations) as well tables of HH, CH and CC coupling constants. There is also material relating to IR and UV spectra. This is a significant improvement over output files from previous versions. Associated with this (and yet to be implemented) is automatic atom renumbering, where the hydrogens have the same numbers as the carbons they are attached to (H12a, H12b for C12 for example).

Graphical Surfaces. Background bleeding has been implemented 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).
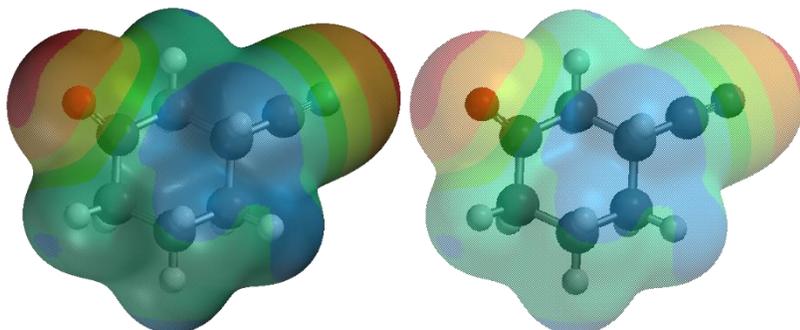
Computational Enhancements.

Spartan'18 Parallel Suite will take advantage of up to 16 cores for parallel jobs, with the option to license >16 cores as well (for high performance multicore systems), will include the latest *Q-Chem* version (5.0.2 at the time this list was compiled) and is the result of continued collaboration (begun with the release of *Spartan'02* in 2002). Through this collaboration our customers benefit from both GUI and computational enhancements in the *Spartan* code-base, as well as a growing range of computational approaches and modern computational methods included in *Q-Chem*. Included in this update are an assortment of additional functionals which can be accessed via type-in the DFT Method Selection dialogue. These include:

Exchange: optB88, PBE-GX
Local XC: HLE16, KT1, KT2, KT3
Hybrid XC: CAM-QTP00, CAM-QTP01, r CAM-B3LYP, WP04, WC04, TPSS0
Double hybrid XC: DSD-PBEPBE-D3, DSD-PBEP86-D3, DSD-PBEB95-D3,
PTPSS-D3, PWPB95-D3, B2GPPLYP, PBE-QIDS, and LS1DH-PBE

Additionally, a new effective core potential has been implemented to enable energy and optimizations for Lanthanides (properly accounting for f orbitals).

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