Automated conformational analysis along with NMR chemical shift calculations from empirically corrected B3LYP/6-31G* or ωB97X-D/6-31G* models provide Boltzmann-averaged NMR spectra for flexible molecules. The DP4 measure is available to determine the best match of calculated and experimental NMR chemical shifts from among a selection of stereo/regio isomers (or the Boltzmann averaged NMR of each isomer) using either B3LYP/6-31G* or ωB97X-D/6-31G* models.

Two, three, four and higher-bond HH, CH and CC coupling constants may be calculated in full or by using only the Fermi contact term. CH coupling constants allow calculation of realistic 2D HMBC plots. For backward compatibility, three-bond HH coupling constants from an extended form of the Karplus equation remain available.

3D to 2D structure conversion is available and resulting 2D sketches may be copied/pasted into spectra and plots.
Spartan’18 Parallel Suite provides convenient access to a number of important computational methods, with emphasis on density functional models among them:

**GGA functionals.** B86PW91, BLYP, BPW91, B97-D2, SOGGA11, PBE-D3, VV10

**GH-GGA functionals.** B3LYP, B3LYP-D3, EDF2, B3PW91, B97-3, MPW3LYP, SOGGA11-X

**RSH-GGA functionals.** ωB97X-D, ωB97X-V, ωB97X, CAM-B3LYP, N12-SX, LC-VV10

**mGGA functionals.** B97M-V, M06-L, BMK, M11-L, TPSS-D3

**GH-mGGA functionals.** M06-2X, M06, M08-HX, M08-SO, MPW1B95

**RSH-mGGA functionals.** M11, ωB97M-V, MN12-SX

Among the wave function based or correlated models are QCISD, QCISD(T), CCSD and CCSD(T) as well as the electric component of G3, G3(MP2), G4 and G4(MP2).

Available basis sets include the full range of Pople sets, the widely-used Dunning correlation consistent sets, and Ahlrich/Weigend def2 sets. Triple-ζ basis sets are now available for transition metals and lanthanides, allowing improved reaction energy calculations. The dual basis set approximation may be employed with double-ζ and larger basis sets, leading to an order of magnitude reduction in computation time.

**From menus:**

**Pople:** STO-3G, 3-21G, 6-31G*, 6-31G**, 6-31+G**, 6-311G**, 6-311+G**, 6-311G(2d,p), 6-311+G(2d,p), 6-311+G(2df,2p), 6-311+G(3df,2p); additional variations on the underlying 6-31G and 6-311G basis sets may be specified

**Dunning:** cc-pVDZ, aug-cc-pVDZ, cc-pVTZ, aug-cc-pVTZ, cc-pVQZ, aug-cc-pVQZ

**Ahlrichs/Weigend:** def2-SV(P), def2-SVPD, def2-TZVP, def2-TZVPPD, def2-QZVP, def2-QZVPPD

Spartan’18 Parallel Suite can be used as a server for both remotely submitted calculations and the Spartan Spectra and Properties Database, extending access to computational tools from remote devices. Remote computation is available from computers running Spartan’14 or later as well as iOS devices (iPad and iPhone) running the iSpartan app.
**SPARTAN’18 PARALLEL SUITE FEATURE SET**

**GRAPHICAL INTERFACE**

Sketch organic, inorganic, organometallic molecules in 2D and automatically convert to 3D structures. Groups, rings and ligands templates are available.

Build organic, inorganic and organometallic molecules, peptides and nucleotides, substituted molecules in 3D.

Auto-convert 3D structures to 2D sketches.

Link seamlessly to ChemDraw®

Display/query molecules in a variety of model styles.

Display dipole vector, hydrogen bonds, points and planes.

Display and customize chemical function descriptors.

Display user-defined annotations.

Align molecules using structure, chemical function descriptors, or atom labels.

Align molecules to pharmacophores.

Build transition states using reaction arrows.

Generate transition states from an extensive reaction library.

Generate and display molecular orbitals, electron densities, spin densities, electrostatic potentials, electrostatic potential maps, orbital maps, and local ionization potential maps.

Optionally silhouette mesh and transparent surfaces for improved visualization.

Generate and display orbital energy diagrams on-the-fly.

Optionally view property maps in Red-White-Blue color scale.

Toggle between default and absolute property ranges for property maps.

Display electron density based on % of enclosed electrons.

Highlight solvent accessible regions on surfaces and property maps.

Display R/S chirality markers, invert chiral centers and absolute chirality.

Integrated reaction energy calculator.

Organize data in spreadsheets.

Print and save calculated spectra tables as PDF files.

Perform regression analysis and make, save and print 2D or 3D plots.

Embed external files such as MS® Office and Adobe® PDF files in Spartan files.

Plot, print, and save calculated and experimental IR, Raman, and UV/vis spectra.

Display calculated 1D (proton, $^{13}$C, DEPT) and 2D (COSY, HSQC, HMBC) and experimental 1D proton and $^{13}$C NMR spectra.

Overlay experimental HMBC and COSY 2D NMR spectra with calculated results.
Calculate strain energy, total energy and heat of formation
Determine gas-phase equilibrium and transition-state geometries
Determine geometries and IR spectra in the presence of solvent; identify global minimum; calculate Boltzmann weights to obtain conformer energy distributions
Build libraries of diverse conformers for use in similarity analysis
Perform similarity analysis on the basis of structure or chemical functionality
Scan geometrical coordinates and generate reaction sequences
Calculate reaction and activation energies
Calculate IR, Raman, UV/vis, and NMR spectra
Determine NMR spectra for flexible molecules
Search SSPD and NIST experimental database for match to calculated NMR spectra
Mine databases of calculated molecular, atomic, and reaction properties

**Molecular Mechanics. SYBYL, MMFF94, MMFF(aq)**
**Semi-Empirical. MNDO, AM1, RM1, PM3 (with transition metal parameters), PM6**
**Hartree-Fock molecular orbital theory**

**Density Functional Theory (functionals available from menus):**
  - GGA functionals: B86PW91, BLYP, BPW91, B97-D2, SOGGA11, PBE-D3, VV10
  - GH-GGA functionals: B3LYP, B3LYP-D3, EDFT, B3PW91, B97-3, SOGGA11-X
  - RSH-GGA functionals: wB97X-D, wB97X-V, wB97X, CAM-B3LYP, N12-SX, LC-VV10
  - mGGA functionals: B97M-V, M06-L, BMK, M11-L, TPSS-D3
  - GH-mGGA functionals: M06-2X, M06, M08-HX, M08-SO, MPW1B95
  - RSH-mGGA functionals: M11, wB97M-V, MN12-SX

Functionals may be customized and additional functionals specified via keywords
Møller Plesset. MP2, MP3, MP4, and RI-MP2

**Wave function based advanced correlated models:**
  - G3(MP2)elect, G3eXct, G4(MP2)eXct, G4eXct, QCISD, QCISD(T), CCSD, CCSD(T)
  - Additional wave function based advanced correlated methods are available from keywords and include CCSD, CCSD(T), OD, OD(T), QCDD, VOD, and VQCCD

**Excited-state methods.** CIS, CIS(D), RI-CIS(D), QCIS(D), QCISD(T) and TDDFT

**Thermochemical Recipes.** T1, G3(MP2), G3, G4(MP2), G4

**Basis Sets (available from menus):**
  - Pople: STO-3G, 3-21G, 6-31G*, 6-31G**, 6-31+G**, 6-311G**, 6-311+G**, 6-311G(2d,p), 6-311+G(2d,p), 6-311+G(2df,2p), 6-311+G(3df,2p); other variations on 6-31G and 6-311G may be specified
  - Dunning: cc-pVDZ, aug-cc-pVDZ, cc-pVTZ, aug-cc-pVTZ, cc-pVQZ, aug-cc-pVQZ
  - Ahlrichs/Weigend: def2-SV(P), def2-SVPD, def2-TZVP, def2-TZVPDD, def2-QZVP, def2-QZVPPD

**Automatic use of pseudopotentials for elements >Kr (including lanthanides and select actinides)**

**Dual basis set approximation available with double-ζ and larger basis sets**

**Import custom basis sets**
PROPERTIES AND QSAR DESCRIPTORS

Mulliken, natural, and electrostatic-fit charges
Dipole and higher moments, polarizabilities and hyperpolarizabilities
Enthalpies, entropies and free energies
Solvation energies from C-PCM, as well as SM5.4, SM8, SM12, SMD and SS(V)PE
Statistical tools for comparing calculated and experimental $^{13}$C NMR shifts
HOMO, LUMO and SOMO energies
Areas, polar surface areas and volumes based on space-filling models
Areas, accessible areas, polar areas, and volumes based on the electron density
Min/Max of electrostatic potential and Min of local ionization potential
Number of conformers and tautomers
Number of hydrogen bond acceptors and donors

SPECTRA

NMR, IR, Raman and UV/visible spectra may be calculated using a variety of theoretical models: Hartree-Fock and density functional models for NMR, semi-empirical, Hartree-Fock, density functional and MP2 models for IR, Hartree-Fock, density functional models for Raman and UV/visible.

◆ ◆ ◆ NMR

A 3rd-generation parameterization scheme for corrections to NMR chemical shifts for the B3LYP/6-31G*, $\omega$B97X-D/6-31G* and $\omega$B97X-D/6-311G* models is available.
Calculated (corrected) chemical shifts together with calculated three-bond HH, CH, and CC coupling constants [using the B3LYP functional with PCJ-0 (PCJ-1 and PCJ-2 basis sets are also available)] allow for a $^1$H $^{13}$C and DEPT 1D spectra and COSY, HSQC and HMBC 2D spectra. Proton spectra may be displayed with or without HH coupling.

◆ ◆ ◆ IR AND RAMAN

Infrared (and Raman) frequencies calculated from $\omega$B97X-D/6-31G*, B3LYP/6-31G* and EDF2/6-31G* density functional models are scaled to account for systematic errors associated with the harmonic approximation. Corrected frequencies and intensities are fit to a Lorentzian function with a line width parameter. Alternatively, scale and line width may be adjusted to best fit a spectrum calculated using any theoretical model to an experimental spectrum.

◆ ◆ ◆ UV/VISIBLE

UV/visible spectra are obtained by explicit calculation of the ground state energies and the low-lying excited states. CIS models are paired with Hartree-Fock models. TDDFT (time dependent density functional) models are paired with density functional models.
Spartan Spectra and Properties Database (SSPD)® comprises two collections, the first of ≈300,000 organic molecules obtained from the EDF2/6-31G* model and the second of ≈300,000 organic molecules and ≈2,000 organometallic molecules obtained from the ωB97X-D/6-31G* model. Both include the optimized geometry, the energy and a selection of molecular properties, the wave function (allowing on-the-fly generation of graphical surfaces), and the NMR spectrum. The infrared spectrum is also provided for molecules in the EDF2/6-31G* collection. Individual SSPD entries can replace user-built structures, and both collections are searchable by substructure, name, formula, and isomer.

Spartan Reaction Database (SRD)® comprises transition states for ≈1,800 reactions searchable by combination of substructure and “reaction arrows” from either 2D sketches or 3D models.

ωB97X-V/6-311+G(2df,2p) ENERGY DATABASE

SSPD entries now include calculated energies from the ωB97X-V/6-311+G(2df,2p) model, providing more accurate reaction energies than provided by the ωB97X-D/6-31G* model. These can be accessed from the Properties or Reactions dialogue as well as from the Spreadsheet.

ADDITIONAL FEATURES

Multi-core parallel processing for Hartree-Fock, density functional, RI-MP2, and thermochemical recipes.

Automatic processing of groups of molecules

Automatic use of molecular symmetry

View recent documents from File menu

Optimize using constraints and/or frozen atoms

NOEs for conformational searching

Identify tautomers and generate tautomer lists

Import experimental IR, Raman, and NMR spectra

Import structures in InChI, SMILES, CDX, CIF, SKC, SDF, TGF, XYZ, Macromodel, PDB, SYBYL MOL and MOL2 format

Retrieve structures from Cambridge Structural Database and Protein Data Bank

Extract ligands and binding sites from proteins (PDB files)

Databases

Spartan Spectra and Properties Database (SSPD)® comprises two collections, the first of ≈300,000 organic molecules obtained from the EDF2/6-31G* model and the second of ≈300,000 organic molecules and ≈2,000 organometallic molecules obtained from the ωB97X-D/6-31G* model. Both include the optimized geometry, the energy and a selection of molecular properties, the wave function (allowing on-the-fly generation of graphical surfaces), and the NMR spectrum. The infrared spectrum is also provided for molecules in the EDF2/6-31G* collection. Individual SSPD entries can replace user-built structures, and both collections are searchable by substructure, name, formula, and isomer.

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Enhanced Parallel Performance

Parallelization now includes shared-memory frequency calculations. Performance has been improved for > 8 core systems.

Summary Output

Provides Tables for NMR chemical shifts and coupling constants, IR and Raman frequencies and intensities and UV/visible absorption frequencies and strengths are provided and may be saved as PDF files.

Chemical Shift Labels

Labels for experimental NMR chemical shifts and differences between calculated (Boltzmann averaged) and experimental chemical shifts are now available.
<table>
<thead>
<tr>
<th>Product</th>
<th>Academic</th>
<th>Government</th>
<th>Commercial</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parallel Suite (up to 16 cores)**</td>
<td>$1,600</td>
<td>$3,200</td>
<td>$4,800</td>
</tr>
<tr>
<td>Parallel Suite (greater than 16 cores)**</td>
<td>$2,400</td>
<td>$4,800</td>
<td>$7,200</td>
</tr>
<tr>
<td>Spartan’18 (single-core version)</td>
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<td>$2,400</td>
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** Academic Lab Pricing**

<table>
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<tr>
<td>20 Seat Lab License</td>
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</tr>
</tbody>
</table>

* Annual campus-wide site license available, contact sales@wavefun.com for pricing.

** Spartan’18 Parallel Suite provides parallel processing for select methods and tasks and includes access/utilization for either up to 16 cores, or greater than 16 cores. The Parallel Suite also includes access to the Spartan Spectra and Properties Database (SSPD), and the ability to act as a computation server for other Spartan licenses or the iSpartan app.

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**SPARTAN’18 PARALLEL SUITE LICENSING**

**MINIMUM SYSTEM REQUIREMENTS**

**WINDOWS**
- Intel or AMD only
- Windows 7, 8.1, or 10**
- 128 GB disk space or higher (SSD recommended)
- 4 GB of RAM (at least 2GB RAM per core)

**MACINTOSH**
- Intel-based Macintosh only
- OS X 10.10, 10.11, 10.12, or 10.13
- 128 GB disk space or higher (SSD recommended)
- 4 GB RAM (at least 2GB of RAM per core)

* Spartan’18 Parallel Suite available for Windows, Macintosh, and Linux. Spartan’18 available for Windows and Macintosh only. Contact Wavefunction for Linux system requirements.

**Fully supports Windows 7, 8, and 10 touch screen computers and tablets.**