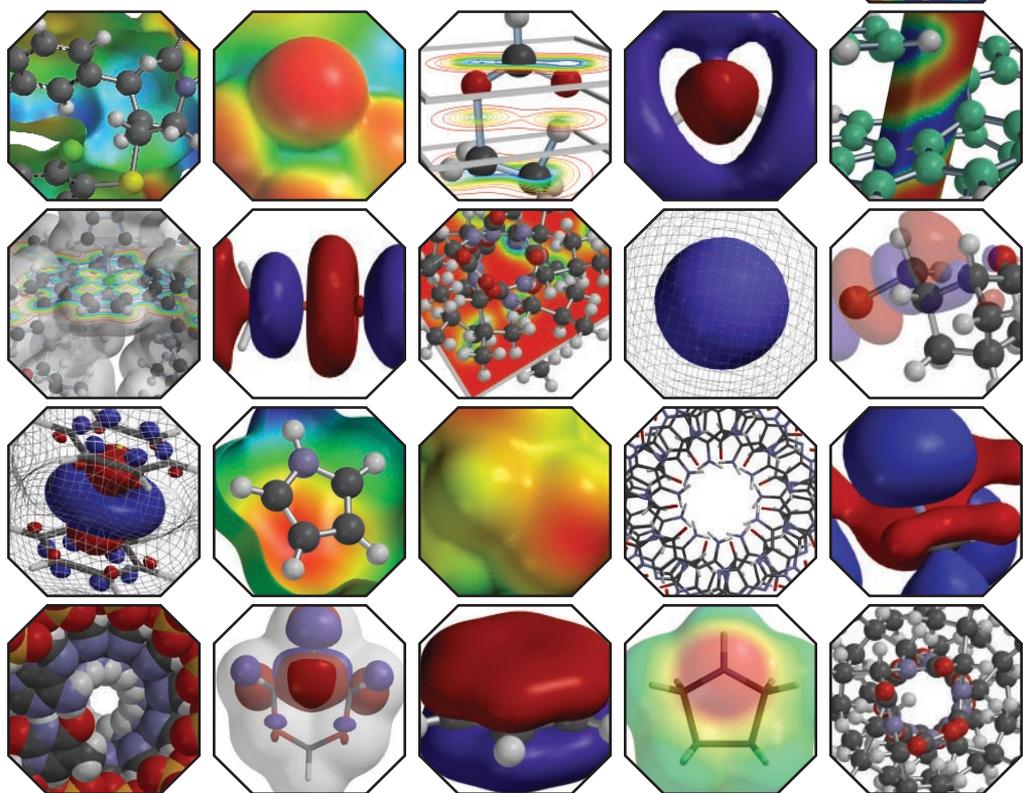
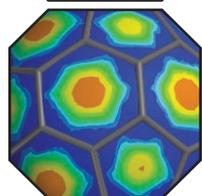


Spartan'18

Parallel Suite



Spartan'18 Parallel Suite is the latest version of Wavefunction's **Spartan** line of molecular modeling software for research and education, representing a significant improvement in access to modern computational methods while new interface developments add to **Spartan's** legacy of user-friendliness. In the latest release, particular attention has been given to the properties of flexible molecules and to NMR spectra. New and improved features include:

AUTOMATED CONFORMATIONAL ANALYSIS



A multi-step recipe for obtaining accurate Boltzmann distributions has been implemented. Combining MMFF, Hartree-Fock, and density functional models, Boltzmann distributions are ultimately obtained from either B97M-V/6-311+G(2df,2p)[6-311G*] energies with B3LYP/6-31G* geometries or ω B97X-V/6-311+G(2df,2p)[6-311G*] energies with ω B97X-D/6-31G* geometries. User-customization is available for theoretical models used to obtain geometry and energy.

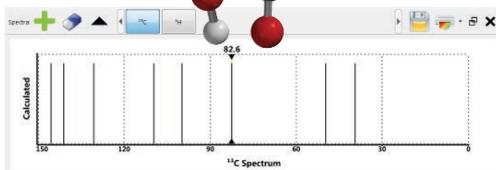
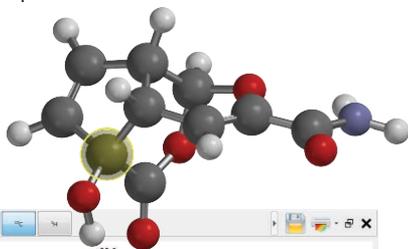


AUTOMATED NMR FOR FLEXIBLE MOLECULES

Automated conformational analysis along with NMR chemical shift calculations from empirically corrected B3LYP/6-31G* or ω B97X-D/6-31G* models provide Boltzmann-averaged NMR spectra for flexible molecules.

DP4 SUPPORT

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 ω B97X-D/6-31G* models.



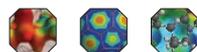
COUPLING CONSTANTS

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.



2D SKETCHES FROM 3D STRUCTURES

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. ω B97X-D, ω B97X-V, ω B97X, 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, ω B97M-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).

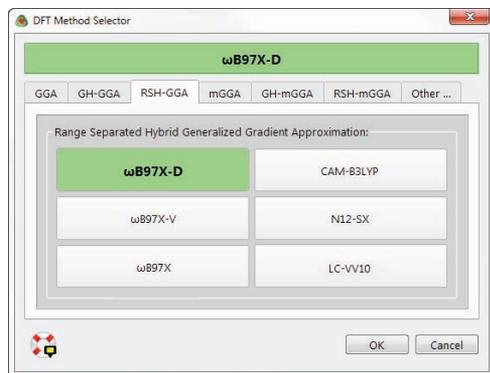
Available basis sets include the full range of Pople sets, the widely-used Dunning correlation consistent sets, and Ahlrich/Weigend def2 sets. Triple- ζ basis sets are now available for transition metals and lanthanides, allowing improved reaction energy calculations. The dual basis set approximation 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

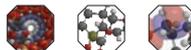


REMOTE SUBMISSION

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, ¹³C, DEPT) and 2D (COSY, HSQC, HMBC) and experimental 1D proton and ¹³C NMR spectra

Overlay experimental HMBC and COSY 2D NMR spectra with calculated results





TASKS

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

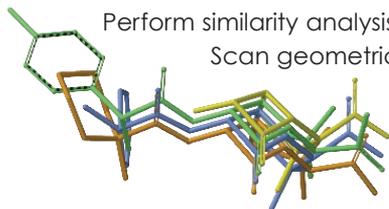
Calculate IR, Raman, UV/vis, and NMR spectra

Determine NMR spectra for flexible molecules

Match calculated and experimental NMR spectra

Search SSPD and NIST experimental database for match to calculated IR spectra

Mine databases of calculated molecular, atomic, and reaction properties



COMPUTATIONAL METHODS



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, EDF2, B3PW91, B97-3, SOGGA11-X

RSH-GGA functionals: ω B97X-D, ω B97X-V, ω B97X, 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, ω B97M-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, G3elect, G4(MP2)elect, G4elect, 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), QCCD, VOD, and VQCCD

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

Gradients available for CIS, CIS(D) 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

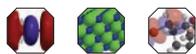
Dunning: cc-pVDZ, aug-cc-pVDZ, cc-pVTZ, aug-cc-pVTZ, cc-pVQZ, aug-cc-pVQZ

Ahlrichs/Weigend: def2-SV(P), def2-SVPD, def2-TZVP, def2-TZVPPD, 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*, ω B97X-D/6-31G* and ω 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 ^1H ^{13}C and DEPT 1D spectra and COSY, HSQC and HMBC 2D spectra. Proton spectra may be displayed with or without HH coupling.

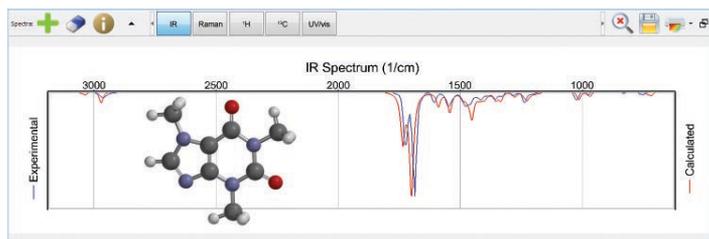
◆ ◆ ◆ IR AND RAMAN

Infrared (and Raman) frequencies calculated from ω 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

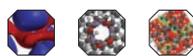
any theoretical model to an experimental spectrum.



◆ ◆ ◆ 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.

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

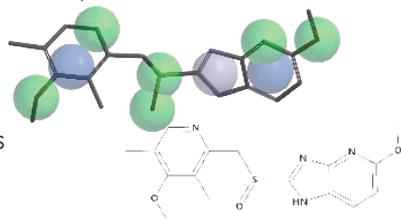
Identify tautomers and generate tautomer lists

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 $\approx 300,000$ organic molecules obtained from the EDF2/6-31G* model and the second of $\approx 300,000$ organic molecules and $\approx 2,000$ organometallic molecules obtained from the ω B97X-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 $\approx 1,800$ reactions searchable by combination of substructure and "reaction arrows" from either 2D sketches or 3D models.

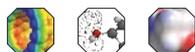
ω B97X-V/6-311+G(2df,2p) ENERGY DATABASE

SSPD entries now include calculated energies from the ω B97X-V/6-311+G(2df,2p) model, providing more accurate reaction energies than provided by the ω B97X-D/6-31G* model. These can be accessed from the Properties or Reactions dialogue as well as from the Spreadsheet.



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.

	Academic	Government	Commercial
Parallel Suite (up to 16 cores)**	\$ 1,600	\$ 3,200	\$ 4,800
Parallel Suite (greater than 16 cores)**	\$ 2,400	\$ 4,800	\$ 7,200
Spartan'18 (single-core version)	\$ 1,200	\$ 2,400	\$ 3,600
Academic Lab Pricing	Spartan'18 Parallel Suite		Spartan'18
5 Seat Lab License	\$ 6,400		\$ 4,800
10 Seat Lab License	\$ 12,000		\$ 9,000
20 Seat Lab License	\$ 16,000		\$12,000

* 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.

MINIMUM SYSTEM REQUIREMENTS*

WINDOWS

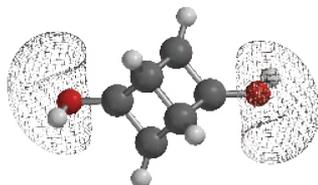
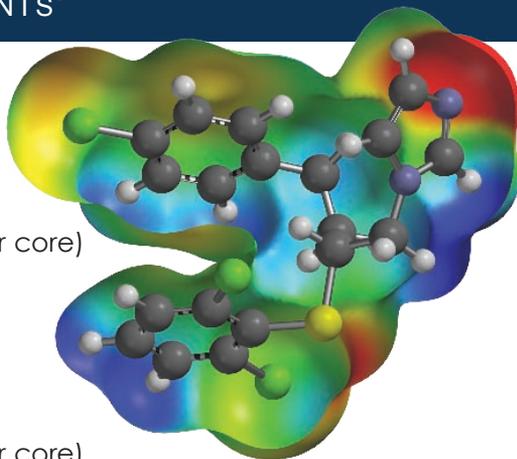
- Intel or AMD only
- Windows 7, 8.1, or 10**
- 128 GB disk space or higher (SSD recommended)
- 4 GB of RAM (at least 2GB RAM per core)

MACINTOSH

- Intel-based Macintosh only
- OS X 10.11, 10.12, 10.13 or 10.14
- 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.



Spartan'18 Parallel Suite

is a collaboration with **Q-CHEM**
A Division of Intel, the leader in security.

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