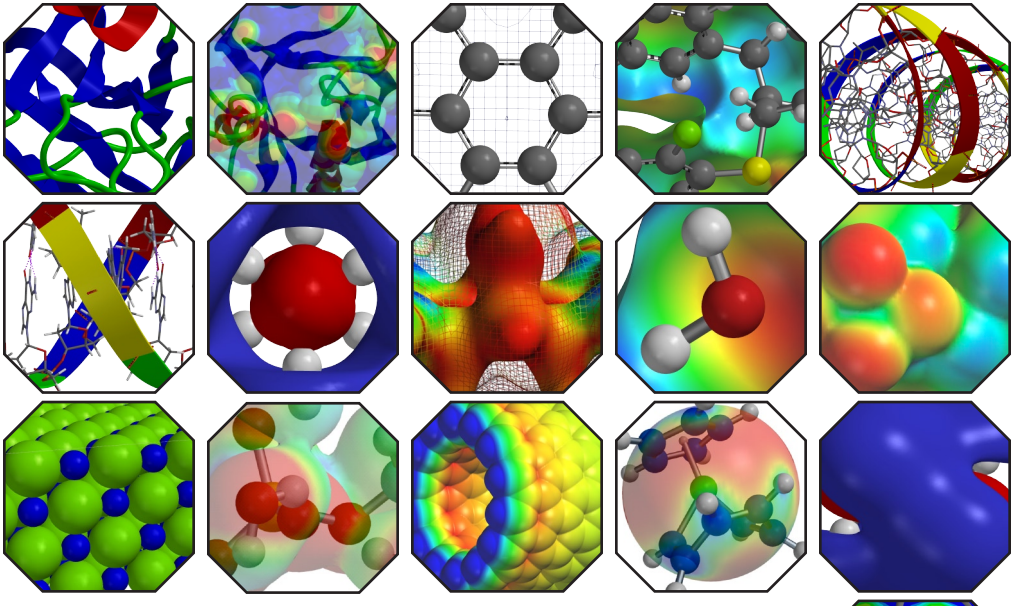
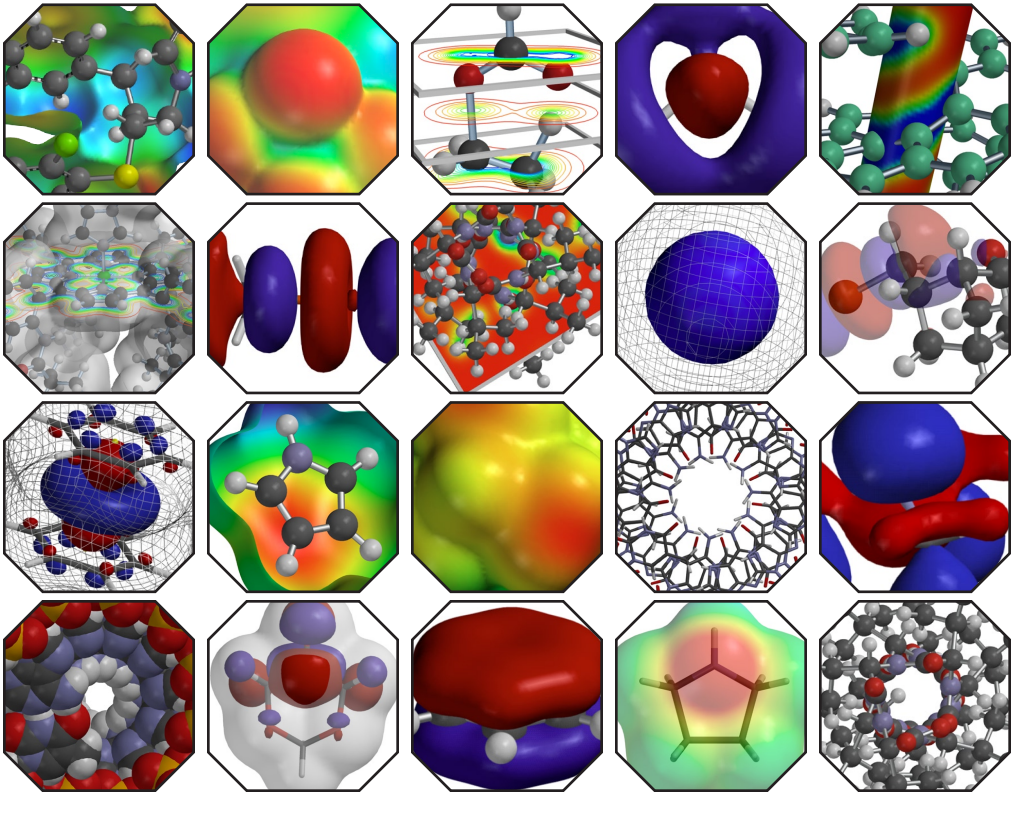


Spartan'20

for Windows, Macintosh and Linux



Spartan'20 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



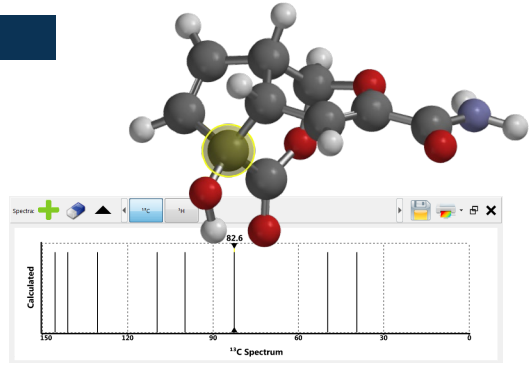
A multi-step recipe for obtaining accurate Boltzmann distributions has been implemented. Combining MMFF, Hartree-Fock, and density functional models, Boltzmann distributions are ultimately obtained from either B97M-V/6-311+G(2df,2p)[6-311G*] energies with B3LYP/6-31G* geometries or ωB97X-V/6-311+G(2df,2p)[6-311G*] energies with ωB97X-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 ωB97X-D/6-31G* models provide Boltzmann-averaged NMR spectra for flexible molecules. Where experimental data are available, a lower-cost alternative procedure provides spectra based on the conformer, which gives the best fit.

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 ωB97X-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. Three-bond HH coupling constants from an extended form of the Karplus equation are available.

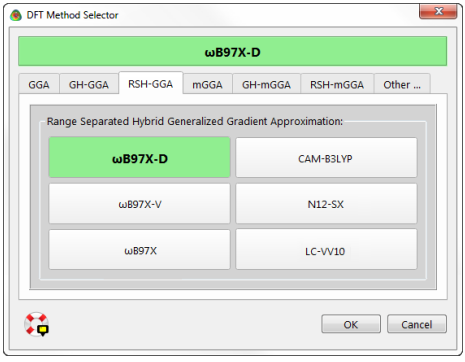


2D SKETCHES FROM 3D STRUCTURES

3D to 2D structure conversion is available and resulting 2D sketches may be copied/pasted into spectra and plots.

MODERN COMPUTATIONAL METHODS

Spartan'20 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

DH-RSH-mGGGA. ωB97M(2)

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) and G4.

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

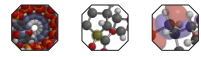
Ahlrichs/Weigend: def2-SV(P), def2-SVPD, def2-TZVP, def2-TZVPPD, def2-QZVP, def2-QZVPPD

REMOTE SUBMISSION

Spartan'20 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*** (2014 release or newer) as well as iOS devices (iPad and iPhone) running the ***iSpartan*** app.

SPARTAN'20 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® (Win Only)

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 lists of regio and stereoisomers

Generate lists of tautomers

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

Input experimental proton and ^{13}C chemical shifts

Input observed 3-bond HH couplings and 2 and 3-bond CH couplings for superposition onto calculated COSY and HMBC plots

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

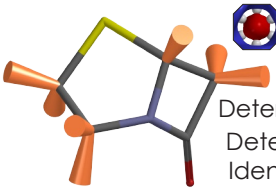
Perform regression analysis and make, save and print 2D or 3D plots

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

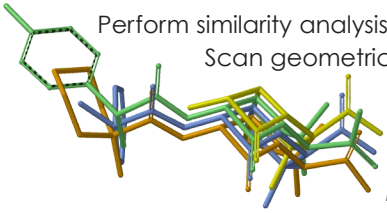
Display calculated 1D (proton, ^{13}C, DEPT) and 2D (COSY, HSQC, HMBC) and experimental 1D proton and ^{13}C NMR spectra

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



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: 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
- DH-RSH-mGGA functionals: ωB97M(2)

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, 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

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 and a number of Truhlar models
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.

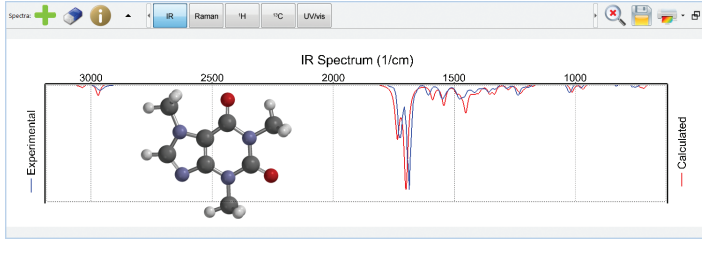
NMR

A 3rd-generation parameterization scheme for corrections to NMR chemical shifts for the B3LYP/6-31G*, ωB97X-D/6-31G* and ωB97X-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. Observed HH and CH couplings may be inputted to construct "experimental" COSY and HMBC plots which can then be superimposed onto calculated plots.

IR AND RAMAN

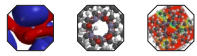
Infrared (and Raman) frequencies calculated from ωB97X-D/6-31G*, B3LYP/6-31G* and EDF2/6-31G* density functional models are scaled to account for systematic errors associated with the harmonic approximation. Corrected frequencies and intensities are fit to a Lorentzian function with a line width parameter. Alternatively, scale and line width may be adjusted to best fit a spectrum calculated using any theoretical model to an experimental spectrum.



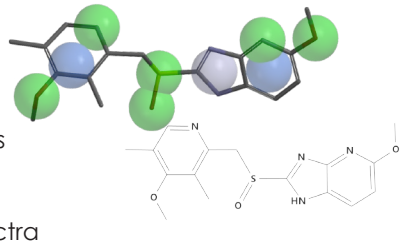
UV/VISIBLE

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.

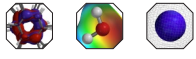
ADDITIONAL FEATURES



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)



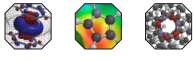
DATABASES

Spartan Spectra and Properties Database *(SSPD)*® comprises two collections, the first of ≈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.

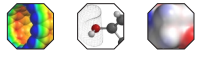
ωB97X-V/6-311+G(2df,2p) ENERGY DATABASE

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.



ENHANCED PARALLEL PERFORMANCE

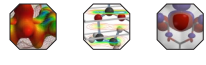
Parallelization now includes shared-memory frequency calculations. Performance has been improved for up to 16 core systems.



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.

SPARTAN'20 LICENSING*

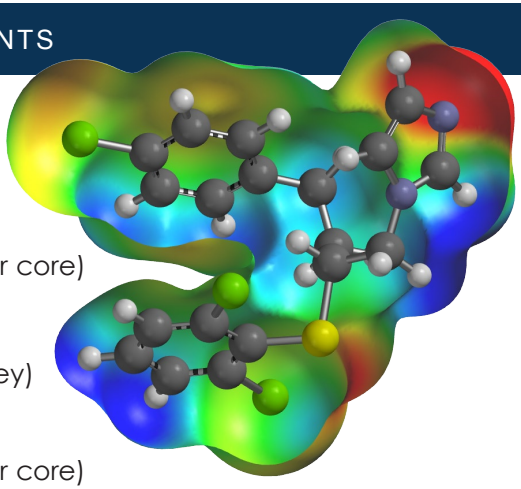
	Academic	Government	Commercial
Spartan'20* (up to 16 cores)*	$ 1,600	$ 3,200	$ 4,800
Spartan'20* (greater than 16 cores)*	$ 2,400	$ 4,800	$ 7,200

Academic Lab Pricing	***Spartan'20 Parallel Suite***
5 Seat Lab License	$ 6,400
10 Seat Lab License	$ 12,000
20 Seat Lab License	$ 16,000

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

** ***Spartan'20*** *provides parallel processing for select methods and tasks and includes access/utilization for either up to 16 cores, or greater than 16 cores.* ***Spartan*** *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

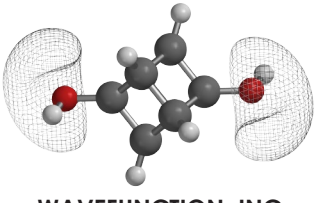


WINDOWS
- Intel or AMD (64-bit only)
- Windows 8.1, or 10*
- 128 GB disk space or higher (SSD recommended)
- 4 GB of RAM (at least 2GB RAM per core)

MACINTOSH
- Intel or M1 chips (only)
- OS X 10.12.6 (Sierra) - 12.X (Monterey)
- 128 GB disk space or higher (SSD recommended)
- 4 GB RAM (at least 2GB of RAM per core)

LINUX
- Modern Intel or AMD Processors (64-bit only)
- Linux RHEL 7 and 8, CentOS 7 and 8, Ubuntu 18.04 and 20.04 LTS
- 128 GB disk space or higher (SSD recommended)
- 4 GB RAM (at least 2GB of RAM per core)

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



Spartan'20

for Windows, Macintosh and Linux

is a collaboration with Q-CHEM

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