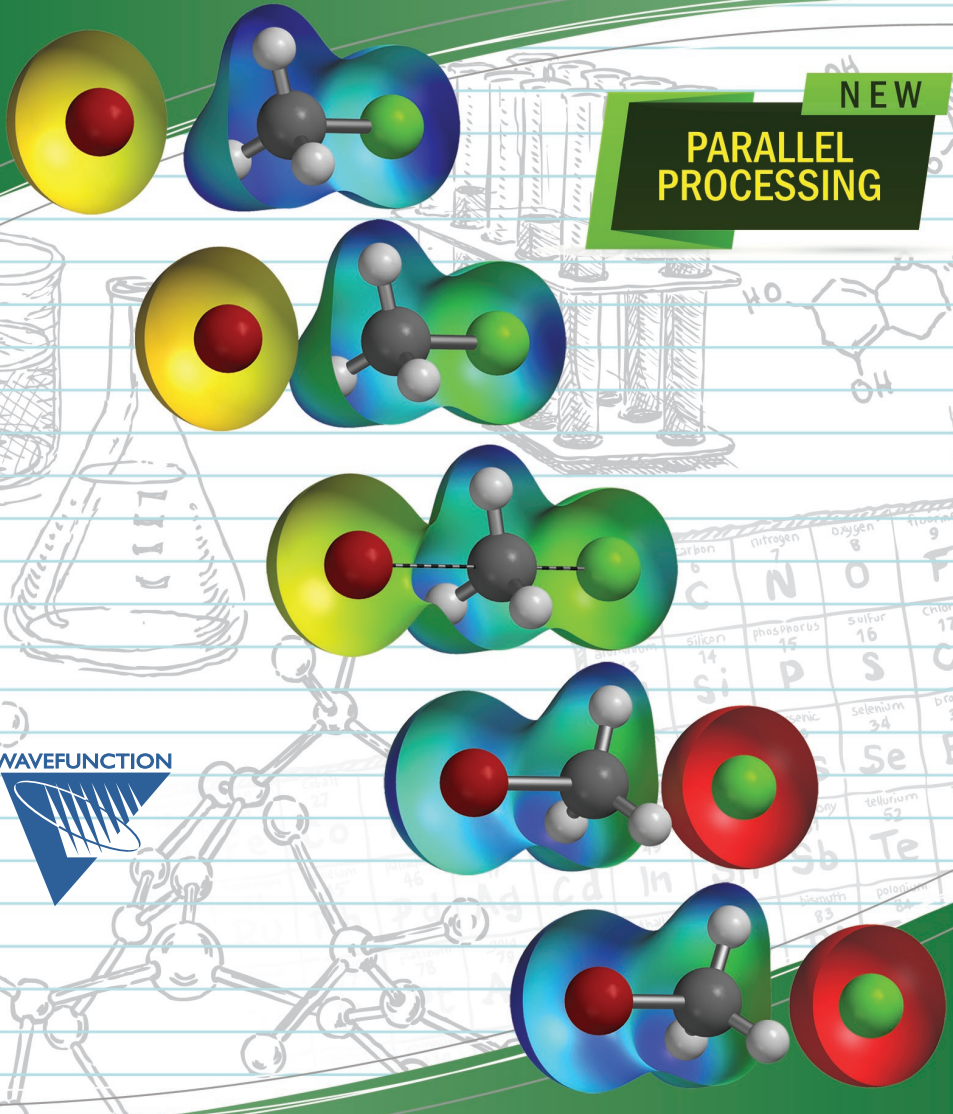
Spartan Student



NEW

PARALLEL PROCESSING

WAVEFUNCTION

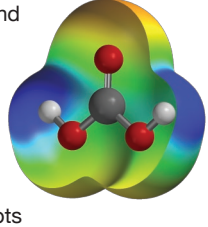
MOLECULAR MODELING
FOR UNDERGRADUATE CHEMISTRY

Spartan Student Edition v. 8

Features in bold are new or improved in the ***Spartan Student version 8*** release. Late 2019.

GRAPHICAL USER INTERFACE

- **Sketch 2D organic and inorganic molecules**
- 2D templates for groups, rings, and ligands
- Automatic conversion from 2D to 3D
- **Automatic conversion from 3D to 2D sketch**
- Build 3D organic, inorganic, and organometallics
- Build 3D polypeptides and polynucleotides
- Automatically display R/S chirality
- Display dipole vector and hydrogen bonds
- Search transition state library from 2D or 3D
- Spreadsheets for data analysis and plotting
- Integrated reaction energy calculator
- **Reaction energy calculations from ΔH° & ΔG°**
- Display calculated NMR and IR spectra
- Display experimental NMR and IR spectra
- Display molecular orbitals, electron density, spin density, electrostatic potential isosurfaces
- Display electrostatic potential, local ionization potential and |LUMO| maps
- **Improved Atom Properties dialog**
- Enhanced visualization models for Polypeptides and polynucleotides



- Display Ramachandran plots
- Display Orbital Energy diagrams
- **New Output Summary**
- Export spreadsheet data as MS Excel or SD file
- Export graphics as JPG, BMP, or (high res) PNG
- Touch/Trackpad commands and gestures
- **Integrated lab activities**

METHODS

- Molecular Mechanics (MMFF)
- Semi-empirical (PM3) up to 75 atoms
- Hartree-Fock molecular orbital up to 30 atoms
- DFT (B3LYP, EDF2 & ω**B97X-D**) up to 30 atoms
- Møller-Plesset (MP2) up to 20 atoms
- **T1 thermochemical recipe** up to 20 atoms

TASKS

- Determine energies and equilibrium geometries
- Determine transition state geometries
- Determine energies and geometries in the presence of water, polar, or non-polar solvent
- Determine global minimum (equilibrium conformer)
- Establish conformer distribution
- Calculate IR spectra, optionally fit to experimental IR
- Calculate NMR spectra with improved accuracy
- Calculate QSAR properties
- **Calculate highly accurate heats of formation**
- Determine orbital energies, vibrational modes, thermodynamic properties, charges & bond orders

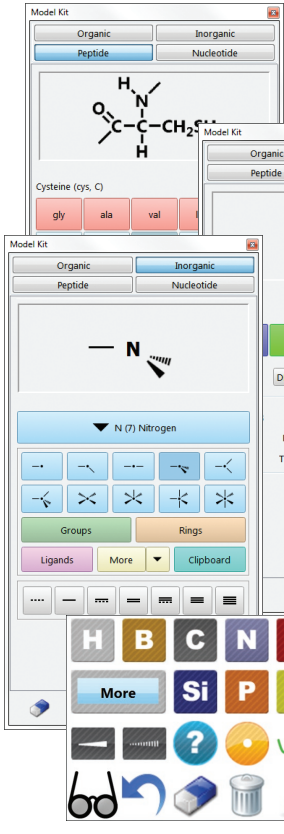
PROPERTIES

- Name, weight, formula, and CAS number
- Atomic charges & chemical shifts
- **Bond Orders**
- HOMO and LUMO energies
- Experimental heats of formation
- Number of conformers and HBAs and HBDs
- Volume, area, polar surface area and ovality
- Polar area based on electrostatic potential
- LogP and polarizability
- Entropy, Enthalpy, Gibbs free energy, zero point energy and heat capacity

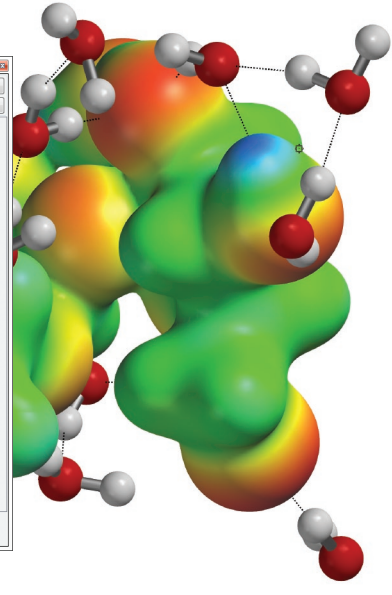
ADDITIONAL FEATURES

- **Parallel processing (up to 16 cores)**
- Automatic processing of list documents
- Align molecules by **structure or label**
- Cartesian optimization subject to constraints
- Automatic use of symmetry
- **Updated Spectra & Properties Database**
- Search and retrieve from the Protein Data Bank
- **Access Wikipedia & ChemSpider by name search**

Providing affordable molecular modeling software and modern computational methods to explore general, organic, physical, and inorganic chemistry topics in undergraduate chemistry.



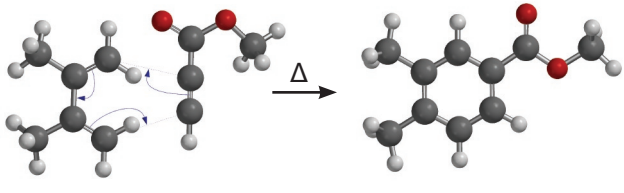
Organic, Inorganic, Peptide, Nucleotide, and 2D builders allow easy construction of a wide variety of molecules, from water to DNA. Transition states are constructed from reactants using familiar arrow-pushing nomenclature and an extensive library of common reactions.

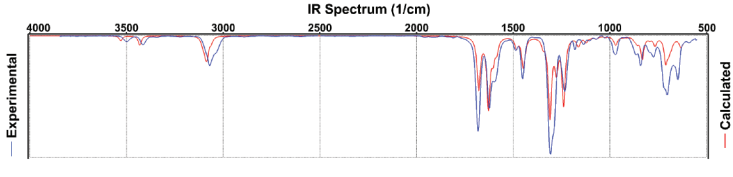


Available features and computational methods enable the exploration of fundamental concepts and molecular properties:

- covalent and ionic bonding
- thermodynamics and kinetics
- reactivity and selectivity
- atomic charges
- atomic and molecular orbitals
- acidity and basicity
- dipole moments
- hydrogen bonding
- IR spectra
- NMR spectra
- solvation
- aromaticity
- stereochemistry
- conformation
- chemical reactions

At Right: Diels-Alder Reaction of 2,3-dimethyl-1,3-butadiene with methyl propiolate





At left Calculated and Experimental IR Spectra for 3-aminobenzophenone

GLOBAL LICENSING

Spartan Student Edition Pricing:

Individual Faculty License	$ 750	5 Seat Lab License	$ 2,500
Individual Student License*	$ 50	10 Seat Lab License	$ 4,500

Campus-wide Annual Site Licenses Available Starting at $ 2,500**

* Academic institutes and students may purchase at the individual student license pricing, provided that the software is installed on student-owned machines only. Wavefunction may require proof of student status before releasing activation codes for individual student licensing. If required for a course, additional discounts may apply. Please contact **sales@wavefun.com** for details.

** Annual Site license pricing is based on total enrollment, includes unlimited access to ***Spartan Student Edition*** on campus machines, and may also include access to the research version of ***Spartan*** software. Please contact **sales@wavefun.com** for details.

SYSTEM REQUIREMENTS

WINDOWS

- 64-bit Intel or AMD only
- Windows* 8.1 or 10
- 2 GB RAM
- 128 GB disk space

MACINTOSH

- Intel or M1 chips (only)
- OS X 10.12.6 (Sierra) - OS 12.X (Monterey)
- 2 GB RAM
- 128 GB disk space

* ***Spartan Student 8*** supports Windows 8, and 10 touch screen computers and tablets.

Q-CHEM

Spartan Student is a collaboration with Q-Chem, Inc.

WAVEFUNCTION

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