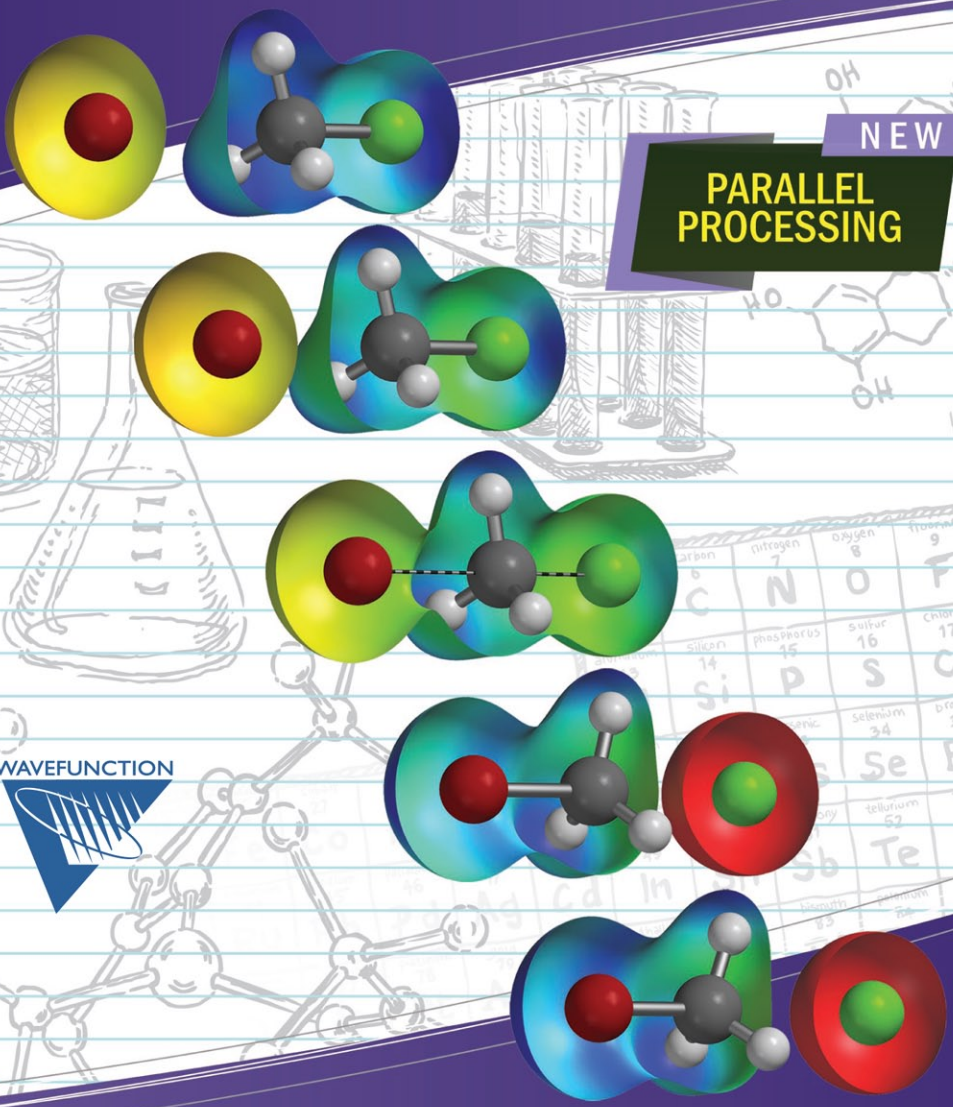
Spartan Student



NEW

PARALLEL PROCESSING

WAVEFUNCTION

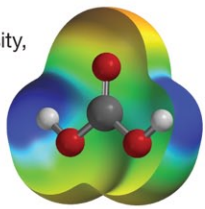
MOLECULAR MODELING FOR UNDERGRADUATE CHEMISTRY

Spartan Student Edition v. 9

Features in bold are new or improved in the ***Spartan Student version 9*** release. Summer 2022.

GRAPHICAL USER INTERFACE

- **Sketch 2D organic and inorganic molecules**
- 2D templates for groups, rings, and ligands
- Automatic conversion from 2D to 3D
- **Improved conversion from 3D to 2D sketch**
- Build 3D organic, inorganic, and organometallics
- Build 3D polypeptides and polynucleotides
- Automatically display R/S chirality
- **Generate Isomers**
- 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°
- **Calculated NMR, IR, and UV/vis**
- **Experimental NMR, IR and UV/vis**
- Display molecular orbitals, electron density, spin density, electrostatic potential isosurfaces
- Display electrostatic potential, local ionization potential and |LUMO| maps



- Improved Atom Properties dialog
- 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 & ωB97X-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 UV/vis spectra**
- Calculate QSAR properties
- Calculate highly accurate heats of formation
- Determine orbital energies, vibrational modes, thermodynamic properties, charges & bond orders

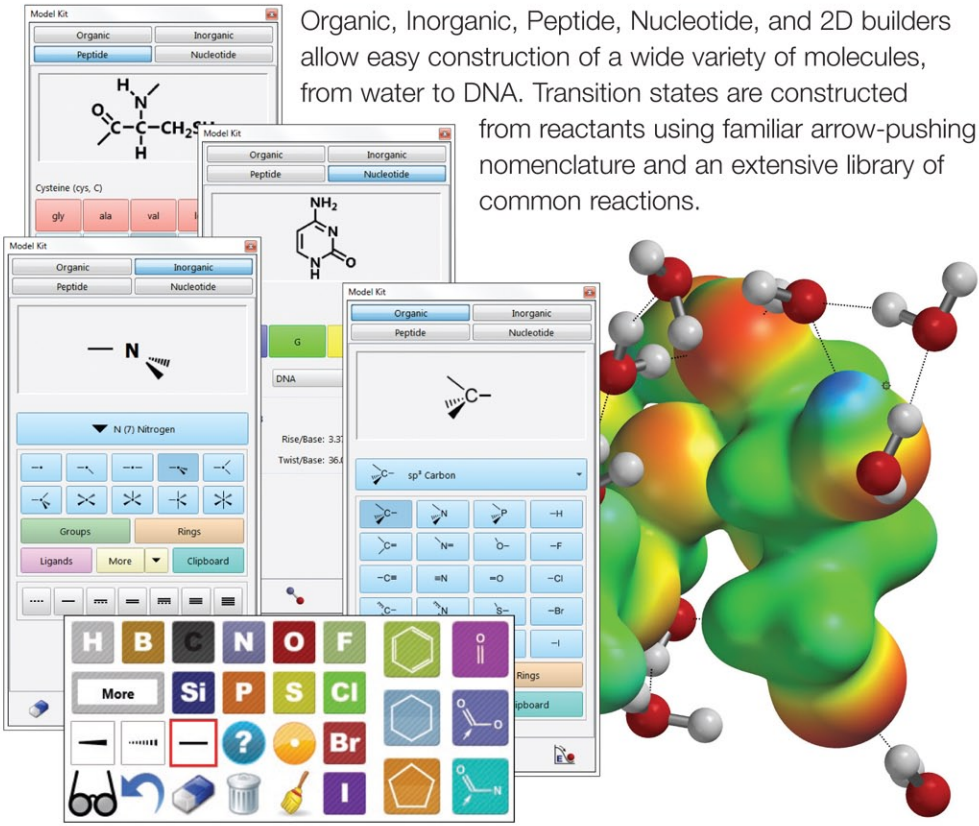
PROPERTIES

- 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

Molecular modeling tools and computational chemistry applied to the undergraduate chemistry curriculum.

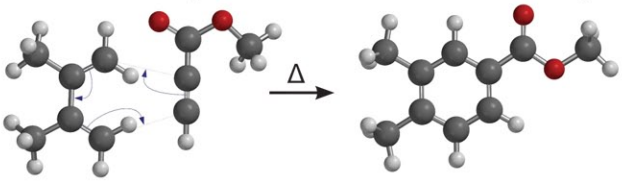


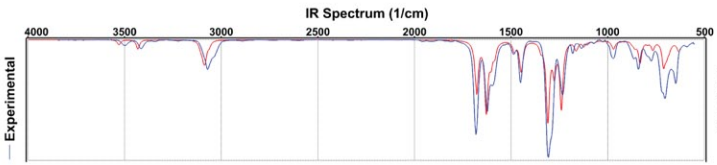
Organic, Inorganic, Peptide, Nucleotide, and 2D builders allow easy construction of a wide variety of molecules, from water to DNA. Transition states are constructed from reactants using familiar arrow-pushing nomenclature and an extensive library of common reactions.

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
- structural and stereo-isomers
- acidity and basicity
- dipole moments
- hydrogen bonding
- IR spectra
- NMR spectra
- UV/vis spectra
- solvation
- aromaticity
- stereochemistry
- conformation
- chemical reactions
- activation energies

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	$ 800	5 Seat Lab License	$ 3,200
Individual Student License*	$ 50	10 Seat Lab License	$ 6,000

Campus-wide Annual Site Licenses Available Starting at $ 2,800**

* Academic institutes and students may purchase at the individual student license pricing, provided that the software is installed on student-owned machines only. 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, 10, or 11
- 2 GB RAM
- 128 GB disk space

MACINTOSH

- Intel or Mx chips (only)
- OS X 10.12.6 (Sierra) - OS 13.X (Ventura)
- 2 GB RAM
- 128 GB disk space

* ***Spartan Student 9*** supports Windows 8.1, 10, or 11 touch screen computers and tablets.

Q-CHEM

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

WAVEFUNCTION

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