



Spartan

'04 Windows

SPARTAN'04 for Windows

F E A T U R E S

Graphical User Interface

- Builders for organic, inorganic and organometallic molecules, polypeptides and polynucleotides
- Automatic generation of transition states from extensive reaction library
- Spreadsheets for data presentation and analysis
- 2D and 3D plots from tabulated data
- Display and query of 3D structure models
- **Display of hydrogen bonds**
- Display of molecular orbitals, electron densities, spin densities, electrostatic potentials and local ionization potentials as isosurfaces, contour plots and property maps
- Import/export of SYBYL MOL and MOL2, PDB, MacroModel and Exchange and Collection files
- Export of Bitmap, AVI, JPEG and PNG files
- **Import/export of SDF, TGF, MOL files (2D)**

Methods

- SYBYL and MMFF94 molecular mechanics
- MNDO, MNDO/d, AM1 and PM3 semi-empirical molecular orbital, including PM3 parameters for transition metals
- Hartree-Fock molecular orbital
- **local, BP, BLYP, EDF1 and B3LYP density functional**
- **MP2, MP3, MP4 and LMP2**
- **CCSD, CCSD(T), OD, OD(T), QCISD, QCISD(T), QCCD, QCCD(T)**
- **G2, G3 and G3 (MP2)**
- **CIS, CIS(D) and TDFT for excited states**
- **STO-3G, 3-21G, 6-31G*, 6-311G*, cc-pVDZ, cc-pVTZ and cc-pVQZ** all-electron basis sets with additional polarization and/or diffuse functions
- **Pseudopotentials for molecules with heavy elements**

Additional Features

- Automatic processing of groups of molecules
- Cartesian optimization subject to constraints and/or fixed atoms
- **Use of NOEs in conformational searching**
- Full and automatic use of symmetry
- **Database of ≈50,000 organic structures at HF/3-21G, HF/6-31G*, EDF1/6-31G*, B3LYP/6-31G* and MP2/6-31G* models**

Tasks

- Determine equilibrium geometries
- Determine transition-state geometries
- Identify lowest-energy conformers
- Establish conformer distributions
- Align molecules
- Scan geometrical coordinates
- Generate reaction sequences
- **Generate and follow intrinsic reaction coordinates**
- Calculate reaction and activation energies
- Identify and generate tautomers
- Calculate and **plot** infrared spectra
- **Calculate and plot NMR spectra**
- **Calculate UV/vis excitation energies**
- **Replace from/search Spartan Molecular Database**
- Search Cambridge Structural Database

Properties

- Mulliken, electrostatic-fit and natural charges
- Dipole **and higher** moments, polarizabilities and hyperpolarizabilities (semi-empirical only)
- Enthalpies, entropies and free energies
- Aqueous solvation energies by SM5.4 model
- **Solvation energies and solvent corrected properties by QM/MM procedure**
- **NMR chemical shifts (Hartree-Fock only)**
- **UV/vis from CIS and TDFT models**

Pricing

- US/Canada/Mexico (NAFTA)
\$3,000 (\$2,000 government, \$1,000 academic)
- International (Pacific Region-call for pricing)
\$4,000 (\$2,500 government, \$1,250 academic)

Essential Edition

- US/Canada/Mexico (NAFTA)
\$2,000 (\$1,250 government, \$600 academic)
- International (Pacific Region-call for pricing)
\$2,500 (\$1,500 government, \$700 academic)

Minimum System Requirements

- Intel Pentium II, AMD Athlon and more recent
- Windows 98 and up
- Microsoft Internet Explorer 4.01

Features in bold are new to Spartan'04.

Features in red are not available in the Essential Edition of Spartan'04 for Windows.