Spartan'10 Licensing*

Spartan'10 for Windows/Macintosh	Commercial	Government	Academic
NAFTA (USA, Canada, Mexico)	$ 3,600	$ 2,400	$ 1,200
International	$ 3,900	$ 2,600	$ 1,200

Spartan'10 for Windows/Macintosh and Linux** Parallel Edition	Commercial	Government	Academic
NAFTA (USA, Canada, & Mexico)	$ 4,500	$ 3,000	$ 1,500
International	$ 4,800	$ 3,200	$ 1,500

* *A lower cost Spartan Student Edition version is available for Academic Labs.*
** *Up to quad core. Contact Wavefunction for cluster licensing.*

Spartan Spectra and Properties Database Licensing

The Spartan Spectra and Properties Database contains infrared and NMR spectra together with diverse molecular and atomic properties and QSAR descriptors for ~50,000 organic molecules (~100,000 by the end of 2011). These derive from EDF2/6-31G* density functional calculations based on the lowest energy conformer from the T1 thermochemical recipe. The wavefunction is stored allowing on-the-fly generation of molecular orbitals and other graphical surfaces and the electrostatic potential and other property maps.

Spartan Spectra and Properties Database	Commercial	Government	Academic
Single User License	$ 2,250	$ 1,500	$ 750
Department/Site License	$ 12,000	$ 8,000	$ 4,000

Minimum System Requirements*

WINDOWS

- Pentium 4 or higher; AMD Athlon
- Windows XP, Vista, or Windows 7
- 2 GB RAM
- 60 GB disk space

MACINTOSH

- Intel-based Macintosh only
- OS X 10.5 or 10.6
- 2 GB RAM
- 60 GB disk space

* *Contact Wavefunction for Linux System Requirements.*

Spartan'10
for Windows, Macintosh and Linux

is a collaboration with

Q-CHEM
WAVEFUNCTION

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Visit **www.computational-chemistry.co.uk**
for a DEMO, pricing and more information.

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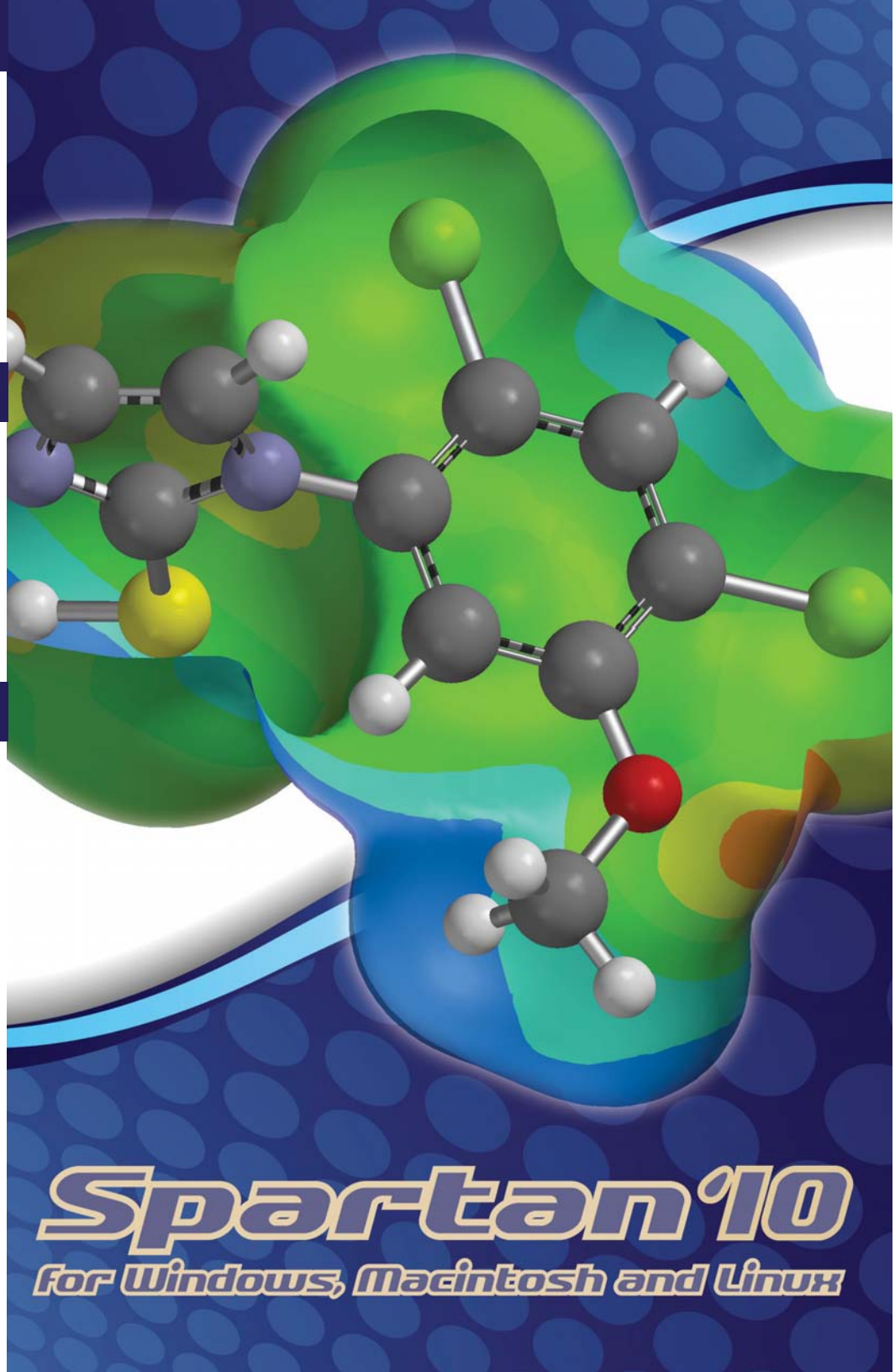

NEW IN SPARTAN'10

Energy orbital diagram display
Refined surfaces dialogue with one-click access to most useful graphical models
Hydride potential surface for exploring nucleophilic selectivity
Surface clipping feature allows visualization inside calculated graphical models
Improved database structure and reaction search options
Improved infrared spectral searching capability
Extended molecular and atomic properties and QSAR descriptors
PM6 semi-empirical method
Extension of T1 thermochemical recipe to silicon and phosphorous
Calculation and display of Raman spectra
NMR spectra display options include DEPT, HSQC, and HMBC
Improved NMR ^{13}C chemical shift accuracy
Data mining, statistical analysis and plotting
Access to Spartan Spectra and Properties Database of IR and NMR spectra, molecular and atomic properties and QSAR descriptors
Tutorials, problems, and Wikipedia accessible from inside Spartan
Parallel implementation of HF and DFT frequencies and of RI-MP2 method
Full 64 bit implementation
Tab-based visualization option for multiple open files; Toolbar customization for icons

TASKS

Calculate strain energy, total energy and heat of formation
Determine gas-phase equilibrium and transition-state geometries
Determine equilibrium and transition-state geometries in the presence of solvent (HF & DFT only)
Identify lowest-energy conformation; Establish conformer distributions and estimate Botlzmann distributions; Build libraries of diverse conformers and use for similarity analysis
Scan geometrical coordinates and generate reaction sequences
Calculate reaction and activation energies
Calculate IR, Raman, UV/vis, and NMR spectra
Match calculated and experimental IR spectra
Estimate NMR spectra for flexible molecules
Mine databases of calculated molecular atomic and reaction properties

PROPERTIES AND QSAR DESCRIPTORS

Mulliken, natural, and electrostatic-fit charges
Dipole and higher moments, polarizabilities and hyperpolarizabilities
Enthalpies, entropies and free energies
Aqueous solvation energies from SM5.4, SM8, and SS(V)PE
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 wavefunction
Min/max of electrostatic potential and min of local ionization potential
Number of conformers and number of tautomers
Empirical NMR HH coupling constants

DATABASES

Spartan Molecular Database®[3]. Structures, energies and properties for ~150k molecules obtained from up to 10 quantum chemical models, searchable by substructure and name; IR spectra of ~30k molecules searchable by spectra; diverse conformers for ~300k molecules obtained from MMFF molecular mechanics for use in similarity analysis.

Spartan Reaction Database®. Transition states for ~1,500 reactions searchable by combination of substructure and "reaction arrows" (included with *Spartan*)

GRAPHICAL INTERFACE

Build organic, inorganic, and organometallic molecules, peptides and nucleotides
Build in 2D with seamless link to ChemDraw®[1], build libraries of substituted molecules
Display and query molecules using a variety of model styles
Display dipole vector, hydrogen bonds, points and planes
Display and customize chemical functional descriptors
Align molecules using structure or chemical function descriptors
Align molecules to pharmacophores
Generate transition states from an extensive reaction library
Generate and display molecular orbitals, electron densities, spin densities electrostatic potentials, local ionization potentials, electrostatic potential maps, hydride potential maps, orbital maps, and local ionization potential maps
Display electron density based on % enclosure
Display solvent accessible regions on surfaces and property maps
Calculate reaction energies with integrated reaction energy calculator
Organize data in spreadsheets, perform regression analysis and make 2D or 3D plots
Embed external files such MS® Word, PowerPoint, Excel and Adobe® PDF files in Spartan files
Plot calculated and experimental[2] IR, Raman, and UV/vis spectra
Plot 1D (proton, carbon, DEPT) and 2D (COSY, HSQC, HMBC) NMR spectra

METHODS

Molecular Mechanics. SYBYL, MMFF94, MMFFaq
Semi-Empirical. MNDO, AM1, RM1, PM3 (including transition metal parameters), PM6
Hartree-Fock molecular orbital theory
Density Functional Theory. Standard functionals: BP, BLYP, B3LYP, EDF1, EDF2, M06, ωB97X-D;
Exchange Functionals. HF, Slater-Dirac, Becke88, Gill96, GG99, B(EDF1), PW91;
Correlation Functionals. VWN, LYP, PW91, P86, PZ81, PBE;
Hybrid Functionals. B3PW91, B3LYP, B3LYP5, EDF1, EDF2, BMK, M05, M05-2X, M06, M06-L, M06-2X, M06-HF, ωB97, ωB97X, and ωB97X-D; Custom functionals may be formulated
Møller Plesset. MP2, MP3, MP4, and RI-MP2
Advanced correlated methods. 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
Thermochemical Recipes. T1, G2, G3, G3(MP2)
Basis Sets include STO-3G, 3-21G, 6-31G*, 6-311G*, cc-pVDZ, cc-pVTZ, cc-pVQZ, cc-pV5Z; with additional polarization/diffuse functions; Dual basis sets; pseudopotentials for heavy atoms; several additional basis sets are available as well as the ability to import custom basis sets

ADDITIONAL FEATURES

Automatic processing of groups of molecules
Full and automatic use of molecular symmetry
Cartesian optimization subject to constraints and/or frozen atoms
Automatic tautomer indicator and generation of list of tautomers
Use NOEs for conformational searching
Import experimental IR, Raman, and NMR spectra in JCAMP format
Import from SMILES, CDX, CIF, SKC, SDF, TGF, XYZ, Macromodel, PDB, SYBYL MOL and MOL2
Export as SMILES, Macromodel, XYZ, PDB, MOL and (MOL2 & SDF) multi-molecule formats
Structure retrieval from the Cambridge Structural Database[4] and Protein Data Bank[5]
Extraction of ligands and binding sites from protein (PDB format) files
Remote submission to external Linux cluster/server resource
Optional multi-core parallel version for Hartree-Fock, DFT, and RI-MP2 calculation

1. ChemDraw® must be licensed from CambridgeSoft®.
2. IR and UV/vis from NIST Chemistry WebBook, NMR from European Bioinformatics Institute. Freely accessible.
3. Subset of 5,000 molecules included with Spartan. Full database included with Spartan maintenance.
4. Cambridge Structural Database® must be licensed from the Cambridge Crystallographic Data Centre®.
5. Protein Data Bank is a freely-acessible on-line resource of biological macromolecules.