



Spartan'08 for Windows/Linux/Macintosh. *Spartan'08* will support Windows (Windows XP, XP64, and VISTA 32bit and 64bit), Macintosh (OS X 10.4 Tiger and 10.5 Leopard), and Linux (RedHat Enterprise 4 and later, SLES 9 or later). *Spartan'08* will access "back-end" computation codes on the local machine and will also (optionally) remotely submit to external Linux systems.

Spartan'08 will be compiled with the latest version Intel compilers. This typically leads to a performance increase on computational codes of $\approx 15\text{-}20\%$ (relative to previous releases), independent of algorithm changes. *Spartan'08* will include Wavefunction, Inc. developed GUI tools and computational algorithms as well as computational algorithms from the latest version of Q-Chem.

1. **Solvation Models.** *Spartan* will include the SM6¹ model from (Cramer-Truhlar) as well as the Continuum Solvation Model SS(V)PE² with improved accuracy for ions

2. **RI-CIS(D).**³ A new RI-CIS(D) code for excited state calculations has been implemented. This provides structures and energies that are nearly identical to those from CIS(D) with an **order of magnitude speed increase** for energy calculations, and a speed increase of a factor of ≈ 3 for structure calculations.

3. **New DFT Functionals.** The non-empirical GGA functional PBE has been implemented. Both M05^{4,5} and M06^{6,7} suites of meta-GGA functionals from the Truhlar group have also been implemented. Additionally, a wider range of functionals will be available as calculation options with the ability to specify model and percentages for exchange and correlation (these include Slater-Dirac⁸, Vokso-Wilk-Nusair⁹, Perdew-Zunger¹⁰, Wigner¹¹, Becke88¹², Gill96¹³, Gilbert-Gill99¹⁴, Lee-Yang-Parr¹⁵, Perdew86¹⁶, GGA91¹⁷, BMK¹⁸, EDF1¹⁹ and EDF2¹⁹)

4. **NMR.** A correction formula has been developed for ¹³C chemical shifts obtained from the B3LYP/6-31G* model. This reduces the mean absolute error with experimental shifts by a factor of two and makes the calculations significantly more reliable (and more useful) in distinguishing spectra of related molecules. An empirical procedure has been implemented to estimate three-bond HH coupling constants and COSY spectra may now be drawn. Both 1D (proton and ¹³C) and 2D COSY spectra may now be averaged over available conformations. NOSY spectra may now be drawn.

5. **Heats of Formation.** The T1²⁰ procedure, delivering highly accurate heats of formation has been improved and now includes support for uncharged, closed-shell molecules comprising H, B, C, N, O, F, P, S, Cl, and Br that can be well represented by conventional Lewis structures ("normal" organic molecules). **T1 is several orders of magnitude faster than G3(MP2)**, and provides results within almost 1 kJ/mol (RMSD) of G3(MP2). This permits accurate thermochemical calculations to be carried out on organic molecules up to molecular weight of ≈ 400 amu. This development has been extended to include a database of T1 (based on best T1 conformer) of $\approx 20,000$ molecules.

6. **Conformer Library Generation.** The capability to provide generation of libraries of diverse conformers has been improved. Based on a systematic search of conformation space using MMFF molecular mechanics, followed by a procedure to eliminate conformers that occupy “similar space”, the best aqueous conformer is now displayed as the structure representing the library. Conformer libraries are intended for use in similarity analysis. Conformer libraries corresponding to common drugs ($\approx 5,000$ entries) and to the Maybridge²¹ compendium, “Compounds for Drug Discovery Chemistry” ($\approx 70,000$ entries) and the Life Chemicals²² “Small Organic Molecules Database” ($\approx 240,000$ compounds) will be available via subscription to the **Spartan Molecular Database (SMD)**.

7. **Spartan Molecular Database²³ (SMD).** The Spartan Molecular Database has grown from to $\approx 200,000$ molecules each available at up to 10 theoretical models: HF/3-21G, HF/6-31G*, HF/6-311++G**, EDF1/6-31G*, B3LYP/6-31G*, B3LYP/6-311G++G**, MP2/6-31G*, MP2/6-311++G**, G3(MP2), and T1 calculations. With the exception of the T1, each data entry corresponds to an optimized structure at the lowest-energy conformer determined from MMFF molecular mechanics and includes the geometry, gas-phase energy, estimated (aqueous) solvation energy, HOMO and LUMO energies, dipole moment and Mulliken, NBO and electrostatic-fit atomic charges, and a 2-D image of the molecule. Calculated infrared spectra are available for all entries, NMR chemical shifts available for $\approx 15,000$ entries and calculated UV/visible spectra for $\approx 1,500$ entries. Approximate van der Waals surfaces and electrostatic potential maps may be instantly generated for all database entries. In addition to substructure searching, The T1 entry is based on a HF/6-31G* geometry and provides only heat of formation. Up to 100 different conformers have been examined for each entry in an attempt to establish the best T1 conformation. SMD may now be searched by name, molecular weight, formula or isomer.

8. **Transition States and the Spartan Reaction Database (SRD).** The library of structures previously forming the basis of **Spartan's** automatic transition state guessing procedure has been extended to include several hundred new organic and organometallic reactions, and has been made available for substructure searching. The transition states in the Spartan Reaction Database (SRD) are each available at one or more of the following models: AM1, PM3, HF/3-21G, HF/6-31G*. Each data entry contains the optimized (transition-state) structure and the vibrational frequencies. Access to SRD is from the reactant (or product) structure together with appropriate “reaction arrows”. **Spartan's** automatic transition-state guessing procedure remains available.

9. **Enhanced Spartan File Structure.** Spartan now includes the ability to embed external files in native Spartan files, experimental data, text descriptions of calculation procedures, journal articles, etc. may now be embedded in a **Spartan** file from external programs (MS[®] Word, PowerPoint, Excel, and Adobe[®] PDF files, for example).

10. **Import/Export.** Spartan now includes the ability to import CIF files, and multi-molecule file types MOL2 and SDF and export multi-molecule files as MOL2 (including atomic charge data) or SDF files.

11. **Reaction Energies Calculator.** Spartan now includes an easy to use tool for calculating reaction energies based either on user data or on information in the Spartan Molecular Database.

12. **Substituent Builder.** Substituents (predefined lists of chemical groups) may now be used as queries in searches of the Spartan Molecular Database and also for calculating reaction energies (see previous item).

13. **ChemDraw²⁴ Thumbnails.** 2D structure drawings provided by ChemDraw may now be put into Spartan's spreadsheet.

14. **Enhanced Spreadsheet/Plotting Capabilities.** Vector quantities may now be stored in Spartan's spreadsheet and plots may be made with vector data.

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