



**Spartan'08 for Windows/Linux/Macintosh.** *Spartan'08* supports 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* accesses "back-end" computation codes on the local machine and will also (optionally) remotely submit to external Linux systems. Beginning with the *Spartan'08* release the interface and functionality for *Spartan* on Windows, Macintosh, and Linux will be identical. A shared memory multi-core parallel version for all Hartree-Fock and DFT models is also available for license.

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

1. **Solvation Models.** *Spartan* includes the Continuum Solvation Model SS(V)PE<sup>1</sup> with improved accuracy for ions as well as the SM8<sup>2</sup> model (Cramer-Truhlar).
2. **RI-CIS(D).**<sup>3</sup> 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** over CIS(D) for energy calculations, and a speed increase of a factor of  $\approx 3$  for structure calculations.
3. **New DFT Functionals.** The non-empirical GGA functional PBE has been implemented. The following functionals<sup>4,5,6,7</sup> from the Truhlar group have been implemented: M05, M05-2X, M06, M06-2X, M06-L, and M06-HF. Additionally, a wider range of functionals are available as calculation options with the ability to specify model and percentages for exchange and correlation (these include Slater-Dirac<sup>8</sup>, Vosko-Wilk-Nusair<sup>9</sup>, Perdew-Zunger<sup>10</sup>, Wigner<sup>11</sup>, Becke88<sup>12</sup>, Gill96<sup>13</sup>, Gilbert-Gill99<sup>14</sup>, Lee-Yang-Parr<sup>15</sup>, Perdew86<sup>16</sup>, GGA91<sup>17</sup>, BMK<sup>18</sup>, EDF1<sup>19</sup> EDF2<sup>19</sup> and  $\omega$ B97X-D<sup>20</sup>).
4. **NMR.** A correction formula has been developed for <sup>13</sup>C chemical shifts obtained from the B3LYP/6-31G\* model. This reduces the mean absolute error with experimental shifts by a factor of two to  $\approx 2$  ppm 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 allowing visually realistic proton NMR and COSY spectra to be drawn. Both 1D (proton and <sup>13</sup>C) and 2D COSY spectra may now be averaged over available conformations. NIOSY spectra may also be drawn.
5. **Heats of Formation.** The T1<sup>21</sup> procedure, delivering highly accurate heats of formation for uncharged, closed-shell molecules comprising H, C, N, O, F, S, Cl, and Br that can be well represented by conventional Lewis structures ("normal" organic molecules) has been improved. **T1 is based on the G3(MP2) recipe for providing heats of formation, but is several orders of magnitude faster than G3(MP2),** and

provides results within 2 kJ/mol (RMSD) of G3(MP2). This permits accurate thermochemical calculations to be routinely carried out on organic molecules up to molecular weight of  $\approx 500$  amu. Against the full NIST Thermochemical Database<sup>22</sup> ( $\approx 2,000$  molecules) T1 yields an (RMSD) error of  $< 9$  kJ/mol. This development has been extended to produce an optional T1 database (based on best T1 conformer) of  $\approx 40,000$  molecules. This not only provides accurate thermochemical data for a diverse collection of organic molecules, but also a large collection of conformational energy differences based on quantum mechanics.

**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 Maybridge<sup>23</sup> compendium, "Compounds for Drug Discovery Chemistry" ( $\approx 70,000$  entries) and the Life Chemicals<sup>24</sup> "Small Organic Molecules Database" ( $\approx 240,000$  compounds) is available via subscription to the **Spartan Molecular Database (SMD)**.

**7. Spartan Molecular Database<sup>25</sup> (SMD).** The Spartan Molecular Database has grown to  $\approx 150,000$  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. With the exception of G3(MP2) and 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  $\approx 40,000$  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. The G3(MP2) entry is based on an MP2/6-31G\* geometry, while 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 and data for the 10 lowest energy conformers is available. In addition to substructure searching, SMD may now be searched by name, molecular weight, formula or isomer.

**8. Input of Experimental IR and NMR Spectra.** The ability to input IR and NMR Spectra (JCAMP format) and search available calculated spectra for the best match against experimental data has been implemented.

**9. 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 and has been extended to cover nearly 2000 reaction types.

10. **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<sup>®</sup> Word, PowerPoint, Excel, and Adobe<sup>®</sup> PDF files, for example).

11. **Discrete Property Maps.** Display of composite calculated surface maps (Electrostatic Potential Map, for example) can now be optionally viewed in discrete bands in addition to the standard continuous color display. This aids in use of property map correlation to acidity, reactivity, and selectivity.

12. **Alternative Density Surface Definition.** A new alternative definition for electron density surfaces based on the % enclosure of total electron density has been implemented.

13. **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 or SDF files (including atomic charge data).

14. **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.

15. **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).

16. **ChemDraw<sup>26</sup> Builder & Thumbnails.** In addition to the use of ChemDraw for building in 2D with automatic conversion to 3D, 2D structure drawings provided by ChemDraw may now be included in Spartan's spreadsheet.

17. **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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For a general discussion and assessment of the techniques and methods and for a review available in Spartan<sup>27, 28</sup> see:

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