Spartan'10 ("***Spartan***") has been designed to address the ever increasing role that calculations play in chemistry and related fields. It represents a continued collaboration between Wavefunction, Inc., and Q-Chem, Inc. Q-Chem codes supplement and extend the traditional strengths of ***Spartan*** as an easy to learn and use tool for molecular mechanics, semi-empirical and Hartree-Fock molecular orbital calculations, as well as a wide variety of graphical models, with a full range of density functional models and a selection of wavefunction based important post-Hartree-Fock models. All models have been implemented using what we believe are the most robust algorithms currently available, and have been tuned for high performance on Intel and AMD processors including multi-core processors.

Spartan is intended to be utilized by chemists, not only computational chemists who are already familiar with the capabilities of molecular mechanics and quantum chemical methods, but also experimental chemists who may have little or no prior experience, but who want to use calculations much in the same way as experimental techniques such as NMR spectroscopy. This ambitious goal is directly reflected in the program's overall design criteria: "convenient access to a full range of modern molecular mechanics and quantum chemical models", and clearly distinguishes ***Spartan*** from other molecular modeling packages.

Spartan is supported under Windows (XP, XP 64, Vista and 7, both 32 and 64-bit), Macintosh (OS 10.5 and 10.6), Linux (Linux Kernel 2.6 or later). The Linux version (only) may be used in a server mode with Windows, Macintosh or Linux acting as a front end, and can also perform calculations locally.

New features in ***Spartan'10*** include the following:

Infrastructure

Tabs. Each open molecule is now given a "tab", any or all of which may either be turned "on" of "off". All tabs "on" mimics ***Spartan's*** previous display paradigm (all open molecules are displayed). Turning tabs "off" simplifies screen clutter.

64-Bit Implementation. The graphical user interface now supports 64 bit chip architectures (64 bit versions of "back-end" codes were released with ***Spartan'08***). This allows ***Spartan*** documents in excess of 2 GB, meaning that very large molecule lists may now be handled. Choice between 32 and 64 bit architectures is automatic and made at the time of installation. (At the time of release, this is available for Windows and Linux only).

File Compression. Files generated from ***Spartan*** (.spartan files) have been significantly reduced in size due to elimination of the part of the wavefunction that is not used, to file compression and (optionally) reduction of precision. This reduction ranges from a factor of five to between one and two orders of magnitude.

Monitor. The ***Spartan*** job monitor has been extended to allow "real-time" visualization of molecular structure. This means that progress of a geometry/transition-state geometry optimization can be followed.

Color Palette. A new color palette has been provided.

Customizable Icons. Spartan's icons may now be individually selected for display.

Graphical User Interface

Simplified Graphics Requests. The most commonly requested graphics (HOMO,

LUMO, electron density, and electrostatic potential, local ionization potential and LUMO maps) may now be requested by the above names instead of as combinations of surfaces and properties.

***Multi-Dimensional Energy Profiles*.** Multi-dimensional energy profiles may now be constructed with arbitrary limits on the number of steps in each dimension. Plots from two-dimensional profiles may be made.

***Ramachandran Plot*[1].** A Ramachandran plot may be made for a protein/nucleotide structure retrieved from PBD.

Formula Editor. A dialog has been provided for construction of quantities (properties or combination of properties) of individual molecules or of molecules related by chemical reaction. These formulas are used in spreadsheet calculations or as queries for database searches ("mining") and subsequent statistical analysis and plotting.

Attachment Points/Reaction Arrows. Specification of attachment points (used in database searches and reaction arrows (used both in database searches and transition-state guessing) have been separated from these functions.

QSAR Descriptors. Descriptors for QSAR type analyses have been collected in one place, and may now be conveniently transferred for data analysis. A series of new descriptors based on the electron density surface and the electrostatic potential and local ionization potential maps have been added.

Computation

RI-CIS(D)*[2] *Gradients. Gradients from RI-CIS(D) models are available allowing efficient calculation of the geometries of excited states.

***Multi-Core Parallel*.** Vibrational frequency calculation has been parallelized for Hartree-Fock and density functional models, resulting in a speed improvement of approximately 1.8 for a two-core machine and 3.2 for a four-core machine. RI-MP2[3,4,5] has been parallelized. The underlying "Hartree-Fock part" (which completely dominates the calculation for less than 500 basis functions) gives speed improvements of approximately 1.9 for a two-core machine and 3.5 for a four-core machine. Speed improvements for the "MP2 part" are not as large. An important practical consequence is that the speed of T1[5] thermochemical calculations now improve significantly on multi-core machines.

PM6*[6].** The PM6 semi-empirical model has been implemented. This offers some improvement over PM3. PM6 becomes the second semi-empirical method available in ***Spartan that may be applied to transition metals.

T1*[7] *Extensions. The T1 thermochemical recipe[5] has been extended to include molecules with silicon and phosphorus. Extension to boron is underway. A procedure for reliably estimating the "best" T1 energy for a flexible molecule has been specified and implemented inside the graphical user interface.

Graphical Models

Orbital Energy Diagram. An orbital energy diagram (spanning up to 20 occupied

valence molecular orbitals and 2 unoccupied molecular orbitals) may now be displayed for the selected molecule. *Clicking* on a line (energy level) in this diagram generates "on-the-fly" and displays the orbital (assuming that the wavefunction is available). These orbitals are not kept when the molecule is closed.

Slicing Planes. Graphical surfaces may now be sliced allowing the "inside" or graphical surfaces (in particular, property maps) to be seen.

***Areas of Banded Property Maps*.** This allows the area of a "color band" on a property map to be determined. It is useful in quantifying the results of graphical models.

Spectroscopy

NMR. The NMR spectra dialog has been completely reorganized allowing (independent or simultaneous) display of six different spectra: 1H, 13C, DEPT, COSY, HMBC and HSQC. Empirically-estimated H-H coupling constants may or may not be included in 1H, COSY, HMBC and HSQC plots, carbon chemical shifts may or may not be empirically corrected in 13C and DEPT plots and all plots may be averaged using Boltzmann weights (if available). At present, experimental 1H, and 13C and DEPT spectra may be displayed on top of calculated spectra.

A second-generation scheme for correcting 13C chemical shifts has been implemented for spectra obtained from the EDF2/6-31G* model (only). The supplements the first-generation scheme (based on topology and applicable only to spectra obtained from the B3LYP/6-31G* model). The new scheme (based on topology and on bond orders to atoms connected to carbon) provides shifts with an (RMS) error of approximately 1.5 ppm (down from approximately 2.5 ppm for the first-generation correction scheme and approximately 4 ppm for uncorrected shifts).

Infrared

Raman. Raman spectra may be calculated from Hartree-Fock and density functional models. Calculated Raman spectra may be fit to experimental spectra the using an overall frequency scale parameter and a width parameter (analogous to what is done for infrared spectra).

Databases

Spartan Molecular Database (SMD). The full (optional) Spartan Molecular Database (provided with maintenance) continues to expand.

Approximately 5,000 transition metal inorganic and organometallic compounds have been added to SMD obtained from calculations using the B3LYP/6-31G* model[8] (or the analogous B3LYP/LACVP* model for second and third-row metals). This model has been shown to provide a good account of equilibrium geometries for organometallic compounds (based primarily on comparisons with X-ray crystal structures). Experimental thermochemical data for organometallic compounds are almost non-existent, and detailed assessment of the B3LYP for reaction energies is not possible. However, the model appears to properly account for observed products in cases where multiple products are possible. All entries correspond to optimized geometries and infrared spectra have been provided for most entries.

Spartan Spectra and Properties Database (SSPD). A new database of IR and NMR spectra and of molecular and atomic properties and QSAR descriptors has been developed and is available as an option to ***Spartan'10***. At first release that

contains ~50,000 molecules and is expected to double in size by the end of 2011. SSPD entries are based on equilibrium geometries from the EDF2/6-31G* density functional model[9] using the best conformation obtained from the T1[7] thermochemical recipe. In addition to spectra, properties and QSAR descriptors, SSPD entries include the vibrational modes (allowing animation of the motions associated with individual frequencies) and the molecular orbitals (allowing on-the-fly generation and display of graphical surfaces) including the molecular orbitals and property maps such as the electrostatic potential map.

Data Mining. Data mining allows access to all information relating to molecular structure, properties and spectra contained in SMD and SSPD (presently >600K entries in total). The primary objective is to allow relationships among different quantities or combinations of quantities to be examined across entire series of molecules. Information retrieved from mining may be presented in the form of histograms or XY plots and may be used as the basis for linear regression. Data mining opens up a wealth of information to exploration.

Data mining is accomplished in a series of steps. Where SMD is the source of data, a ***structural query*** is devised and all entries containing this query are retrieved. For example, were the structural query the molecule phenol with an open valence at the *para* position, all *para*-sustituted phenols available in SMD would be retrieved. Next, one or more ***property queries*** are formulated. These might simply refer to individual quantities such as the dipole moment or the charge on a particular atom. More generally, they may reference a combination of properties, for example, the charge on one atom times the charge on another atom. By associating reaction arrows with a structural query, property queries can be extended to refer to one of the products of a chemical reaction (fully defined give the structural query and the reaction arrows) or to a property of the reaction itself, most conspicuously, the energy of the reaction. Finally, one or more properties queries and brought together with the retrieved data from SMD either for the purpose of both the results of the search and are combined

Spartan Infrared Database (SIRD). The interface to the Spartan Infrared Database has been completely reworked. Matching to an unknown (experimental) spectrum may now be accomplished with or without functional group, formula and substructure filters.

Documentation

Tutorials and Problems. The full set of Spartan tutorials and a selection of problems may be opened inside of ***Spartan***. Tutorials are indexed by chapter (in this manual) and problems according to topic.

Wikipedia Access. A Wikipedia page may be brought up from ***Spartan***.

Changes from ***Spartan'10*** and ***Spartan'08*** include the following:

On-Line PDB Access. PDB access has been moved from the **Search** menu to the **File** menu.

Since the release of ***Spartan'08***, ***Spartan*** users have diligently reported program bugs via ***support@wavefun.com***. All reported bugs have been addressed. Wavefunction would like to thank our customers for their help in making ***Spartan*** a better program. User-feedback is greatly appreciated!

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