Spartan Student Overview

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Chapter 1

*Spartan Student*

This chapter describes the architecture of *Spartan Student*, focusing on the connectivity of computational, graphical and database components to the user interface. Available molecular mechanics and quantum chemical methods are enumerated and their utility and applicability assessed.

*Spartan Student* comprises a series of independent molecular mechanics and quantum chemical calculation modules tightly connected via a graphical user interface that is highly functional, yet simple and uncluttered. It has been designed not only to greatly reduce the drudgery and possibility for human error associated with the preparation of input for calculations, but also to guide the interpretation of output from the calculations. The interface is perhaps best viewed as an interactive and intuitive window into modern molecular mechanics and quantum chemical techniques.

![Diagram of the Spartan Student architecture]

Included in the interface are 3D builders for organic, inorganic and organometallic molecules, polypeptides and polynucleotides, and a procedure for guessing transition states. 2D sketch capability for organic molecules has been introduced with this version of *Spartan*.
**Student.** Additionally, access to ChemDraw\(^1\) is provided without having to exit the interface. A \(\sim 6,000\) molecule subset of the Spartan Spectra and Properties Database (SSPD)\(^2\) contains structures, infrared and NMR spectra as well as a wide variety of molecular properties obtained from the EDF2/6-31G* density functional model. The wavefunction is included, allowing quick access to a variety of graphical surfaces and property maps. On-line access to the Protein Data Bank (PDB)\(^3\), a collection of \(>95,000\) biological macromolecular structures, is provided. Experimental infrared spectra are available from the NIST website\(^4\) and experimental NMR spectra from NMRShiftDB website.\(^5\)

**Spartan Student**'s interface provides the gateway to a range of modern computational methods\(^6\). The simplest of these is the MMFF molecular mechanics model, available to determine equilibrium geometries and equilibrium conformers of molecules comprising upwards of several thousand atoms. It is the only computational technique that is applicable to biopolymers.

Quantum chemical models are required to account for the geometries of transition states as well as for reaction and activation energies.\(^8\) The simplest of these are semi-empirical molecular orbital models. The PM3 model, supported in Spartan Student, has proven successful for determining equilibrium geometries including the geometries of transition-metal compounds, but it is not reliable for the calculation of the reaction or activation energies.

Hartree-Fock molecular orbital models are a mainstay of quantum chemical techniques, in particular, for determining equilibrium and transition-state geometries and reaction energies, and are supported in Spartan Student with the STO-3G, 3-21G, 6-31G* and 6-311+G** basis sets. Hartree-Fock models generally provide suitable descriptions of many types of reactions, but are **not adequate** for thermochemical comparisons where bonds are broken or formed. In addition, they do not provide a proper account of the geometries of molecules incorporating transition metals. Supported in Spartan Student are the B3LYP and EDF2 density functional models and the MP2 Møller-Plesset model. All properly account for the energies of reactions.
that involve bond making and breaking and both density functional models (but not the MP2 model) properly account for the geometries of molecules incorporating transition metals. B3LYP, EDF2 and MP2 models are supported with the 6-31G* and 6-311+G** basis sets.

**Spartan Student** provides access to infrared spectra (MMFF, PM3, Hartree-Fock, B3LYP, EDF2 and MP2 models) and NMR spectra (B3LYP/6-31G* and EDF2/6-31G* models only). These are available both as numerical data (vibrational frequencies, chemical shifts) as well as spectral plots. **Spartan Student** provides internet access to experimental IR and NMR databases, allowing direct comparison with calculated spectra. Infrared spectra from the EDF2/6-31G* model have been corrected using both a multiplicative scale of calculated frequencies and peak width at half height as parameters. Proton, $^{13}$C and $^{19}$F chemical shifts obtained from the EDF2/6-31G* density functional model have been empirically corrected to account for local environment.

**Spartan Student** provides a variety of graphical tools to assist in interpreting the results of calculations. These include molecular orbitals, electron and spin densities, local ionization potentials and electrostatic potentials that can be displayed as surfaces, slices and property maps. **Spartan Student** provides the ability to distinguish accessible and inaccessible regions on a density surface and on property maps based on this surface. Animations can be created and used to depict conformational changes or the progress of chemical reactions. Animations can be saved as QuickTime files.
1. ChemDraw is not included with Spartan Student, but may be obtained from CambridgeSoft (www.cambridgesoft.com). Seamless access to ChemDraw is not available in the Macintosh version although both Windows and Macintosh versions are able to read ChemDraw files.

2. The full Spartan Spectra and Properties Database contains ~250,000 entries from the EDF2/6-31G* density functional model and is available to license. Contact info@wavefun.com for more information.


5. NMRShiftDB web reference: http://nmrshiftdb.ice.mpg.de


7. Chemical shifts only. HH coupling constants and splitting patterns are evaluated empirically.

8. QuickTime is a multimedia framework developed by Apple, Inc.
Chapter 2
Operating Spartan Student

This chapter describes the general operating features of Spartan Student.

Opening and Quitting Spartan Student

To open on Windows, click on the Start button, then click on All Programs, and finally click on Spartan Student (or double click on the Spartan Student icon on your desktop). To open on Macintosh, double click on the Spartan Student icon in the Applications Folder. To exit, select Exit from the File menu (select Quit Spartan Student from the Spartan Student menu on Mac), or click the Close button (⩲) at the top right (⩲ top left on Mac) of the Spartan Student interface.

Menus and Icons

Program functions may be accessed either from the menu bar of from icons in the toolbar which is directly underneath the menu bar. The menu bar may either be accessed as pull-down menus (Classic List), for example, the Setup menu.

![Menu Bar and Icons]

or from a list of icons presented in a palette (Button Pad), for example, the Display menu
Selection is made in the Settings Preferences dialog (Preferences... under the Options menu; Chapter 10).

Icons for all menu functions (as shown alongside text in both Classic List and Button Pad styles) are available on screen above the menus. There are too many icons to be simultaneously displayed and the choice (beyond the default initially supplied with Spartan Student) is made in the Icons Preferences dialog (Preferences... under the Options menu; Chapter 10). Icon size is also user selectable in the Setting Preferences dialog (Preferences... under the Options menu; Chapter 10). The default settings are for 20 medium size icons.
Allows you to build or sketch a new molecule or read in a molecule that you have previously saved, to retrieve the structure, properties and IR and NMR spectra from a molecule in Spartan Student's database from its name, to retrieve a protein structure from the Protein Data Bank, to print what is on screen or save it as an image file, and to make QuickTime movies.

**Edit**

![Edit buttons]

Allows you to transfer information to and from the clipboard, to undo the last operation, to find text strings and molecule fragments, to center molecules on screen, and to clear the active molecule by deleting it.

**Model**

![Model options]

Allows you to control the style of your model, to display hydrogen bonds and to couple or decouple molecules in a multi-molecule document. Allows you to display of a Ramachandran plot for a protein structure brought in from PDB.
Geometry

Allows you to measure and constrain bond lengths, angles and dihedrals, define points and planes, specify atoms to be “frozen” and align molecules.

Build

Allows you to build or sketch and edit molecules, and to estimate a transition state geometry based on a library of reactions.

Setup

Allows you to specify the task to be performed and the theoretical model to be employed for this task, to specify graphical surfaces and property maps and to submit jobs for calculation.
**Display**

Allows you to display text output, molecular and atomic properties, orbital energy diagrams, surfaces and property maps and infrared and NMR spectra, as well as to access experimental IR and NMR over the internet. Allows you to present data in a spreadsheet and make plots from and perform regression analysis on these data, and to compute reaction energies based either on user data or from entries in the database associated with *Spartan Student*.

**Options**

 Allows you to set display standards, specify the location of the database, monitor executing jobs and customize colors, icons and other aspects of the graphical user interface.

**Activities**

Allows you to display tutorials and topics inside of *Spartan Student* and to search Wikipedia.
Help

Provides access to information on *Spartan Student*’s general operation, the *A Guide to Molecular Mechanics and Quantum Chemical Calculations*, and a number of computational FAQ’s.

A complete listing of menu functions is provided in **Appendix B**.

### Additional Icons

A variety of other icons appear in *Spartan Student*, both in individual dialogs and in bars at the bottom of the screen.

- ![Post to Spreadsheet](image1.png)
- ![Search Transition State Library](image2.png)
- ![Lock/Unlock Constraints](image3.png)
- ![Move Up/Down Dialog](image4.png)
- ![Play](image5.png)
- ![Pause](image6.png)
- ![Step](image7.png)
- ![Revert to Fullscreen](image8.png)
- ![Extend to Fullscreen](image9.png)
- ![Play](image10.png)
- ![Look Up in Wikipedia](image11.png)

### Tabs

*Spartan Student* assigns a tab to each open document. When more than a single document is open, these appear in a single row along the bottom of the screen in the order that the documents were created or read. Backward and forward step keys ([◀] and [▶]) at the far right provide access to tabs outside of those displayed. Documents are selected for display by *clicking* on its tab. To the left of each tab is a check box, which if checked indicates that the document will be displayed on screen even if it is not the selected document. By default, tabs are not checked. Selecting **Pin New Documents** from the **Settings Preferences** dialog (**Preferences...** under the **Options** menu; **Chapter 10**) changes the behavior and checks all tabs.
Mouse/Keyboard Operations

The following functions are associated with the (two-button) mouse and keyboard.

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<th>button</th>
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<tbody>
<tr>
<td></td>
<td>left</td>
</tr>
<tr>
<td>–</td>
<td>selection, X/Y rotate, atom/fragment exchange(^a), fragment insertion(^a)</td>
</tr>
<tr>
<td>Shift</td>
<td>range selection, Z rotate</td>
</tr>
<tr>
<td>Ctrl</td>
<td>global X/Y rotate(^c)</td>
</tr>
<tr>
<td>Ctrl + Shift</td>
<td>multiple selection, global Z rotate(^e)</td>
</tr>
<tr>
<td>Ctrl (edit build mode)</td>
<td>fragment X/Y rotate(^c)</td>
</tr>
<tr>
<td>Ctrl + Shift (edit build mode)</td>
<td>fragment Z rotate(^c)</td>
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<td>absolute configuration invert(^e,d)</td>
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<td>Alt (Windows), option (Mac)</td>
<td>group selection(^e), bond rotation(^f)</td>
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<td>X/Y translate</td>
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<tr>
<td></td>
<td>scaling(^b)</td>
</tr>
<tr>
<td></td>
<td>global X/Y translate</td>
</tr>
<tr>
<td></td>
<td>scaling(^b)</td>
</tr>
<tr>
<td></td>
<td>global X/Y translate</td>
</tr>
<tr>
<td></td>
<td>scaling(^b)</td>
</tr>
<tr>
<td></td>
<td>bond stretching</td>
</tr>
<tr>
<td></td>
<td>bond stretching</td>
</tr>
</tbody>
</table>

a) Requires double clicking.
b) Scaling is always applied to all open molecules and all fragments. The scroll wheel may also be used to scale molecules.
c) Global rotations can be either molecule or screen centered. This is controlled by Global Rotate in the Miscellaneous Preferences dialog (Preferences... under Options menu; Chapter 10).
d) For Macintosh, command key replaces Ctrl key for chirality inversion.
e) In View mode only.
f) In Edit Build mode with bond selected (red arrow visible).

These broadly fall into two categories: selection (picking) and manipulation (translation/rotation).

Selection. Clicking (left button) selects objects on screen and/or of menu items. Left and right buttons together are used to define a selection box for copying to the clipboard, as well as for multiple model selection. Together with the Shift key, the left button allows for selection over a range. Together with the Ctrl (Control) key, the
left button allows for multiple selection. Both range and multiple selection apply not only to text items in lists, but to atoms and bonds in molecules as well. Together with the Alt key (option key for Mac), the left button allows for selection of an entire group (detached molecular fragment).

In Edit Build mode (only), double clicking (left button) on an atom exchanges it with the atom or atomic fragment selected in the model kit. Double clicking on an atom while holding down the Ctrl key leads to inversion in chirality of the atom and double clicking on an atom while holding down both the Ctrl and Shift keys inverts the absolute configuration of the molecule. These operations are not available in the 2D skinner (Edit Sketch mode). Once an initial fragment, group or ring has been drawn, double clicking on the background will insert it alongside (but not bonded to) whatever fragments currently exist on screen.

Manipulation. The left button is used for rotation and the right button is used for translation and scaling of objects on screen. With no keys depressed, moving the mouse while holding down the left button gives rise to rotation about the X and Y (screen) axes, while moving the mouse while holding down the right button gives rise to translation in the X and Y (screen) directions. Together with the Shift key, moving the mouse while holding down the left button gives rise to rotation about the Z direction, while moving the mouse while holding down the right button gives rise to scaling. The center (scroll) wheel on the mouse may also be used for scaling.

The Ctrl key in conjunction with the left or right mouse buttons and (optionally) the Shift key, signifies a change in focus away from the default for the purpose of rotations and translations. Outside of Edit Build/Edit Sketch mode, the default is focus on a single molecule (the selected molecule). Use of the Ctrl key changes focus to the entire set of molecules on screen, meaning that rotations and translations are carried out globally. In Edit Build mode (only), the default is focus on the full set of fragments that make up the molecule being constructed, and rotations and translations refer to this set of fragments as a whole. Use of the Ctrl key changes focus to a single
fragment (the selected fragment), and rotations and translations now refer only to this fragment. Does not apply to Edit Sketch mode.

In Edit Build mode (only), moving the mouse while holding down the Alt key (option key for Mac) together with the left mouse button rotates about the selected bond and, with the right mouse button, changes the length of the selected bond. Bond rotation (only) may also be accomplished by moving the mouse up and down inside the marked area at the left of the screen while holding down the left button. Does not apply to Edit Sketch mode.

Additional keys control various Spartan Student functions.

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<td>3 selects red-cyan stereo display. Pressing again returns to non-stereo display.</td>
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<tr>
<td>Page Up, Page Down Home, End</td>
<td>Moves up (Page Up), down (Page Down), to the top (Home) and to the bottom (End) of the set of open molecules. Also, moves up and down pages in the Output dialog.</td>
</tr>
<tr>
<td>Insert (option for Mac)</td>
<td>In Edit Build/Edit Sketch fragment mode only, inserts a new fragment on screen. This is accomplished by selecting the fragment from the model kit, holding down the Insert key and clicking on screen. Insertion may also be accomplished by double clicking on the background following selection of a fragment.</td>
</tr>
<tr>
<td>Delete</td>
<td>Deletes a fragment, free valence, reaction arrow or the contents of a selection box. This is accomplished by holding down the Delete key and clicking on the fragment, etc.</td>
</tr>
<tr>
<td>Enter (return for Mac)</td>
<td>Required following text or data entry into spreadsheet or dialogs.</td>
</tr>
</tbody>
</table>
Touch-Screen Operations

*Tap*ping is equivalent to *clicking* and *double tapping* is equivalent to *double clicking*. Touch commands for range and multiple selection has not as of yet been implemented. One finger motions on screen are equivalent to left button motions (object and bond rotation). Two finger motions are equivalent to right button motions (object translation). Two finger pinching is equivalent to scroll wheel operations (zooming).

Selecting Molecules

While two or more molecules may be simultaneously displayed in *Spartan Student*’s window (see *Tabs* earlier in this chapter), only one molecule may be selected. Only the selected molecule has access to all capabilities. Molecule selection occurs by *clicking* on its structure model or on any of its associated graphical surfaces. The previously selected molecule is deselected.

Where the molecule belongs to a document with more than a single molecule, selection from among the different molecules may be made using either the [ ] and [ ] buttons or the scroll bar at the bottom left of the screen. *Clicking* on [ ] at the bottom left of the screen animates the display of molecules in the document, that is, steps through them sequentially. Animation speed is controlled from the *Settings Preferences* dialog (*Preferences...* under the *Options* menu; *Chapter 10*). *Clicking* on [ ] (that replaces [ ]) stops the animation. If the spreadsheet associated with the document is open (*Spreadsheet* under the *Display* menu; *Chapter 9*), selection can also be made by *clicking* on the molecule label at the left of the spreadsheet.

Two or more molecules from the same document may be displayed at once (although only one may be selected). Molecules are marked for display by *checking* the box immediately to the left of the molecule label in the spreadsheet.
Database

Included with *Spartan Student* is a ~6,000 molecule subset of the Spartan Spectra and Properties Database (SSPD).* This provides infrared and NMR spectra in addition to a variety of molecular properties obtained from the EDF2/6-31G* density functional model. The database may be accessed either by molecule name (see Chapter 3) or by molecule structure (see below).

The existence of the selected molecule in the database is signaled by its name being displayed at the bottom of the screen.

Details are provided by clicking on ▲ to the immediate left of the molecule name (it then changes to ▼). This brings up a dialog that allows a 3D model of the entry in the database to be rotated, translated and scaled using the usual mouse/keyboard commands (you need to position the cursor inside the viewing area). Model style may not be changed.

The selected (on-screen) molecule may be replaced by the selected database entry by clicking on Replace at the bottom of the dialog. (Replacement can be undone by selecting Undo from the Edit menu; Chapter 4). If Update molecule names when replaced is checked, the name of the molecule in the database will replace the

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* The SSPD is a growing collection of >250,000 organic molecules along with associated properties and 1R and NMR spectra data. Contact sales@wavefun.com for licensing options.
name previously associated with the molecule.

In the event that the selected (on-screen) molecule belongs to a multi-molecule document, it is possible to replace all molecules in the document for which database entries for the specified level of calculation are available. In this case, clicking on Replace will give rise to a second dialog. Clicking on All will replace all the molecules in the document, while clicking on Current will replace only the selected molecule.

**Stereo Displays**

*Spartan Student* supports red-cyan stereo. Red/blue glasses must be worn. To enter stereo mode, press the 3 key. Press again to return to non-stereo mode. Does not apply to the 2D sketcher.

**Changing Colors and Setting Preferences**

Colors and Preferences... under the Options menu (Chapter 10) allow for changing default background and graphical object colors, and for setting (and resetting) program defaults, respectively.

**Monitoring and Terminating Jobs**

Monitor under the Options menu (Chapter 10) allows for monitoring of executing jobs as well as for terminating jobs.
Chapter 3

The File Menu

Operations under the **File** menu access to a 2D sketch pad, model kits to build, edit and substitute molecules in 3D and the file system to read and write both native and non-native files, print text and on-screen graphics, save on-screen graphics as image files, access the database of quantum chemical results by name, access the online PDB database of protein and nucleotide structures, documents and create QuickTime movies.

![Image of File Menu Options]

**New Build** (.addButton)

Brings up a model kit and clears the screen. Model kits are discussed in **Chapter 7**.

**New Sketch** (.addButton)

Brings up the 2D sketch pane and clears the screen. The 2D sketch pane is discussed in **Chapter 7**.
Open... (ē)

Opens a file that contains all information associated with a particular molecule (or list of molecules). In addition to native (.spartan) files (documents) including 2D sketch files, supported are files containing 2D drawings, 3D structures and 1D strings. Also supported are file formats for experimental IR and NMR spectra. Non-native files are normally hidden from view, but may be seen by selecting All Files from the Files of type menu at the bottom of the dialog.

Close (ē)

Closes the document containing the selected molecule, as well as any document specific dialogs. If the document has not previously been saved, a name is requested. If a previously-saved document has been altered, verification that the changes are to be saved is requested.

Save (ē)

Save As... (ē)

Save Image As... (ē)

Saves the document containing the selected molecule exactly as it appears on screen. Opening the document will bring it on screen exactly as it was last saved. If the document has not previously been named, Save behaves as Save As.... Documents may be either be saved in native format or in one of the formats listed under Open. In addition, Bitmap (.bmp), JPEG (.jpg) and PNG (.png) graphics file formats are supported. Support is also provided for writing QuickTime (movie) files (see discussion later in this chapter). Selection is made under the Save as type menu in the Save As dialog. Save Image As... allows for saving molecules as JPEG, PNG or BMP files of specified resolution.
Build New Molecule ( )

Brings up a model kit and clears the screen. Build New Molecule differs from New Build, in that the resulting molecule is appended to the end of the document associated with the molecule (or sketch) that is presently selected.

Sketch New Molecule ( )

Brings up the 2D sketch pane and clears the screen. The menu bar is still accessible, but only the View ( ) and Sketch New Molecule ( ) icons are available. Sketch New Molecule differs from New Sketch in that the resulting sketch is appended to the end of the document associated with the molecule (or sketch) that is presently selected.

Delete Molecule ( )

Deletes the selected molecule(s) from a document. Deleting the last molecule leads to an empty document.
Append Molecule(s)... ( )

Appends one or more documents onto the end of the document that contains the selected molecule. **Append Molecule(s)...** leads to a file browser from which one or more documents need to be selected.

Access Database By Name... ( )

Included with **Spartan Student** is a ~6,000 molecule subset of the Spartan Spectra and Properties Database (SSPD). The individual entries correspond to calculations from the EDF2/6-31G* density functional model and each includes the structure, gas and (estimated) aqueous phase energies, infrared and NMR spectra, as well as a variety of molecular and atomic properties. The wave function is available allowing graphical surfaces and property maps to be computed on-the-fly. Selection brings up a dialog.

A name search is initiated by entering a name (or partial name) in the box to the right of **By Name:** at the bottom of the **Access**

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* Alternatively, molecules may be appended onto an existing document either by copy/paste operations using the clipboard or by dragging from an external window. Both require that the spreadsheet associated with the destination document be open on screen. To copy a molecule open on screen onto the clipboard, first select (click on) it, and then select **Copy** from the **Edit** menu. Alternatively, click on its label in its spreadsheet (in the leftmost column), and then select **Copy** from the **Edit** menu. The latter permits several molecules to be selected (and copied) at once using the **Shift** and **Ctrl** keys in the usual manner. Once on the clipboard, the molecule or molecules may be moved to the destination list by clicking on an empty row header in the spreadsheet (for the destination document), and then selecting **Paste** from the **Edit** menu.

To copy a document from an external window, drag it onto the open spreadsheet (associated with the destination document) inside of **Spartan Student**. Several documents can be dragged at once using the **Shift** and **Ctrl** keys in the usual manner.
**Database by Name** dialog. The search will return all entries that include whatever text string is entered into this box. For example, typing in *toluene* will not only result in toluene, but also molecules like para-toluenesulfonic acid and 4-chloro-2-fluorotoluene.

Following the search, one or more hits may be retrieved by selecting them from the hit list and then *clicking* on **Retrieve**. **Shift** and **Ctrl** keys are used in the usual way to select multiple entries from the hit list.

**Access PDB Online...**

Provides access to the online **Protein Data Bank (PDB)*** comprising more than 90,000 protein and nucleotide structures. Selection results in a dialog.

To access a PDB structure, enter the four character identification code in the box to the right of **PDB ID** and *click* on **Open**. If the PDB entry contains more than one structure and/or the PDB ID yields more than one entry, all structures will be returned in a single document.

PDB access will typically require a few seconds. The PDB ID will appear at the right and a ribbon model of the protein or nucleotide will appear on screen. A Ramachandran plot associated with a protein structure may either be drawn upon initial retrieval of the PDB file by *checking* the box to the left of **Draw Ramachandran Plot** or later from **Ramachandran Plot** under the **Model** menu (Chapter 5).

**Print**

Selection leads to a dialog in order to designate a printer, specify print layout and number of copies. It also allows printing to a file.

* The web address is http://www.rcsb.org.
The contents of the spreadsheet (Spreadsheet under the Display menu; Chapter 9) may be printed using Print from the contextual menu. The results of a reaction energy calculation (Reactions... under the Display menu; Chapter 9), may be printed using Print from the contextual menu.

Start/Stop QuickTime Recording ( )

This allows QuickTime movies to be created. To start making a movie, select Start QuickTime Recording. Any motions of all molecules in Spartan Student’s main screen will be captured. Dialogs (including the builders) will not be captured. Note the use of “tumbling” (see Settings Preferences under Preferences in the Options menu; Chapter 10) in making QuickTime movies. To stop making a movie, select Stop QuickTime Recording (which has replaced Start QuickTime Recording in the File menu) and supply the requested file name.

Note that the QuickTime entry in the File menu will only appear if QuickTime is actually installed on your machine.

Exit ( )

Exits Spartan Student, that is, clears the screen and closes all open documents. A prompt for a name is provided for each document that has not previously been saved.
Operations under the Edit menu provide for undoing commands, copying items to and from the clipboard, finding text and graphics, centering molecules on screen and clearing the selected molecule.

**Undo**

Undoes the last operation from the Build and Edit menus. Undoes transition-state formation (see Guess Transition State in Chapter 7).

**Cut**, **Copy**, and **Paste**

Cut moves the selected item to the clipboard and removes it from the document. Copy copies the item to the clipboard. The item is unaffected. Paste transfers the contents of the clipboard to the selected location. The contents of the clipboard are unaffected. Among the important uses of the clipboard are:

(i) Transferring on-screen graphics into other applications such as Microsoft Word® and PowerPoint®.

(ii) Temporary storage of a 3D molecular structure for use in molecule building. Temporary storage of a 2D sketch is accomplished using Copy/Paste under a contextual menu (see Chapter 7).

(iii) Transferring data between Spartan Student spreadsheets and between a Spartan Student spreadsheet and other applications such as Microsoft Excel®.
(iv) Making multi-molecule documents and/or transferring molecules between documents.

**Cut** operations for (i) and (ii) require drawing a selection box. Position the cursor slightly above and slightly to the left of the item to be transferred, hold down both buttons and *drag* the mouse to a location slightly below and slightly to the right of the item to be transferred and release both buttons. **Copy** operations for (i) and (ii) also refer to the contents of a selection box *if one has been drawn*, but to the selected molecule if a box has not been drawn. **Copy** operations from a spreadsheet refer to all information associated with a molecule if selection is made on the header cell of the leftmost column, but only to the selected (text) information if selection is made on any other column. Further discussion relating to use of the clipboard in molecule building is provided in *Chapter 7* and for moving data in and out of the spreadsheet in *Chapter 9*.

**Select All ( )**

Selects all atoms in the selected molecule.

**Find... ( ), Find Next ( )**

**Find** locates a text string defined in the **Find** dialog if an output window or a spreadsheet is selected, or a structure sequence defined on the clipboard if an on-screen model is selected. **Find Next** locates the next occurrence of a text string or a structure sequence.

**Center ( )**

Centers on screen all molecules in the document for which the selected molecule is a member (only the selected molecule is displayed).

**Clear ( )**

Clears (deletes) the structure and other information for the selected molecule, and brings up a model kit. Information is not removed from the file system until the document is saved.
Chapter 5

The Model Menu

Structure models available under the Model menu include wire, ball-and-wire, tube, ball-and-spoke and space-filling (CPK) models, with or without hydrogens, with or without hydrogen bonds indicated, and with or without atom labels, as well as ribbon displays for polypeptides and polynucleotides, with or without labels and with or without hydrogen bonds indicated. It allows drawing a Ramachandran plot for a protein structure retrieved from the Protein Data Bank (PDB). The menu also provides for configuring atom labels to display element name, R/S chirality, mass number, charge or chemical shift, and for specifying color coding and display style for ribbon labels, as well as turning a variety of other labels on and off. Finally, it allows model style to be applied globally (to all molecules in a document) and models to be manipulated in concert.

Only one model style Wire, Ball and Wire, Tube, Ball and Spoke, Space Filling or Hide) may be selected. The selected model is designated by a check mark \( \checkmark \) in front of its entry in the menu or by a blue highlighted button in the case of the button pad option. Global Model, Coupled, Hydrogens, Labels, Ribbons and Hydrogen...
**Bonds** operate as toggle switches. A ✓ in front of the entry in the menu indicates that it is selected.

All structure models, and graphics may be displayed either in orthogonal or perspective projections. The latter may be valuable in helping to visualize large molecules. Selection is done in the **Settings Preferences** dialog (Preferences... under the **Options** menu; Chapter 10). Both structure models and graphics may be presented in 3D stereo. This is also controlled from the **Settings Preferences** dialog as well as from the 3 key. Stereographic displays require perspective projections.

**Wire ( )**

This represents the molecule as a wire model where the vertices represent the atoms.

The bonds are drawn in two colors, one for each of the atoms making up the bond. Default atom colors are given in **Table 5-1**.

Atom colors apply globally (to all atoms of given type), and may be changed using the **Set Colors** dialog (Colors under the **Options** menu; Chapter 10). All models use the same color scheme for atoms, and provide for the same mechanism of changing colors globally or individually.

**Ball and Wire( )**

This represents atoms by small balls and bonds by wires.
### Table 5-1: Default Atom Colors

<table>
<thead>
<tr>
<th>main group</th>
<th>main group (con’t)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>white</td>
</tr>
<tr>
<td>Lithium</td>
<td>orange</td>
</tr>
<tr>
<td>Beryllium</td>
<td>green</td>
</tr>
<tr>
<td>Boron</td>
<td>orange</td>
</tr>
<tr>
<td>Carbon</td>
<td>gray</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>blue-gray</td>
</tr>
<tr>
<td>Oxygen</td>
<td>red</td>
</tr>
<tr>
<td>Fluorine</td>
<td>pale yellow</td>
</tr>
<tr>
<td>Sodium</td>
<td>yellow</td>
</tr>
<tr>
<td>Magnesium</td>
<td>purple</td>
</tr>
<tr>
<td>Aluminum</td>
<td>magenta</td>
</tr>
<tr>
<td>Silicon</td>
<td>gray</td>
</tr>
<tr>
<td>Phosphorus</td>
<td>orange</td>
</tr>
<tr>
<td>Sulfur</td>
<td>yellow</td>
</tr>
<tr>
<td>Chlorine</td>
<td>green</td>
</tr>
<tr>
<td>Potassium</td>
<td>red</td>
</tr>
<tr>
<td>Calcium</td>
<td>red</td>
</tr>
<tr>
<td>Gallium</td>
<td>orange</td>
</tr>
<tr>
<td>Germanium</td>
<td>gray</td>
</tr>
<tr>
<td>Arsenic</td>
<td>dark orange</td>
</tr>
<tr>
<td>Selenium</td>
<td>red orange</td>
</tr>
<tr>
<td>Bromine</td>
<td>dark red</td>
</tr>
<tr>
<td>Rubidium</td>
<td>red</td>
</tr>
<tr>
<td>Strontium</td>
<td>red</td>
</tr>
<tr>
<td>Indium</td>
<td>orange</td>
</tr>
<tr>
<td>Tin</td>
<td>gray</td>
</tr>
<tr>
<td>Antimony</td>
<td>orange</td>
</tr>
<tr>
<td>Tellurium</td>
<td>orange</td>
</tr>
<tr>
<td>Iodine</td>
<td>violet</td>
</tr>
<tr>
<td>Scandium-Zinc</td>
<td>green</td>
</tr>
<tr>
<td>Yttrium-Cadmium</td>
<td>green</td>
</tr>
<tr>
<td>Lanthanum-Mercury</td>
<td>green</td>
</tr>
<tr>
<td>Cerium-Lutetium</td>
<td>violet</td>
</tr>
<tr>
<td>Thorium-Lawrencium</td>
<td>dark blue</td>
</tr>
<tr>
<td>Helium</td>
<td>dark orange</td>
</tr>
<tr>
<td>Neon</td>
<td>dark orange</td>
</tr>
<tr>
<td>Argon</td>
<td>dark orange</td>
</tr>
<tr>
<td>Krypton</td>
<td>dark orange</td>
</tr>
<tr>
<td>Xenon</td>
<td>orange</td>
</tr>
</tbody>
</table>
The balls are color coded according to atom type, and the wires representing bonds are drawn in two colors (as in wire models).

**Tube**

This is similar to the wire model, except that tubes instead of wires are used to represent bonds.

Tubes may either be solid cylinders or be split to represent multiple bonds depending on whether **Split Tubes** in the **Settings Preferences** dialog (**Preferences...** under the **Options** menu; **Chapter 10**) is turned off or on. As with wire models, bonds are drawn in two colors.

**Ball and Spoke**

This represents atoms by balls (the color of which depends on atom type), and bonds by spokes.

Spokes may either be cylinders or be split to represent multiple bonds depending on whether **Split Tubes** in the **Settings Preferences** dialog
(Preferences... under the Options menu; Chapter 10) is turned off or on. Bond (spoke) color is gray by default but it may be changed using the Set Colors dialog (Colors under the Options menu; Chapter 10).

**Space Filling ( )**

This represents the molecule as a composite of spheres, the radii of which have been chosen to approximate van der Waals contact distances.* Also known as CPK models, space-filling models are intended to portray overall molecular size and shape.

![Space-Filling Model](image)

Volume, surface area and polar surface area (PSA)** are displayed in the Molecule Properties dialog (Properties under the Display menu; Chapter 9) and correspond to a space-filling model.

**Hide ( )**

This removes the structure model from the screen. This may be desirable where its display may lead to unnecessary crowding, for example, in proteins where ribbon displays are more appropriate. A structure model may be restored by selecting it from the Model menu.

**Global Model ( )**

If checked (turned on), this signifies that all molecules in a document will share attributes. These include presentation of hydrogens, atom and other labels, hydrogen bonds and ribbon displays. Global model style is controlled from the Molecule Preferences dialog

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* Default values for van der Waals radii may be changed from the VDW Radii dialog accessible from Preferences under the Options menu (Chapter 10). Settings apply to all atoms of given atomic number.

** Polar surface area is defined as the area due to nitrogen and oxygen and any hydrogens attached to nitrogen and oxygen.
Global Model acts in a toggle manner, switching between global and local display. **Global Model** is normally on.

**Coupled** (🔧)

If **checked** (turned on), this signifies that all molecules in a document selected for simultaneous display will be moved together. **Coupled** is turned on following molecule alignment (see **Align** under the **Geometry** menu; Chapter 6). **Coupled** acts in a toggle manner, that is, repeated selection couples and decouples the molecules.

**Hydrogens** (💧)

If **checked**, this signifies that hydrogens are to be included in the model. **Hydrogens** acts in a toggle manner, that is, repeated selection turns the display of hydrogens on and off.

**Labels** (🔍)

If **checked**, this signifies that labels associated with atoms, ribbons and bonds as well as with other attributes specified in **Configure**... (see discussion later in this chapter) are to be displayed in the model. **Labels** acts in a toggle manner, that is, repeated selection turns display of labels on and off. **Labels** is automatically turned on following selection of **Apply** or **OK** in the **Configure** dialog.

**Ribbons** (🎨)

If **checked**, this signifies that ribbons are to be displayed along with the selected model. (If only ribbons are desired, for example, in proteins, select **Hide** for the model.) **Ribbons** acts in a toggle manner, that is, repeated selection turns display of ribbons on and off.

**Ramachandran Plot** (🔍)

If **checked**, this draws a Ramachandran plot for a protein input from the Protein Data Bank (see **Access PDB Online** under the **File** menu; Chapter 3). **Ramachandran Plot** acts in a toggle manner, that is, repeated selection turns the plot on and off. Note that coloring of
the points on the plot (red for α-helices, blue for β-sheets, green otherwise) is not based on the actual 3D geometry but rather on assignments in the PDB file.

**Hydrogen Bonds**

If checked, this signifies that hydrogen bonds are to be drawn as part of the model. **Hydrogen Bonds** acts in a toggle manner, that is, repeated selection turns display of hydrogen bonds on and off.

**Configure...**

This selects the types of labels attached to atoms and ribbons.

**Configure Labels**

![Configure Labels](image)

Atom labels may be selected from among the following: **Labels**, a unique element/number combination that may be changed from the **Atom Properties** dialog (accessible from **Properties** under the **Display** menu; Chapter 9), **Element**, **Mass Number**, **R/S** (chirality), **Electrostatic Charge**, **Strand: Res\Label** (polypeptides and polynucleotides), and **Exposed Area** (of an atom in a space-filling model) and **Chem Shift**. In addition, **Bond Labels**, **Point Labels**, **Plane Labels**, **Constraint Labels**, **Residue Labels** and/or **Reaction Labels** may be provided. Default settings
(for a new molecule) are made in the Molecule Preferences dialog (Preferences under the Options menu; Chapter 10).

Configure Objects

Clicking on the Objects tab leads to the Configure Objects dialog.

![Configure Objects dialog](image)

If checked, Constraint and Frozen markers, Points and Planes and Reaction arrows attach to the model. If not checked, these are shown only in the respective modes, for example, Frozen markers are shown only if Freeze Center is selected.
Configure Ribbons

*Clicking* on the **Ribbons** tab leads to the **Configure Ribbons** dialog.

![Configure Ribbons dialog]

Ribbon coloring may be selected from among the following: **Monochrome**, **By Secondary Structure**, **By Strand** or **By Residue**. Ribbon style may be selected from among the following: **Ribbons**, **Beads** or **Lines**.

The **Configure** dialog is removed from the screen with all selections maintained by *clicking* on **OK**. *Clicking* on **Cancel** or on **x** removes the dialog but selections are lost. *Clicking* on **Apply** maintains the selections but leaves the **Configure** dialog on screen. Note, that **Labels** (from the **Model** menu) will be turned on following either *clicking* on **OK** or on **Apply**.
Chapter 6

The Geometry Menu

Functions available under the Geometry menu allow querying, changing and constraining bond lengths, angles and dihedral angles, defining points, ligand points and planes, freezing atomic centers and aligning molecules in a document.

Measure Distance (؟)
Measure Angle (؟)
Measure Dihedral (؟)

Measure Distance displays the distance (in Ångstroms) between two atoms, whether or not they are bonded. Selection results in a message at the bottom left of the screen.

Clicking on two atoms displays the distance at the bottom right of the screen.

Alternatively, clicking on a bond displays its length.

Measure Distance may also be used to alter the distance between atoms (as long as both are not incorporated into the same ring), by altering the contents of the box to the right of Distance \( (A,B) = \) or Length \( (A)= \), and then pressing the Enter key (return key on Mac).
The distance (length) may be entered into the spreadsheet by \textit{clicking} on \( \square \) to the right of its display (see \textbf{Spreadsheet} under the \textbf{Display} menu; \textbf{Chapter 9}). Alternatively, the label “\textbf{Distance (A,B)=}” or “\textbf{Length (A)=}” may be \textit{dragged} into the spreadsheet.

Angle and dihedral angle queries are handled in a similar manner. Angles require that three atoms or two bonds be identified in the proper order while dihedral angles require that four atoms or three bonds be identified in the proper order.

\textbf{Constrain Distance (\( \square \))}
\textbf{Constrain Angle (\( \square \))}
\textbf{Constrain Dihedral (\( \square \))}

These introduce one or more geometrical constraints during structure minimization (in build mode), and during equilibrium or transition-state geometry optimization or conformational searching using methods specified in the \textbf{Calculations} dialog (\textbf{Calculations...} from the \textbf{Setup} menu; \textbf{Chapter 8}). They also allow for setting a range of constraints needed for generation of energy profiles. Constraints may be useful in a number of situations, among them:

(i) constructing conformational energy profiles where one or more dihedral angles need to be fixed while other geometrical variables are optimized,

(ii) optimizing molecular structures where the values of certain key parameters are known, for example, optimizing the geometry of a molecule with an intramolecular hydrogen bond or a disulfide linkage, and

(iii) building molecules with unusual geometries, for example, molecules with very long bonds, as might be required in the construction of transition states and intermolecular complexes.

Selecting \textbf{Constrain Distance} results in a message at the bottom left of the screen.

\begin{quote}
Select two atoms, a bond,...
\end{quote}

\textit{Clicking} on two atoms, or a bond results in a message at the bottom right of the screen.
Clicking on \(\vdash\) changes it to \(\checkmark\) and shows the current distance.

This (constraint) distance can now be changed by altering the contents of the box and then pressing the Enter key (return key on Mac). Alternatively, the existing distance may be used as the constraint distance. If the selected distance had previously been constrained, the icon \(\vdash\) would have been initially displayed. In this case, clicking on \(\checkmark\) turns the constraint off and returns the icon to \(\vdash\). Finally, the value of the constraint (that may be different from the value of the current distance*) may be entered into the spreadsheet by clicking on \(P\) to its right. Alternatively, the label **Constraint \((A,B)\)** may be dragged into the spreadsheet.

This sequence of operations (bond identification followed by turning the constraint on and off) may be repeated as many times as necessary. Any bonds or non-bonded distances on which constraints are to be imposed are indicated by magenta colored markers. Any constraints introduced are automatically enforced.

Angle and dihedral angle constraints are handled in a similar manner. Note that **points and planes may not be used to define constraints**.

Locking in a constraint leads to two additional text boxes at the bottom right of the screen. This allows a sequence of constraints to be defined (from some initial value to some final value in a given number of steps) for the purpose of constructing an energy profile along a predefined set of coordinates (see **Calculations...** under the Setup menu; **Chapter 8**).

The leftmost box sets the initial value of the constraint, the middle box to the right of **to** sets the final value, and the rightmost box to the right of **Steps**: sets the number of steps. For example, were the

* Note, however, that you should not start a constrained geometry optimization from a structure that is very different from that satisfying one or more constraints.
initial value set to 0°, the final value to 180° and the number of steps to 10, then a series of ten constraints (0°, 20°, 40°, ... 180°) would be specified. This can also be accomplished using the Constraint Properties dialog, (see Properties under the Display menu; Chapter 9) and the value of the constraint posted to the spreadsheet.

Whether or not constraint markers are included as part of the model (outside of constrain distance, constrain angle or constrain dihedral mode) is controlled from the Molecule Preferences dialog (Preferences... under the Options menu; Chapter 10).

**Freeze Center ( 

This forces atoms to be held in place during minimization (in the 3D builder) or during equilibrium or transition-state geometry optimization, conformational searching, or energy profile generation using methods specified in the Calculations dialog (Calculations... from the Setup menu; Chapter 8). Any frozen centers specified are automatically enforced.

Atom freezing may be useful in a number of situations, among them guessing a transition-state geometry for a reaction that is closely related to one for which a transition state is available. For example, a good guess at the transition state for pyrolysis of cyclohexyl formate will be obtained by modifying the transition state for pyrolysis of ethyl formate, freezing all but the modified sections (designated in bold in the figure below) and then minimizing.

![Diagram showing the freezing process](image.png)

Selection of **Freeze Center** leads to a message at the bottom left of the screen.
Clicking on an atom or free valence*, freezes it; clicking again thaws it. Buttons at the bottom right of the screen allow for freezing all atoms (Freeze All), freezing all heavy (non-hydrogen) atoms (Freeze Heavy) and for thawing all atoms (Thaw All).

Frozen atoms are indicated by magenta colored markers ( ). Whether or not these are included with the model (outside of freeze center mode) is controlled from the Molecule Preferences dialog under Preferences... in the Options menu (Chapter 10).

**Define Point ( )**

This defines a point as the geometric (unweighted) center of selected atoms (or points) previously defined. Selection results in display of a message at the bottom left of the screen.

Clicking on atoms (or points) in any order, and clicking a second time on any one of the atoms (or points) defines a point (depicted as a small sphere). As many points as desired can be defined and these are treated in the same way as an atom in defining distances, angles, etc. Points move with the molecule as its geometry is altered.

Selecting Define Point (or clicking on ) while holding down on the Shift key, followed by clicking on the appropriate atoms, leads to a ligand point. This is a point of attachment directed perpendicular to the geometric center of the plane defined by three atoms (or best plane in the case of four or more atoms). A ligand point shares all the characteristics of a normal point, but may also be used to bond to atomic fragments, functional groups, etc. See Make Bond under the Build menu (Chapter 7) for a discussion. Ligand points move with the molecule as geometry is altered.

Delete from the Build menu ( ) or the Delete key may be used to remove a point or ligand point.

Whether or not points and ligand points are shown as part of the model

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* The bond distance in this case is that appropriate for hydrogen being added to the free valence.
is controlled from the Molecule Preferences dialog (Preferences... under the Options menu; Chapter 10).

**Define Plane ( )**

This defines and displays a reference plane. Selection results in display of a message at the bottom left of the screen.

*Clicking* on three atoms or points defines a plane. As many planes as desired may be defined, and these may be used in defining distances, angles, etc. Planes move with the molecule as its geometry changes.

Whether or not planes are included as part of the model for an is controlled from the Molecule Preferences dialog (Preferences... under the Options menu; Chapter 10).

**Align ( )**

This aligns the selected molecule to all other molecules in the same document. Selection of Structure from the Align by menu results in a message at the bottom left of the screen.

*Clicking* on an atom designates it as an alignment center, and marks it with a red circle. *Clicking* on the circle removes the designation (and the circle). Following selection of alignment centers, *clicking* on the Align by button at the bottom right of the screen aligns the molecules. If no atoms are selected prior to *clicking* on Align by, then alignment is based on all (non-hydrogen) atoms.

Following alignment, two or more molecules may be displayed at once using spreadsheet functions (see Spreadsheet under the Display menu; Chapter 9). Their motions (coordinates) will be coupled following alignment, but may be uncoupled allowing the
aligned molecules to move independently (see Coupled under the Model menu; Chapter 5). Note that alignment center selections are kept and molecules can be realigned by again selecting Align from the Geometry menu (or clicking on ⏯) followed by clicking on the Align by button.

The alignment score from 0 to 1 (where 1 designates perfect alignment), is available in the spreadsheet. This is accessed by clicking on the Add button at the bottom of the spreadsheet, and selecting Alignment Score from the list of available properties (see Spreadsheet under the Display menu; Chapter 9). A score of 0 is assigned to molecules that cannot be aligned to the selected molecule.
Chapter 7

The Build Menu

The Build menu provides a sketch palette for drawing organic molecules in 2D, model kits and associated tools for building and editing organic, inorganic and organometallic molecules as well as polypeptides and polynucleotides in 3D, 2D to 3D conversion and 3D structure refinement using molecular mechanics.

Spartan Student provides a variety of tools for specification of 3D molecular structure, a necessary first step to any molecular mechanics or quantum chemical calculation. Organic molecules can either be rendered as 2D sketches and later brought into 3D*, or directly constructed from 3D fragments. Inorganic and organometallic molecules as well as polypeptides and polynucleotides need to be built in 3D.

2D Sketch Palette

The 2D sketch palette contains tools for making and manipulating drawings. There are also tools for specifying charges and radical sites and for adding cues to designate stereochemistry.


* The Windows version of Spartan Student allows seamless access to ChemDraw installed and licensed on the same computer. 2D drawings are automatically brought into 3D. Both Windows and Mac versions of Spartan Student are able to read ChemDraw files. Information is provided in Appendix E.
**Element/Functional Group Library.** A “wildcard” icon which appears below the H and B icons allows any atom to be specified by its element symbol, for example, **Na** or **Al**, as well as a variety of standard groups, for example, **Ph**, **OCH3**, **OMe**, **NO2**, or **TMS**. About 60 functional group symbols are presently recognized, a list of which may be found under the **Help** menu. The meaning of this icon can be changed by **double-clicking** the icon and entering a new symbol. Case is not important, for example, **sn**, **sN**, **Sn** and **SN** are all interpreted as **Sn**.

**Common Rings.** Three icons facilitate the rapid addition of benzene (**C**), cyclohexane (**O**) and cyclopentane (**P**) rings to drawings.

**Common Carbonyl Groups.** Three icons facilitate the rapid addition of carbonyl (**i**), carboxylic acid/ester (**e**) and amide (**a**) groups to drawings.

**Stereochemical Markers.** Wedges and dashes, represented by **-** and **-**, can be used to designate in-out stereochemistry. Once a stereochemical marker has been added to a drawing, it is possible to designate the orientation of hydrogen atoms and/or substituents bonded to six-member rings as **ax(ial)** or **eq(uatorial)** (**ax** and **eq** labels appear only on the drawing, not in the palette).

**Charge/Radical Markers.** Conventional bonding rules (neutral C makes 4 bonds, neutral N makes 3 bonds, and so on) are enforced when 2D perspective drawings are converted into 3D models. This is accomplished by adding hydrogen atoms to the drawing. For example, a single carbon on screen will give methane, a single line, ethane, and a double line, ethylene. (Hydrogen atoms are added to nitrogen, oxygen, phosphorous and sulfur in the 2D drawings.) When another outcome is desired, for example, for an ion or free radical, charge or radical markers must be added to the drawing.

Two icons, **+** and **-**, are used to label atoms that bear formal charges. **+** is used to label atoms that are neutral, open-shell radicals. Each of these markers affects the number of electrons and the number of hydrogen atoms added to the 3D model. For
example, O will produce a 3D model of water, H$_2$O. However, adding the appropriate marker will result in 3D models of H$_3$O$^+$ ( ), HO$^-$ ( ), or HO radical ( ), respectively. Only one charge/radical marker can be assigned to an atom.

Only one charge/radical marker is displayed on the palette, but clicking on the icon will cause each marker to appear in turn.

**Drawing Tools.** left arrow undoes the most recent drawing operation. right arrow removes or modifies parts of a drawing. can delete an entire drawing (a warning is provided). left arrow tries to improve the readability of a drawing by applying various “clean up” procedures.

**Making a Sketch**

To start a sketch, first select (click on) an atom, group, ring or wildcard icon in the sketch palette and then double click in the white portion of the screen (the drawing area). To draw a bond, first click on an atom, group, ring or wildcard icon in the sketch palette to designate what is at the end of the bond, then position the cursor over the atom in the drawing area where you want the bond to start, move the cursor while holding down the left button (drag the cursor) to the place in the drawing area where you want the bond to end and release the button. Multiple bonds are made by dragging over existing bonds.

To make a bond touch the screen where you want it to start, move one finger to where you want it to end and lift. Replace position by touch, drag by move and release by lift in the diagram above.
Manipulating a Sketch

To translate the sketch, move the mouse over the screen while holding down the right button. To rotate the sketch (in the plane of the screen), move the mouse up and down while holding down both the left button and Shift key. Use the scroll wheel to resize the sketch.

Sketch Operations

Add an Atom, Ring, or Carbonyl Group. To add an atom, click on that atom’s icon. Position the cursor over the atom in the drawing that will connect to the new atom, drag it away and release the button. To add a common ring or carbonyl group, click on that ring’s (group’s) icon, position the cursor over the atom in the drawing that will connect to the new ring (group) and drag it away and release the button. The carboxylic acid/ester and amide icons contain an arrow that shows which atom in these groups will be connected to the existing drawing. To change the location of this connection point (arrow), click on the group’s icon until the arrow reaches the desired location.

Add Multiple Bonds. To add a multiple bond, first draw a single bond at the location where the multiple bond is needed, then redraw this line once to make a double bond, and redraw it again to make a triple bond (in other words, position the cursor over one end of the bond, drag to the other end, and release the button).

Fuse 5 and 6-Member Rings. Click on an icon for the first ring and double click on the screen. Next, click on the icon for the second ring and double tap the bond that the rings will share. This will create a drawing with a fused bicyclic ring system. Note that the (cis or trans) stereochemistry of the ring juncture is ill-defined.

This technique can also be used to add 5 and 6-member rings to an existing bond in any drawing. Click on the icon for the ring to
be added and *double click* on the bond that will become part of the ring.

**Replace an Atom with Another.** If a drawing contains atom A where atom B is needed, *click* on the icon for B, then *double click* on A in the drawing. This allows the drawing of heterocycles. First, draw an all-carbon ring and then replace specific carbons with heteroatoms.

**Access an Element or Functional Group from the Library.** *Click* on the icon underneath H and B (this icon will initially be labeled with the name of the group that was previously selected and will change each time you select a new element or group). A dialog results.

![Substituent dialog](image.png)

To define an element, type the one or two-letter standard chemical symbol for the element and *click* return. To define a group, type the atoms in the group (for example, OCH3 or NO2) or a standard abbreviation for the group (for example, OMe, Ph, or TMS) and *click* on OK. Case is not important, for example, sn, sN, Sn and SN are all interpreted as Sn. A listing of available groups is provided under the Help menu.

The element/group can be added to a drawing, replaced, or removed using the same drawing techniques used for standard atoms. The element/group can also be redefined. *Double click* on the icon and type the symbol for the new group.

**Add a Stereochemical Marker (Dash or Wedge).** 3D information can be added to a drawing by replacing single bonds with stereochemical markers: dashes or wedge. The single bond must be drawn before a marker can be added.

To replace a single bond with a marker, *click* either or , then *re-draw* the single bond. To reverse the orientation of the marker,
**re-draw** the bond or marker in the opposite direction. One type of marker can be replaced directly by the other. **Click** on the desired marker and then **re-draw** the existing marker. Markers can also be converted back into single bonds. **Click** on \[\text{ },\] then **double click** on the marker.

For best results during 2D-to-3D conversion, all substituent bonds to the ring should be drawn with stereochemical markers.

**Add an Axial or Equatorial Marker** (6-member rings only). The orientation of a hydrogen/substituent on a 6-member ring can be specified by marking **one** ring substituent as either \text{ax(ial)} or \text{eq(uatorial)}. If the molecule contains multiple rings, the conformation of each ring can be specified by marking **one** substituent per ring. Axial or equatorial markers can only be added to stereochemical markers (dashes, wedge) so the bond connecting the substituent to the ring must be drawn with a stereochemical marker first.

To add an \text{axial} or \text{equatorial} marker to a stereochemical marker, **click** on either \[\text{ },\] or \[\text{ },\] then **double click** on the stereochemical marker. ax will appear on top of the stereochemical marker. To replace ax with eq, **double click** on the stereochemical marker again. To remove the marker, **double click** on the marker again.

Although it is possible to produce a drawing in which several bonds are marked as \text{axial} or \text{equatorial}, **only one** marker is used when converting a 2D ring drawing into a 3D model.

**Assign Charges and Radical Sites.** Formal charges and unpaired electrons can be assigned to individual atoms using charge/unpaired electron markers. To assign a **positive** formal charge to an atom, **click** on \[\text{ },\] and **double click** on the atom in the drawing. To assign a **negative** formal charge or **unpaired electron**, **click** on the charge/unpaired electron marker until the desired icon appears (tapping the marker rotates it through three possibilities: \[\text{ },\], \[\text{ },\], and \[\text{ },\]) and double tap the atom in the drawing.

To replace a charge/unpaired electron marker on an atom with a different marker, **click** on the desired charge/unpaired electron icon.
and double click the marked atom. To remove a marker, click on and double click on the marker.

Charge/unpaired electron markers play an important role during the conversion of 2D drawings into 3D models in that they determine the number of hydrogens that need to be added to the model (it is usually unnecessary to draw hydrogens unless they are needed to mark stereochemistry).

Hydrogens are not shown in 2D perspective drawings unless they have been drawn explicitly (exceptions: hydrogens attached to neutral N, O, P, and S are shown). When a drawing is converted into a 3D model, hydrogens are added to the model according to conventional bonding rules. A neutral carbon atom is assumed to form four bonds, nitrogen three bonds, oxygen two bonds, and so on. Analogous logic is used for atoms that carry a formal charge or unpaired electron marker.

Charge and unpaired electron markers are carried over into specification of quantum chemical calculations (Calculations... from the Setup menu; Chapter 8). The total charge is set equal to the sum of the formal charges in the 2D drawing. A model with one unpaired electron is treated as a free radical (drawings that contain more than one unpaired electron may give unanticipated results).

**Undo the Last Action.** Click on to return to the drawing as it existed before the last action. Only a single level of undo is presently supported.

**Clean Up a Drawing.** Click on to clean up a drawing, that is, to equalize bond lengths, bond angles, and so on. Clean up can improve the appearance of a 2D drawing, but not every clean up will produce a desirable result. To undo an unsatisfactory clean up operation, click on.

**Remove an Atom or Bond.** Click on and then double click on the atom or bond. If you click an atom, all bonds to that atom will also be removed. Removing a bond, either by clicking on an atom or by clicking on the bond itself, will also remove terminal atoms,
that is, atoms not connected to any other atoms in the drawing will be removed along with the bond.

**Remove a Multiple Bond.** To remove a multiple bond, *click* on \( \text{bond} \) then *double click* on the multiple bond. This reduces the bond order by one. Repeated *double clicks* on a triple bond will reduce the bond order: triple \( \rightarrow \) double \( \rightarrow \) single \( \rightarrow \) no bond.

**Remove a Stereochemical Marker.** *Click* on \( \text{marker} \), then *double click* the marker. This replaces the marker with a single bond.

**Change or Remove an Axial or Equatorial Label from a Stereochemical Marker.** Tap either \( \text{axial} \) or \( \text{equatorial} \), then *double click* on the stereochemical marker where an axial or equatorial label appears. This cycles the label (in order) among ax (axial), eq (equatorial) and nothing. The stereochemical marker itself will not be affected.

**Remove a Charge or Radical Marker.** *Click* on \( \text{marker} \) and *double click* on the marker.

**Clear the Screen.** *Click* on \( \text{clear} \). A warning message will ask you to confirm this operation.

A 3D structure is obtained from the 2D sketch by *clicking* on \( \text{3D model} \).

**3D Model Kits**

*Spartan Student* provides four different model kits for assembling a variety of molecular systems: an organic model kit for most organic molecules, an inorganic model kit for organic molecules not well represented in terms of an uncharged (non-zwitterionic) valence structure, as well as inorganic and organometallic molecules, and model kits for polypeptides and polynucleotides. The organic and inorganic model kits utilize atomic fragments, functional groups and rings (and ligands in the inorganic model kit), while the peptide model kit uses the set of natural amino acids as building blocks, and the nucleotide model kit the set of nucleotide bases.

3D molecule construction in *Spartan Student* proceeds much in the same manner as a chemist would assemble a structure from a model...
kit, that is, pieces are taken from the kit one at a time and added sequentially to the molecule under construction.

**Organic Model Kit**

The organic model kit contains a suite of molecule building/editing tools specifically designed to construct organic molecules.

![Organic Model Kit](image)

In the center of the model kit are a selection of atomic fragments, which from left to right and then top to bottom, correspond to:

- C(sp$^3$)
- N(sp$^3$)
- P(sp$^3$)
- H
- C(sp$^2$)
- N(sp$^2$)
- O(sp$^3$)
- F
- C(sp)
- N(sp)
- O(sp$^2$)
- Cl
- C(aromatic)
- N(aromatic)
- S(sp$^3$)
- Br
- Si(sp$^3$)
- N(planar)
- S(sp$^2$)
- I

A fragment is chosen by *clicking* on its icon, which is then displayed at the top of the model kit. Once selected, the fragment may be used to initiate building, to add alongside of an existing structure or appended onto an existing structure. To initiate building, *click* anywhere on screen. To add alongside of an existing structure, *click* on the appropriate icon and then position the fragment so that it is aligned with the existing structure.
structure, hold down the **Insert** key (**option** key on Mac), and then **click** anywhere on screen or **double click** in a blank area on screen. To bond to an existing structure, **click** on a free valence (**not an atom**). (Free valences are colored yellow on the selected molecule.) Bond type in the case of atomic fragments with multiple bond types, for example, sp² carbon, depends on the nature of the free valence selected.

While only H, C, N, O, F, Si, P, S, Cl, Br and I are available from the organic model kit, other elements may be substituted using atom replacement feature available in the inorganic model kit (see **General Molecule Building Functionality** later in this chapter). Similarly, bond types may be altered in the inorganic model kit. Atom and bond types may also be altered using the **Atom** and **Bond Properties** dialogs, respectively (accessible from **Properties** under the **Display** menu; Chapter 9).

Menus inside the model kit provide access to a number of pre-built fragments corresponding to functional groups (**Groups**) and rings (**Rings**), and to additional libraries of rings (as well as any user-defined structures) stored in **Spartan**’s file system (**More**). The model kit also accesses the clipboard (**Clipboard**).

**Groups**

Clicking on **Groups** brings up a menu of groups, and displays an icon of one group in a box at the top of the model kit.

Once selected from the menu, a group may be used to initiate building, to add alongside of an existing structure on screen, or to add to an existing structure.

The amide and carboxylic acid/ester groups have more than one different free valence. The free valence that is to be used is marked with a gold • (in the icon at the top of the model kit).
The marked position circulates among the possible positions with repeated clicking on the icon.

Rings

Clicking on Rings brings up a menu of hydrocarbon rings, and displays an icon of one ring in a box at the top of the model kit.

Once selected from the menu, a ring may be used to initiate building, to add alongside of an existing structure on screen, or to add to an existing structure.

Cyclohexane, cycloheptane, napthalene, anthracene, phenanthrene, indene and fluorene have more than one different free valence. The one that is to be used is marked with a gold • (in the icon). The marked position circulates among the available positions with repeated clicking on the icon. Selection of an axial or equatorial free valence in cyclohexane and cycloheptane is indicated by the label ax or eq appearing alongside the icon. All rings in this menu are hydrocarbons, but heteroatoms may be substituted (see General Molecule Building Functionality later in this chapter).

More

This provides access to a broader selection of rings as well as to access user-defined entities (rings, groups, ligands, etc.). Upon initial entry, the menu to the right of More will be empty. It can be populated, by clicking on to the far right. This brings up a file browser that has been set to point toward a directory containing documents of common rings.

nitrogen heterocycles saturated nitrogen rings
oxygen heterocycles saturated oxygen rings
sulfur heterocycles  saturated sulfur rings
mixed heterocycles  saturated mixed rings

*Clicking* on a document followed by *clicking* on **Open** or *double clicking* on a document fills the menu to the right of **More**. Menu entries are selected in the usual way. In response, a ball-and-wire model of the selected ring will appear in a box at the top of the model kit. This may be manipulated (rotated, translated, zoomed) using the usual mouse/keyboard commands (you need to position the cursor inside the box) or with the usual one and two-finger touch commands. The ring may be used to initiate building, to add alongside of an existing structure, or to add to an existing structure. In the latter case, the attachment point (on the ring in the window) needs to be identified by *clicking* on the appropriate free valence.

Documents containing ligands, chelates and high-coordination fragments intended for use with the inorganic model kit (discussed in the next section) are also available. In addition, any **Spartan Student** document may also be accessed.

**Clipboard**

*Clicking* on **Clipboard** accesses the clipboard. A ball-and-wire model of whatever is on the clipboard is displayed in a box at the top of the model kit. This may be manipulated using the usual mouse/keyboard commands (you need to position the cursor inside the box or with the usual one and two-finger touch commands). Once selected, the contents of the clipboard may be used to initiate building, to add alongside of an existing structure, or to add to an existing structure. In the latter case, the attachment point needs to be identified by *clicking* on the appropriate free valence.

An empty clipboard will be signaled by:
Inorganic Model Kit

*Spartan Student*’s inorganic model kit allows construction of a much wider class of molecules (including inorganic and organometallic species) than possible with the organic model kit. Structures that violate conventional bonding rules may be constructed, as this model kit purposefully provides no checking. The inorganic model kit is reached by selecting Inorganic from among the tabs at the top of the model kit.*

Atoms may be selected by clicking on the atom button near the center of the model kit. This brings up a full *Periodic Table*. Main-group elements are colored red, transition metals are colored green and lanthanides and actinides are colored blue. The Model menu inside the *Periodic Table* contains a selection of theoretical models (basis sets except for semi-empirical models).

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* Tabs may require too much vertical space on computers or tablets with very small screens. Alternative **Builder Selection Methods** are available in the **Miscellaneous Preferences** dialog (**Preferences** from the **Options** menu; **Chapter 10**).
Selecting an entry from this menu leads to recoloring of the Periodic Table. A light green color is used to indicate elements for which the selected model may be used.* Immediately below is a selection of atomic hybrids.

Selection of atom type is effected by clicking on the appropriate element in the Periodic Table. The entry will be highlighted. Selection of an atomic hybrid follows by clicking on the appropriate icon which will then be highlighted.** This combination (atom type + atomic hybrid) may be used to initiate building, to add alongside of an existing structure or to append onto an existing molecular fragment. To initiate building, click anywhere on screen. To add alongside of an existing structure, hold down the Insert key (option key on Mac) and click anywhere on screen, or double click in a blank area on screen. To bond to an existing fragment, click on the appropriate free valence.

Two of the hybrids (trigonal bipyramidal and square-based pyramidal) may bond either axially or equatorially. Selection of the appropriate bonding point, marked by a •, is effected by repeatedly clicking on the icon; the bonding point alternates between the two sites.

Atoms are connected with whatever bond type (partial single, single, aromatic, double, triple or quadruple) is selected from a menu near the bottom of the model kit. A bond type may be changed by first selecting a type and then double clicking on the bond. Bond types have no impact on quantum chemical calculations, but do affect molecular mechanics calculations which reference a Lewis structure (including minimization in the builder; see discussion

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* Note that while molecular mechanics models are available for all elements, they have been carefully parameterized for only a relatively few of these.

** Hybrids for a number of high-coordination centers are available as a library reachable from More (see discussion under Organic Model Kit).
later in this chapter).

No valence checking is performed in the inorganic model kit, and the user is free to construct any arrangement of atoms.

Menus under **Groups**, **Rings** and **More** are the same as those described for the organic model kit as is **Clipboard**. One additional fragment collection is provided:

**Ligands**

This provides access to a number of pre-built ligands, useful in the construction of inorganic and organometallic molecules. Its operation is analogous to that for the **Groups** and **Rings** menus. **Clicking** on **Ligands** brings up a menu of available ligands, and results in an icon of one ligand from this menu being displayed in a box at the top of the model kit.

A ligand may be used to initiate building or to add alongside or to an existing structure. Additional ligands are accessible from **More** (see previous discussion). Ligands may also be built with the aid of ligand points (**Define Point** in the **Geometry** menu; **Chapter 6**).
Peptide Model Kit

The peptide model kit available in Spartan Student is not intended to be used for constructing proteins (although this is actually possible). Rather, it is primarily intended to build idealized helix and sheet structures. Protein structures are best entered from the Protein Data Bank (see Access PDB Online... under the File menu; Chapter 3). A model kit for construction of polypeptides is reached by selecting Peptide from among the tabs at the top of the model kit.

At the middle of the peptide model kit are icons designating the amino acids (specified by their usual three-letter codes). An amino acid is selected by clicking on its three-letter code, following which either an icon of the amino acid is displayed in the box at the top of the model kit, or the three-letter code for the amino acid is appended to the sequence of codes in the box. Amino acids replace atoms, functional groups, rings and ligands as the building blocks in the peptide model kit. Because these other building blocks are
missing, modifications of peptides, aside from modifications in sequence and in overall conformation, need to be carried out using the organic or inorganic model kits.

There are two different modes of operation: single amino acid mode and polypeptide mode. The former is used to initiate building with a single amino acid, to add a single amino acid alongside of an existing structure or to add a single amino acid to an existing structure, while the latter is used to construct amino acid sequences (polypeptides). Sequence off (unchecked) corresponds to single amino acid mode, and on (checked) corresponds to polypeptide mode.

Peptide construction (Sequence on) is accomplished in three steps:

**Specify Amino Acid Sequence**

This is accomplished by clicking in the desired order on the amino acid codes. Building occurs from the N end to the C end of the peptide. In response to each selection, the three-letter code is appended to the sequence of codes in the box at the top of the model kit. The stereochemical configuration of the amino acid is by default the l configuration; this may be changed to the d configuration prior to selection of the amino acid, by checking d to the right of stereoisomer in the model kit. (It may be changed back to l by checking l). d amino acids are indicated by .d following the code in the box.

The sequence may be altered by changing the text in the box. Existing amino acid codes may be deleted or changed or new codes can be added. The entire sequence may be specified in this way if desired. Specification of a non-existent code will result in an error message. The sequence can be cleared by clicking on Clear.

**Specify Macroscopic Structure**

Once sequencing is complete, macroscopic structure (ψ and φ angles), is specified by clicking on one of α Helix, β Sheet or Other. In the case of the first two, preset angle values are displayed on the right. In the case of specification of Other, boxes appear, into which the desired dihedral angles need to
be entered.

**Terminate**

The peptide is not yet terminated, and the two ends are still set up for addition of further amino acids.

\[ \text{O} \longrightarrow \text{C} \quad \text{N} \longrightarrow \text{H} \]

\[ \text{C end} \quad \text{N end} \]

where the \* indicates a free valence. *Clicking* on **Terminate** at the bottom of the model kit leads to the **Terminate** dialog.

C and N terminating groups may be selected by repeated *clicking* on the C and N icons, respectively. Selection will rotate among the available terminating groups. *Clicking* on **OK** removes the dialog and terminates the polypeptide. *Clicking* on **Cancel** or \( \text{X} \) removes the dialog but does not terminate the polypeptide.

The peptide (or single amino acid) may now be used either to initiate building, by *clicking* anywhere on screen or added alongside of an existing structure, by holding down the **Insert** key (option key on Mac) and *clicking* anywhere on screen, or by *double clicking* in a blank area on screen. If unterminated, it may also be joined onto an existing structure by *clicking* on a free valence. In the latter case, attachment is made from the N end, unless the free valence corresponds to an unterminated peptide fragment, in which case the appropriate end required to make an amide bond is used.
Nucleotide Model Kit

Finally, *Spartan Student* provides a model kit for construction of polynucleotides. It is reached by selecting **Nucleotide** from among the tabs at the top of the model kit.

At the middle of the model kit is a menu designating the type of polynucleotide.

- DNA
- DNA (single strand)
- DNA-RNA
- RNA
- RNA (double strand)
- RNA-DNA

Immediately below this menu are icons, designating the nucleotide bases. Selection of DNA, DNA (single strand) or DNA-RNA from the menu leads to one set of icons.
Selection of RNA, RNA (double strand) or RNA-DNA leads to a second set, the only difference is that uracil (U) has been substituted for thymine (T).

A nucleotide base is selected by clicking on its letter, following which either an icon of the base is displayed in the box at the top of the model kit, or the letter for the base is appended to the sequence of letters in the box. Nucleotide bases replace atomic fragments, functional groups, rings and ligands as the building blocks in the nucleotide model kit. Because these other building blocks are missing, modifications of nucleotides, aside from modifications in sequence and helical structure, need to be carried out using either the organic or inorganic model kits.

There are two different modes of operation: single base mode and polynucleotide mode. The former is used to place a single base or base pair on screen, to add a single base or base pair alongside of an existing structure, or to add a single base or base pair to an existing structure, while the latter is used to construct strands of DNA or RNA (or mixed strands). Sequence off (unchecked) corresponds to single base (base pair) mode and on (checked) corresponds to polynucleotide mode.

Polynucleotide construction (Sequence on) is accomplished in two steps:

**Specify Base Sequence**

This is accomplished by clicking in order on the base codes. In response to each selection, the letter code is appended to the sequence of codes in the box at the top of the model kit. The sequence may be altered by editing the contents of the box. Existing base codes may be deleted or changed or new codes added. The entire sequence can be specified in this way if desired. The sequence may be cleared by clicking on Clear.

**Specify Helical Structure**

Once sequencing is complete, a helical structure may be
specified by clicking on A or B. These correspond to A and B helices, respectively. Selecting Other allows user modification of the rise (in Å) per base (Rise/Base) and twist (in degrees) per base (Twist/Base).

Note that the polynucleotide is not yet terminated, and the two ends are still set up for addition of further bases or base pairs.

* indicates a free valence. Hydrogens occupy all free valences (except the *’ed positions at the two ends of the chain).

The polynucleotide (or single base pair) may now be used to either initiate building, by clicking anywhere on screen, added alongside of an existing structure, by first holding down the Insert key (option key on Mac) and clicking anywhere on screen, or double clicking in a blank area on screen, or joined onto an existing structure by clicking on a free valence. In the latter case, attachment is made from the phosphate end.

**General Molecule Building Functionality**

Additional capabilities are available with Edit Build selected:

**Multiple Fragments**

Multiple fragments may result either from bond breakage (see Break Bond later in this chapter) or from use of the Insert key (option key on Mac), or double clicking in a blank area on screen. A fragment is selected by clicking on it, following which the associated free valences are colored gold (free valences for any non-selected fragments are colored white). All builder functions apply to the selected fragment only. Rotation and translation also apply to the selected fragment, but may be made to apply to the entire set of fragments by holding down the Ctrl key while carrying out these operations.
Fragments may be attached using **Make Bond** (see discussion later in this chapter).

**Rotate/Stretch Bonds**

In addition to molecule rotation, translation and scaling, the mouse is used to rotate about and stretch bonds not incorporated into rings. This is accomplished via the following sequence of operations:

(i) *Clicking* on the bond, which is then marked by a red cylindrical arrow. (The bond connecting the last atom, group, ring or substituent added to the molecule is automatically selected.)

(ii) Simultaneously holding down the **Alt** key (**option** key on Mac) and the left mouse button while *dragging* the mouse up and down, for bond rotation, or the **Alt** (**option**) key and the right mouse button for bond stretching. Bond rotation (only) also follows from moving the cursor up and down inside the shaded area at the right of the screen while holding down the left button.

**Replace Atom/Fragment**

Another function of the mouse is atom replacement. This behaves differently in the organic and inorganic model kits. *Double clicking* on an atom (not a free valence) while an atomic fragment in the organic model is highlighted, replaces the atom by selected fragment. Free valences are adjusted to accommodate the replacement, for example, replacement of sp$^3$ carbon by sp$^3$ oxygen results in two free valences being removed. Atom replacements that violate valence rules or that would disrupt substituents are not permitted. *Double clicking* on an atom (**not a free valence**) while an element in the *Periodic Table* from the inorganic model kit is selected, replaces the atom by the selected element, that is, changes the atomic number. No changes in the number or arrangement of free valences is made, and no checking is done. Atom replacement is not available in the peptide, nucleotide and substituent model kits.
Invert Chirality

In the Add Fragment mode, double clicking on a chiral atom with the Ctrl key (command key on Mac) depressed inverts the chirality of the atom (R→S or S→R). This is not available in fused ring systems. Double clicking on any atom with both Ctrl (command key on Mac) and Shift keys depressed inverts the absolute configuration of the molecule.

Building/Editing Menu Functions

Molecule building/editing functions are found under the Build menu.

Icons for Delete, Make Bond, Break Bond and Minimize are also found at the bottom of the model kit. They may also be included in the set of icons above the menus at the top of the screen.

View (👀)

This exits build mode, and removes the model kit from the screen.

Initial entry into the 3D builder is by way of New Build or Build New Molecule under the File menu (Chapter 3). Edit Build, Delete, Make Bond, Break Bond and Minimize are for modifying existing structures.

Edit Build (👤)

In addition to the capabilities discussed under General Molecule
Building Functionality, this allows access to the libraries of atomic fragments, groups, rings, ligands and substituents, as well as the file system and the clipboard. Clicking on any buttons or menus in the organic, inorganic, peptide, nucleotide or substituent model kits, leads to Edit Build. (If a model kit is not already on screen, selection brings up the last-accessed model kit.) A fragment may be used to initiate building by clicking anywhere on screen, to add alongside an existing structure on screen by holding down the Insert key (option key on Mac) and by clicking anywhere on screen, or by double clicking in a blank area on screen, or be added to an existing structure by clicking on the appropriate free valence. Fragment addition can be terminated by selection of any other function.

Edit Sketch (✍)

This allows a 2D sketch to be modified in the 2D sketcher after it has been converted to a 3D structure. Note, however, that 2D → 3D conversion (as occurs upon exiting the sketcher) is one way. A 2D sketch may be brought back into the sketcher only if it has not been modified from one of the 3D model kits or has not been replaced with an entry from the database. In these cases, Edit Sketch is unavailable (greyed out). Of course, 3D structures originating from 2D sketches can be modified using the 3D model kits.

Delete (🗑)

This allows atom, free valence and substituent library removal from a structure. Selection leads to a message at the bottom left of the screen. Clicking inside a selection box results in deletion of everything inside the box. Selection of Delete does not bring
up a model kit nor does it remove a model kit that is present on screen. **Delete** is a one-time operation. Upon deleting, whatever was previously selected is again selected.

**Delete** is also used to delete points and planes.

Deletion may also be accomplished by holding down on the **Delete** key while *clicking* on the item to be deleted. This mode (only) allows multiple deletions.

**Make Bond (● ●)***

This allows bonds to be drawn between free valences and/or atoms. Selection leads to a message at the bottom left of the screen.

*Clicking* on two free valences (on different atoms) will cause these atoms to be linked by a single bond. Alternatively, *double clicking* on each of two atoms will bond them, and *clicking* on a free valence on one atom and *double clicking* on a different atom will bond the two atoms. Note that available free valences are consumed as a result of bond formation, irrespective of whether free valences or atoms are selected.* If the selected atoms are already bonded, this will result in the bond order being increased by one, that is, single $\rightarrow$ double, double $\rightarrow$ triple. Selection of **Make Bond** does not bring up a model kit nor does it remove a model kit that is already present on screen. **Make Bond** may be terminated by selection of any other function.

**Break Bond (● ●)***

This allows breaking an existing bond resulting in free valences. Selection leads to a message at the bottom left of the screen.

*Free valences can be protected without altering the molecule by adding hydrogens to them (●H from the organic model kit).
Clicking on a bond breaks it and restores free valences. Note that bond breaking may result in detached fragments. Selection of Break Bond does not bring up a model kit nor does it remove a model kit that is present on screen. Break Bond may be terminated by selection of any other function.

Replace click with tap and double click with double tap for delete, make bond and break bond operations.

Minimize (متاز)

This uses MMFF molecular mechanics to refine the geometry. Selection leads to a message at the bottom left of the screen.

The molecular mechanics energy* in kJ/mol, displayed at the bottom right of the screen, is continually updated during the minimization process. Minimization may be stopped at any time by clicking on the icon at the bottom right of the screen. Any geometrical constraints imposed on the structure (see Constrain Distance, Constrain Angle, Constrain Dihedral under the Geometry menu; Chapter 6) are enforced during minimization. Also, any frozen atoms in the structure (see Freeze Center under the Geometry menu; Chapter 6) remain frozen.

Following completion, Minimize reverts back to Edit Build.

Guess Transition State (دبت)

Spartan Student provides a facility for automatically guessing the geometries of transition states based on the similarity of the reaction of interest with one or more entries in Spartan Student’s reaction database. Where an exact match is not available, Spartan Student will attempt to provide as close a match as possible. This will generally involve a less substituted system or one in which substituents differ. Here, the procedure is to use those parts of the

* The mechanics energy is a combination of the strain energy which is either zero or positive and the non-bonded or intramolecular interaction energy which can be either positive or negative. It will most commonly be a positive quantity, although it can be slightly negative.
structure of the transition state in the database that are common, and to optimize the remaining parts (using molecular mechanics).

It may be essential for the reactants to be properly oriented to reflect the desired stereochemical outcome of the reaction.

Where a reaction is completely unknown to the database, a fallback technique similar to the linear synchronous transit method is automatically invoked.

Input to *Spartan Student’s* transition-state guessing procedure will be very familiar to (organic) chemists, in that it is based on reaction arrows. The difference is that arrows are superimposed onto a three-dimensional structure rather than a two-dimensional drawing. The reaction is specified using curved arrows, where each arrow identifies the movement of one electron pair. The direction of electron flow follows customary practice:

![Diagram of reaction arrows](image)

There are two possible sources of an electron pair and three possible destinations, leading to six combinations:

- lone pair → lone pair
- lone pair → bond
- lone pair → space between atoms
- bond → lone pair
- bond → bond
- bond → space between atoms

<table>
<thead>
<tr>
<th>Source</th>
<th>Destination</th>
</tr>
</thead>
<tbody>
<tr>
<td>lone pair</td>
<td>lone pair</td>
</tr>
<tr>
<td>lone pair</td>
<td>bond</td>
</tr>
<tr>
<td>lone pair</td>
<td>space between atoms</td>
</tr>
<tr>
<td>bond</td>
<td>lone pair</td>
</tr>
<tr>
<td>bond</td>
<td>bond</td>
</tr>
<tr>
<td>bond</td>
<td>space between atoms</td>
</tr>
</tbody>
</table>

The first of these is a null operation, and its inclusion has no effect.

Selecting **Guess Transition State** results in a message at the bottom left of the screen.
The tail of the arrow corresponds to the source of the electron pair. If the source is a lone pair, then select (click on) the atom that holds the lone pair. If the source is a bond, then select (click on) the bond. Clicking on an atom or bond highlights (colors gold) the atom or bond and leads to a new message at the bottom left of the screen. Clicking again on the same atom or bond deselects (dehighlights) it and leads back to the first message.

The head of the arrow corresponds to the destination of the electron pair. If the destination is an atom (leading to a lone pair), then select (click on) the atom that will hold the lone pair two times. If the destination is an existing bond (leading to an increase in bond order from single $\rightarrow$ double $\rightarrow$ or double $\rightarrow$ triple), then select (click on) the bond. If no bond presently exists, then select (click on) the two atoms that will become bonded upon reaction. These operations result in a curved arrow being drawn on the reactant structure. This extends from an atom, or the center of a bond to an atom, or the center of a bond, or the center of a dotted line that has been drawn between atoms that are to be bonded. The original message returns to the bottom left of the screen.

The process (tail selection followed by head selection) is repeated as necessary to fully define the reaction. Incorrect reaction arrows may be removed by selecting Delete from the Build menu (🗑️) followed by clicking on the arrow to be deleted. It is necessary to again select Guess Transition State (✔️) in order to continue arrow specification. Alternatively, click on the arrow(s) to be deleted while holding down the Delete key.

After all reaction arrows have been properly designated, click on at the bottom right of the screen to replace the reactant with a guess at the transition state. In the event that the guess is unreasonable, this operation may be undone (select Undo from the Edit menu). This allows you to review your assignment of arrows and make changes as needed.
Examples

Diels-Alder reaction of 1,3-butadiene and ethylene

\[ \text{a, b. double bond to empty space leading to a single bond and to a new single bond} \]
\[ \text{c. double bond to single bond leading to a single bond and a double bond} \]

\[ \text{S}_\text{N}2 \text{ reaction of chloride and methyl iodide} \]

\[ \text{a. atom to empty space leading to a new single bond} \]
\[ \text{b. single bond to an atom leading to the loss of the single bond} \]

Ene reaction of 1-pentene

\[ \text{a. single bond to empty space leading to loss of the single bond and to a new single bond} \]
\[ \text{b. double bond to single bond leading to a single bond and a double bond} \]
\[ \text{c. single bond to single bond leading to loss of the single bond and to a double bond} \]
Ring closure of 1-hexenyl radical to methylcyclopentyl radical

a. atom to empty space leading to a new single bond
b. double bond to an atom leading to a single bond
Chapter 8

The Setup Menu

This chapter describes functions available under the Setup menu. Calculations... is used to specify MMFF molecular mechanics calculations, PM3 semi-empirical molecular orbital calculations, Hartree-Fock molecular orbital calculations, B3LYP and EDF2 density functional calculations and MP2 calculations. Tasks include calculation of energy, equilibrium geometry, equilibrium conformation and transition-state geometry and constructing energy profiles. STO-3G, 3-21G, 6-31G* and 6-311+G** basis sets are provided for Hartree-Fock calculations and 6-31G* and 6-311+G** basis sets for B3LYP, EDF2 and MP2 calculations. Calculations... also requests IR and NMR spectra, and extended printing.

Surfaces is used to designate graphical surfaces, including electron and spin densities, electrostatic potentials, local ionization potentials and molecular orbitals, for later display as surfaces, property maps and contour plots. Inaccessible regions on electron density surfaces and property maps based on these surfaces may be demarked.

Submit is used to initiate calculation.

Calculated by ( )

The MMFF molecular mechanics model, the PM3 semi-empirical molecular orbital model, Hartree-Fock molecular orbital models, B3LYP and EDF2 density functional models and MP2 Møller-Plesset models are available to calculate energy, equilibrium geometry and make energy profiles. All models except MMFF are available for calculating transition state geometry. The MMFF molecular mechanics
model is also available to calculate equilibrium conformation. STO-3G, 3-21G, 6-31G* and 6-311+G** basis sets are available for Hartree-Fock calculations and 6-31G* and 6-311+G** basis sets for B3LYP, EDF2 and MP2 calculations.

The aqueous solvation energy obtained by the SM5.4 model is added to the energy of any molecular mechanics or quantum chemical calculation and provided in the Molecule Properties dialog (Properties under the Display menu; Chapter 9).

Quantum chemical calculations also provide atomic charges, IR and NMR spectra. IR spectra are available for all models but NMR spectra are only available for the B3LYP/6-31G* and EDF2/6-31G* models.

Selection of Calculations... results in the Calculations dialog.

This contains pull-down menus, buttons and check boxes:

**Calculate**

This section is used to specify the task to be accomplished, theoretical model to be employed and spectra to be supplied.

Specification of a task is by way of a pull-down menu:

**Energy** specifies calculation of energy (and in the case of quantum chemical methods, a wave function) at a single geometry.
Spartan Student reports energies from molecular mechanics calculations in kJ/mol, from semi-empirical calculations as heats of formation in kJ/mol, and from Hartree-Fock, B3LYP, EDF2 and MP2 calculations as total energies in atomic units (hartrees).

The molecular mechanics energy comprises two parts: the strain energy and the non-bonded energy. The strain energy is the difference in energy between a molecule and its “strain free” analog. It is nearly always positive and less than a few hundred kJ/mols in magnitude. The non-bonded energy accounts for attraction or repulsion between atomic centers that are not connected due to van der Waals and Coulombic interactions. Because the strain energy of every molecule relates to a different standard, molecular mechanics energies cannot be used to obtain reaction energies (unless there are no changes in bonding between reactants and products).

The heat of formation is to the enthalpy at 298K of a balanced chemical reaction in which a molecule is converted to a set of standard products. For example, the heat of formation of ethylene is given by reaction,

\[ \text{C}_2\text{H}_4 + \rightarrow 2\text{C} \text{ (graphite)} + 2\text{H}_2 \text{ (gas)} \]

where graphite and hydrogen molecule are the carbon and hydrogen standards, respectively. In practice, the actual measurement is typically carried out for a combustion reaction, for example, for ethylene:

\[ \text{C}_2\text{H}_4 + 3\text{O}_2 \rightarrow 2\text{CO}_2 + 2\text{H}_2\text{O} \]

Heats of formation may either be positive or negative quantities and generally span a range of only a few hundred kJ/mol.

Heats of formation are not suitable for presenting energy data from quantum chemical calculations, simply because the standards for several important elements (most notably, carbon) are not well-defined isolated species. In its place is the energy of a reaction that splits a molecule into isolated nuclei and electrons, for example, for ethylene:

\[ \text{C}_2\text{H}_4 \rightarrow 2\text{C}^{++6} + 4\text{H}^+ + 16\text{e}^- \]

Total energies, as the energies of such reactions are termed, are always negative and may be very large (tens of thousands of kJ/mol). They are most commonly given in atomic units (hartrees).

1 atomic unit = 2625 kJ/mol

It is possible to relate total energies to heats of formation by incorporating data on atomic species. Heats of formation reported from T1 calculations
(part of the information provided in *Spartan Student’s* database) relate directly to experimental heats and are given in kJ/mol.

To summarize, the heat of formation differs from the total energy both with regard to the standard reaction and with regard to units. Either provides a suitable basis for thermochemical calculations.

**Equilibrium Geometry** specifies that the nearest energy minimum will be located, **Equilibrium Conformer** specifies that the lowest energy conformer will be located and **Transition State Geometry** specifies that the nearest transition state (energy maximum in one dimension and energy minima in all other dimensions) will be located. **Energy Profile** steps along user-defined coordinates.

Except for **Equilibrium Conformer**, a theoretical model needs to be specified by way of pull-down menus. (**Equilibrium Conformer** is limited to MMFF Molecular Mechanics.) The first provides a choice among different classes of models.

![Molecular Mechanics Menu](image)

Selection of **Molecular Mechanics** leads to a single method, MMFF. Selection of **Semi-Empirical** leads to a single method, PM3. Selection of **Hartree-Fock** leads to a second menu of available basis sets.

![Basis Sets for Hartree-Fock](image)

Selection of either **B3LYP, EDF2** or **MP2** leads to an abbreviated menu of available basis sets.

![Basis Sets for B3LYP, EDF2, MP2](image)

**Transition State Geometry** is not available for **Molecular Mechanics**.
Spectra

If checked, **Infrared Spectra** calculates vibrational frequencies and intensities together with the corresponding vibrational modes. These are available in the output (**Output** under the **Display** menu; **Chapter 9**) along with zero-point energies and thermodynamic properties (enthalpies, entropies, heat capacities and Gibbs energies). Vibrational motions (**normal modes**) may be animated and an IR spectrum displayed from the **IR** dialog accessible from **Spectra** under the **Display** menu (**Chapter 9**). Frequency calculations involving MP2 models are very costly in terms of computation and are not recommended.

Infrared frequencies from B3LYP/6-31G* and EDF2/6-31G* calculations (only) have been uniformly scaled to account for known systematic errors. Calculated frequencies from all other models have not been scaled. However, the lines in the calculated infrared spectrum obtained from all models have been broadened to account for the fact that the calculations correspond to 0K, whereas experimental measurements are carried out at finite temperature.

If checked, **NMR Spectra** specifies that NMR chemical shifts from the B3LYP/6-31G* and EDF2/6-31G* models (only) will be calculated. These are then available in the output (**Output** under the **Display** menu; **Chapter 9**) as well as from the **Atom Properties** dialog (**Display** menu) and as atom labels (**Configure...** under the **Model** menu; **Chapter 5**). $^{13}$C (proton decoupled) and $^1$H spectra may be displayed from the **NMR Spectra** dialog accessible from **Spectra** under the **Display** menu (**Chapter 9**). Proton, $^{13}$C, and $^{19}$F chemical shifts (only) have been empirically corrected for local environment. Line intensities are assumed to be proportional to the number of equivalent carbons or hydrogens. Three-bond $HH$ coupling constants for $^1$H spectra are estimated empirically and these have been used to simulate splitting patterns.

---

* Chemical shifts for other nuclei are available in the **Output** dialog (**Output** under the **Display** menu) and may also be attached as labels (**Configure...** under the **Model** menu; **Chapter 5**).
**Total Charge**

Total charge. The default setting (**Neutral**) may be changed either by clicking on \[\text{\textbullet}\] and selecting Anion, Dianion, -3, etc. from the menu, or by typing a number in the. **Total Charge** is ignored for molecular mechanics calculations.

**Unpaired Electrons**

The number of unpaired electrons. The default setting (0) may be changed either by clicking on \[\text{\textbullet}\], and selecting 1 or 2 from the menu, or by typing in the menu. **Unpaired Electrons** is ignored for molecular mechanics calculations.

**Print**

If checked, writes the quantity to the output window. Text output may be seen by selecting **Output** from the **Display** menu (Chapter 9) and printed by first selecting the output dialog and then selecting **Print Output** from the **File** menu (Chapter 3).

If checked, **Orbitals & Energies** writes the orbitals and energies to the output. An orbital energy diagram may also be displayed (**Orbital Energies** under the **Display** menu; Chapter 9) and HOMO and LUMO energies are also available in the spreadsheet (**Spreadsheet** under the **Display** menu; Chapter 9).

If checked, **Vibrational Modes** writes vibrational frequencies and modes to the output. This requires that the infrared spectrum has been calculated.

If checked, **Charges and Bond Orders** writes atomic charges and bond orders to the output.

**Global Calculations**

If checked, signifies that settings in the **Calculations** dialog are to be applied to all molecules in the document.

The **Calculations** dialog may be exited by clicking on **Submit**, **Cancel** or **OK** at the bottom right of the dialog, or on \[\text{\textbullet}\] at
Chapter 8

Surfaces (Surfaces)

*Spartan Student* allows graphical display of the HOMO and LUMO among other molecular orbitals, the electron density, the spin density for molecules with unpaired electrons, the electrostatic potential and the local ionization potential.

The **electron density** is the number of electrons found at a point in space. It is the quantity measured in an X-ray diffraction experiment that is then used to locate atomic positions, that is, most electrons are closely associated with atoms. While the electron density is non-zero everywhere, it is possible to define surfaces of constant density. The most important of these contains most of a molecule’s electrons and that roughly corresponds to a space-filling model, that is, a van der Waals surface. We will refer to this as the **electron density**. It is interesting because it reveals overall molecular size and shape and demarks the steric barrier seen by encroaching molecules. Another important surface, that we will refer to as the **bond density**, contains fewer electrons in total and demarks atomic connectivity.

The **spin density** is the difference in the number of electrons of $\alpha$ and $\beta$ spin at a point in space. It indicates the location of the unpaired electron in a radical or unpaired electrons in a triplet.

The **electrostatic potential** is the energy of interaction of a positive charge with a molecule. This assumes a fixed electron distribution for the molecule. It represents a balance between repulsive interactions involving the positively-charged nuclei and attractive interactions involving the negatively-charged electrons. Regions where the balance tips toward attraction are said to be electron rich (basic) and subject to attack by electrophiles, while regions where the balance tips toward repulsion are said to be electron poor (acidic) and subject to attack by nucleophiles. Electron-rich regions such as lone pairs are typically located outside the van der Waals surface. As such, they may be easily identified by constructing a surface of negative (attractive) electrostatic potential. While interesting electron-poor areas such as acidic hydrogens also lie outside the van der Waals surface, the electrostatic potential is also
positive (repulsive) throughout the region inside this surface.

The **local ionization potential** indicates the ease or difficulty of electron removal (ionization). Like the negative regions of the electrostatic potential, regions of low local ionization potential are likely to be subject to attack by electrophiles.

Note that neither electrostatic potential nor the local ionization potential are experimental observables, although they relate to quantities that can be given clear chemical interpretation.

Additionally, any one of the quantities listed above (except the electron density) may be mapped onto any surface (except a molecular orbital surface). In practice, the only maps to have received widespread attention are those based on the electron density surface (depicting overall molecular size and shape). Most common are the electrostatic potential map, the local ionization potential map and the LUMO map. Some regions of an electron density surface are inaccessible and are not available for interaction with their environment (or with an incoming reagent). **Spartan Student** allows these regions to be identified.*

The **electrostatic potential map** paints the value of the electrostatic potential onto an electron density surface. By convention, colors toward red depict negative potential, while colors toward blue depict positive potential, and colors in between (orange, yellow, green) depict intermediate values of the potential. Thus, an electrostatic potential map for \( p\text{-}\text{tert}\)-butylphenol will show oxygen to be red, its attached (acidic) hydrogen to be blue, the \( \pi \) faces of benzene to be orange or yellow and the \( \text{tert}\)-butyl group to be green.

* A region on a density surface is designated as inaccessible if a sphere of radius 1.0 Å centered on a line normal to the surface and touching a point in the middle of the region, impinges on any other regions of the density surface. The sphere radius may be changed in the **Settings Preferences** dialog (Preferences under the Options menu; Chapter 10).
The main advantages of this presentation relative to separate electron density and electrostatic potential surfaces are its clarity and its compactness. The main disadvantage is that it provides information only about the contact surface and does not reveal how far electron-rich and electron-poor areas extend beyond the surface.

An alternative to an electrostatic potential map, referred to as an exposed electrostatic potential surface, is a composite of three different surfaces: an electron density surface depicting overall molecular size and shape, a negative electrostatic potential surface identifying electron-rich regions and a positive electrostatic potential surface identifying electron-poor regions. These surfaces need to be generated and then displayed simultaneously. The electron density may either be displayed as an opaque solid or as a transparent solid (in order that the molecular skeleton may be seen inside). The two potential surfaces are best represented as transparent solids, the negative surface colored red and the positive surface colored blue. The exposed electrostatic potential surface for \( p\text{-}\text{tert-} \)butyl phenol is shown on the next page.

Note that the exposed electrostatic potential surface provides the same information as the electrostatic potential map. Red areas in the map correspond to regions when the negative electrostatic potential surface is likely to protrude from the electron density while blue areas correspond to regions where the positive electrostatic potential surface is likely to stick out.

The local ionization potential map paints the value of the local ionization potential onto an electron density surface. By convention, colors toward red indicate low ionization potential, while colors toward blue indicate high ionization potential. Thus, the local ionization potential map for aniline shows that the \textit{ortho} and \textit{para} ring positions have a lower ionization potential than the \textit{meta} positions, consistent with the known directing ability of an amino group in electrophilic aromatic substitution.
The **LUMO map** paints the absolute value of the lowest-unoccupied molecular orbital (the LUMO) onto an electron density surface. By convention, colors near blue indicate high concentration of the LUMO, while colors near red indicate low concentration. Given that the LUMO designates space available for a pair of electrons, a LUMO map indicates where nucleophilic attack would likely occur. For example, a LUMO map for cyclohexenone shows concentration in two regions, one over the carbonyl carbon and the other over the β carbon, consistent with both carbonyl addition and Michael (conjugate) addition.

![LUMO Map Example](image)

The **spin density map** paints the value of the spin density onto an electron density surface. By convention, colors near blue indicate high concentration of spin density, while colors near red indicate low concentration. For example, a spin density map for the radical resulting from loss of hydrogen from 3,5-di-tert-butylhydroxytoluene (BHT) shows that the spin has delocalized from oxygen onto the *ortho* and *para* ring positions.
This radical would be expected to be particularly stable, which explains why BHT acts as an antioxidant (scavenging less favorable localized radicals).

Surfaces (including those underlying maps) connect points of equal value (they are isosurfaces), and may be displayed as an arrangement of dots, a mesh, or an opaque or translucent solid. Examples of graphical output in orthogonal projection are provided in Figure 8-1. Surfaces (and maps) may also be rendered in perspective (see Chapter 5) and in stereo (see Chapter 2).

Calculated quantities may also be displayed as two dimensional contour plots (slices). Unlike surfaces and maps, these can be translated, rotated and zoomed independently of the molecular skeleton. An example of a slice display is provided in Figure 8-1.

Several different surfaces, maps and slices may be simultaneously displayed. In addition, any of the usual structure models may be displayed along with the graphic. The total display can become very complex, and selective use of meshes and/or translucent solids (as opposed to opaque solids) may facilitate visualization.

Selection of Surfaces leads to the Surfaces dialog.
### Figure 8-1: Examples of Graphical Displays Available in *Spartan Student*

<table>
<thead>
<tr>
<th>Frontier orbitals for a symmetry-allowed Diels-Alder reaction, showing interaction of the HOMO of 1,3-butadiene and the LUMO of ethylene.</th>
<th>Space-filling model and electron density surface of cyclohexanone, showing overall molecular size and shape.</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Frontier orbitals" /></td>
<td><img src="image2.png" alt="Space-filling model" /></td>
</tr>
<tr>
<td><strong>Electron density surface (0.08 electrons/au^3) of transition structure for pyrolysis of ethyl formate,</strong> showing bonding in the transition state.</td>
<td><strong>Electrostatic potential surfaces (-40 kJ/mol) of trimethylamine (left) and dimethyl ether (right),</strong> showing the lone pairs on nitrogen and oxygen, respectively.</td>
</tr>
<tr>
<td><img src="image3.png" alt="Electron density surface" /></td>
<td><img src="image4.png" alt="Electrostatic potential surfaces" /></td>
</tr>
<tr>
<td><strong>Electron density slice for acetic acid dimer,</strong> showing hydrogen bonding.</td>
<td><strong>Simultaneous display of the LUMO and the electron density surfaces of cyclohexanone,</strong> showing accessibility for nucleophilic attack.</td>
</tr>
<tr>
<td><img src="image5.png" alt="Electron density slice" /></td>
<td><img src="image6.png" alt="Simultaneous display" /></td>
</tr>
</tbody>
</table>
This contains a box at the top for listing requested surfaces and property maps.

**Common Surfaces and Property Maps**

*Add* at the bottom of the dialog is used to specify a number of commonly-used graphical surfaces and property maps*. Clicking on it leads to a menu.

![Common Surfaces and Property Maps Menu](image)

Selection of all but the last entry in the menu leads to a request for the analogous surface or map. A surface and property map specified from this menu will be calculated at medium resolution and will assume a fixed isovalue unless a different resolution has been selected and/or an adjustable isovalue has been requested.

**More Surfaces**

Additional surfaces and maps or the same surfaces or maps at different resolution and with adjustable isosurfaces may be requested by selecting **More Surfaces...** from the menu (or by clicking on **More Surfaces...** at the bottom of the **Surfaces** dialog). This leads to the **Add Surfaces** dialog that contains three menus and a check box:

* Additional selections are provided if the molecule has unpaired electrons.
Surface

Available surface types appear under the Surface menu.

Density is the total electron density which may be used to reveal bonding as well as overall molecular size and shape, HOMO\text{-}, HOMO, LUMO, LUMO\text{+}, SOMO* are molecular orbitals, potential is the electrostatic potential, ionization is the local ionization potential and spin density* is the spin density.

Selection of HOMO\text{-} and LUMO\text{+} results in display of a box to decrement the HOMO and increment the LUMO. This allows any molecular orbital to be specified..

Slice designates that a plane will cut through the graphic defined by Property.

Property

Properties for maps appear in the Property menu.

* These menu entries appear only for molecules with one or more unpaired electrons.
Available properties are the molecular orbitals (HOMO{-}, HOMO, LUMO, LUMO{+}, SOMO*), the electrostatic potential (potential), the local ionization potential (ionization) and the spin density (spin density)*. none indicates that no property is to be mapped onto the surface). As with Surface above, selection of HOMO{-} and LUMO{+} leads to a decrement (increment) box.

A Spin button will be displayed if Unpaired Electrons (in the Calculations dialog) is set to a value other than 0, and if HOMO{-}, HOMO, LUMO or LUMO{+} has been selected for Surface or for Property. Clicking on Spin toggles it between Alpha and Beta. Alpha designates that the molecular orbital either to be displayed as a surface or mapped as a property corresponds to $\alpha$ spin; Beta designates that the molecular orbital corresponds to $\beta$ spin.

Resolution

Selection of surface resolution is from the Resolution menu.

High resolution is necessary for surfaces based on percentage enclosure. Both calculation time and disk storage increase significantly in moving from medium to high resolution.

Isovalue

Checking the box to the left of Fixed specifies calculation of a surface with fixed isovalue. In the case of a density surface, the default value of 0.002 electrons/bohr$^3$ corresponds roughly to enclosure of 99% of the total number of electrons and closely resembles a space-filling model. Fixed surfaces take less time to
compute and require less storage.

Following **Surface, Property, Resolution, Isovalue** and (optionally) spin selection, *clicking* on **OK** adds the requested graphic to the list and removes the (**Add Surfaces**) dialog. **Clicking** on **Apply** adds the requested graphic to the list but leaves the dialog on screen. **Clicking** on **Cancel** does not add a graphic to the list but removes the (**Add Surfaces**) dialog.

The process (*clicking* on **Add...**, followed by selection from the menu or *clicking* on **More Surfaces...** followed by selection of surface, property, resolution and isovalue and *clicking* on **OK** or **Apply**) may be repeated as required.

An existing graphic may be deleted from the list by first highlighting (*clicking* on) it and then *clicking* on **Delete**.

**Global Surfaces**

If *checked*, signifies that the requested surfaces will be calculated for all members of the list.

Only one copy of the **Surfaces** dialog may appear on screen, and any actions relate to the currently selected molecule. The dialog may be removed by *clicking* on **×**.

**Submit (🏃)**

Following setup of a molecular mechanics or quantum chemical calculation, including any requests for spectra and/or graphical displays, the required calculations will begin when **Submit** is selected. If the job has not previously been saved or submitted, selection of **Submit** triggers a request for a name. If the document contains only a single molecule and that molecule exists in the Spartan Spectra and Properties Database, the name in the database will be presented as a default name. Otherwise, the default name presented will be **spartan** for the first job and **spartanx** (x an integer starting with 1 for all successive jobs). After a name has been provided (or if a name already exists or if the default name is accepted) a dialog appears
indicating that the job has actually been submitted.*

* The job is submitted to a job queue and will be submitted for execution only when released from this queue. See Monitor under the Options menu (Chapter 10) for discussion.

Click on OK to remove it. After a job has started, and until it has completed, all associated files will be designated read only.

Another dialog appears following completion of a calculation.

Click on OK to remove it.

Upon completion, an energy profile calculation leads to an additional document being created for each molecule in the original document. These new documents are named document.Prof.identifier where document is the name given to the original document and identifier identifies the molecule inside the original document. A query dialog is provided asking whether the resulting document is to be opened.
Chapter 9

The Display Menu

Functions available under the **Display** menu provide for text, dialog, spreadsheet and graphical displays. Functions are also available to query a variety of on-screen objects, display both calculated and (if available) experimental IR and NMR spectra, animate vibrational motions, prepare plots from spreadsheet data and calculate reaction energies.

![Output Menu](image)

**Output (**)**

Selection of **Output** opens a window.

![Output Window](image)

A menu at the top left of the window selects the type of output.
Summary provides a brief summary of the calculated data, in particular, the energy and any spectral quantities. Output provides normal output. Verbose Output contains more detailed output, but is eliminated upon normal completion unless Keep Verbose is checked in the Setting Preferences dialog (Preferences under the Options menu; Chapter 10). Job Log contains diagnostic information.

The contents of the output window may be scrolled and may be paged up or down by clicking above or below the scroll bar. The contents may be printed or copied by right clicking inside the Output window and selecting Print or Copy from the menu that results. Alternatively, if Confined has been selected for Output/Spreadsheet Windows (from the Preferences menu, Chapter 10), printing is accomplished by selecting Print Output... from the File menu (this replaces Print... when an output window is selected). Similarly, copying is accomplished by selecting Copy from the Edit menu when an output is selected. Find... and Find Next functions from the Edit menu are also available.

Only one output window is associated with each document, and changes focus as different molecules from the document are selected. Output windows for different documents may be simultaneously open on screen. An output window may be closed by clicking on .

Output from jobs that are currently executing or are in the execution queue, is unavailable. Output for jobs that are executing may be viewed using the Monitor under the Options menu (Chapter 10).

Properties ( )

Spartan Student provides specialized dialogs for reporting and (in some cases) changing the properties of molecules, atoms, bonds, graphical surfaces and geometrical constraints. Only one Properties dialog may be opened at a time. Dialog selection operates in a toggle mode. The default Properties dialog is Molecule Properties. Other Properties dialogs may be accessed by clicking on an atom, bond, surface, or constraint. For example, clicking a second time on an atom, bond, or constraint reverts the currently displayed Properties
dialog back to **Molecule Properties**.*

Most **Properties** dialogs have an associated **Utilities** or **Style** dialog. For example, associated with the **Molecule Properties** dialog is a **Molecule Utilities** dialog. These access additional information about the molecule and its components/attributes, or provide style and color controls. This is useful for highlighting (or deemphasizing) a particular molecule, component or attribute. **Utilities/Style** dialogs are reached by *clicking on* ![button](at the bottom right of the appropriate **Properties** dialog. Return to the **Properties** dialog follows from *clicking on* ![button](at the bottom right of the associated **Utilities/Style** dialog.

The **Properties** (or **Utilities/Style**) dialog may be removed from the screen by *clicking on* ![button](.

**Molecule Properties**

The dialog under this tab includes the name, formula, CAS number, molecular weight (in amu), surface area and polar surface area (PSA) of a space-filling model (in Å²), volume of a space-filling model (in Å³) and the point group. It provides the energy (in au) of a Hartree-Fock, B3LYP, EDF2 or MP2 calculation, the heat of formation (in kJ/mol) of a PM3 calculation, or the sum of the strain energy and non-bonded energy (in kJ/mol) of an MMFF calculation, the energy (heat of formation, strain energy)

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* The exception to this involves *clicking* on a property map to obtain the value of the property at a particular surface location. *Clicking* a second time on a new location will report a new value of the property. *Clicking* on the background leads to the **Molecule Properties** dialog.
corrected for an aqueous environment (in the same units as the non-corrected quantity), the solvation energy (in kJ/mol) as the difference between aqueous and gas-phase energies, (if available) the heat of formation from the T1 model (in kJ/mol), (if available and in parenthesis) the experimental heat of formation (in kJ/mol) and the dipole moment (in debyes). With the exception of experimental heat of formation, any or all of these may be posted to the spreadsheet using the buttons to the left of their values. Label (also referred to as identifier) identifies the molecule in a document. It appears in the first column of the spreadsheet (see Spreadsheet later in this chapter) and will be the name of the molecule if it has been retrieved from the Spartan Spectra and Properties Database. Finally, the dialog permits display of the dipole moment vector by checking the box to the right of Display Dipole Vector.

**Atom Properties**

Selection of an atom with a Properties dialog on screen, or selection of Properties following selection of an atom, leads to the Atom Properties dialog.

![Atom Properties dialog](image)

This displays the element name (and allows changing the element), R/S chirality, electrostatic-fit charges (in electrons), calculated

* If the molecule does not appear in the Spartan Spectra and Properties Database, the name will be \textit{M000X} (X=1,2,\ldots) unless altered by the user.
NMR chemical shift (in ppm relative to the appropriate standard; tetramethylsilane for both proton and $^{13}$C) and exposed surface area of a space-filling model (in Å$^2$). It also allows freezing the atom (see Freeze Center in Chapter 6), eliminating the line due to the atom from the displayed proton or $^{13}$C NMR spectrum, changing its mass number and the default label, and posting atomic charges, chemical shifts and exposed areas to the spreadsheet.

**Bond Properties**

Selection of a bond with a Properties dialog on screen, or selection of Properties following selection of a bond leads to the Bond Properties dialog (not shown). This displays the bond length (in Å), Mulliken bond order (in electrons) and bond type (and allows changing the bond type). Note that the results of quantum chemical calculations do not depend on bond types.

**Constraint Properties**

Selection of a constraint marker with a Properties dialog on screen, or selection of Properties following selection of a constraint marker, leads to the Constraint Properties dialog (expanded form shown).

![Constraint Properties dialog](image)

This allows setting the value of a constraint, posting it to the spreadsheet and changing the default constraint label. Checking Dynamic leads to the expanded dialog shown above. This allows
specifying a sequence of constraints for an energy profile (see Calculations... under the Setup menu; Chapter 8). The value of the starting constraint is given in the box to the right of Value, and the value of the ending constraint is given in the box to the right of to. The number of steps in the profile is given in the box to the right of Steps. Initially, the numbers in both boxes to the right of Value will be the same, and Steps will be set to 1. These may be altered by typing the desired numbers into the appropriate boxes and then pressing the Enter key (return key on Mac). This functionality may also be accessed from Constrain Distance (Angle, Dihedral) under the Geometry menu (Chapter 6). If Global Steps is checked, the independent variables are moved in concert, meaning that the number of steps must be the same for each variable (the constraint ranges may be different). If unchecked, the variables are moved independently and the number of steps may differ from one to another. In this case, the total number of steps in the profile is the product of the number of steps for each variable. An energy profile may involve constraints on more than one geometrical variable.

Point and Plane Properties

Selection of a user-defined point or plane with a Properties dialog on screen, or selection of Properties from the Display menu following selection of a point or plane, leads to the Point Properties or Plane Properties dialog (not shown). These allow changing point or plane labels.

Surface Properties

Selection of a graphical display with a Properties dialog on screen, or selection of Properties following selection of a graphical display, leads to the Surface Properties dialog.
This allows changing display style, isovalue (and in the case of electron density surfaces), percentage of the electrons contained inside the surface, turning on mapped properties, selecting between continuous and banded displays and setting the range of the property, displaying accessible area of surfaces and maps and changing the default labels. The dialog also reports (and optionally posts to the spreadsheet) the area and volume of the graphic, the accessible area*, the polar area of an electrostatic potential map**, maximum and minimum value of the mapped property and its value at the cursor position***. If checked, Legend displays a scale. If checked, Global Surfaces designates that the settings apply to all molecules in the document.

If the selected graphical surface is a slice, the Slice Properties dialog replaces the Surface Properties dialog.

---

* A region on a density surface is designated as inaccessible if a sphere of radius 1.0 Å centered on a line normal to the surface and touching a point in the middle of the region, impinges on any other regions of the density surface. The default radius (Accessible Area Radius) may be changed in the Settings Preferences dialog (Preferences under the Options menu; Chapter 10).

** This is defined as that part of the surface area for which the absolute value of the electrostatic potential is > 100 kJ/mol. The cutoff (Polar Area Range) may be changed in the Settings Preferences dialog (Preferences under the Options menu; Chapter 10).

*** To determine property value at another position click on it. To bring up the Molecule Properties dialog, click on the background.
This contains similar controls to that found in the previous dialog. Specification of isovalue has been replaced by specification of the number of contours to be displayed. A sphere or a cylinder may be selected instead of a plane, and check boxes allow for a frame around the slice and for a grid.

**Regression Properties**

Following a linear regression analysis, a new row, labeled \textbf{Fit1*}, appears near the bottom of the spreadsheet. This contains information about the fit. \textit{Clicking} on this line with a \textbf{Properties} dialog on screen, or selecting \textbf{Properties} from the \textbf{Display} menu (\textbullet) after \textit{clicking} on the line, leads to the \textbf{Regression Properties} dialog.

* More precisely, a row will be written for each fit, and labelled \textbf{Fit1, Fit2, . . . .}
This reports RMSD and $R^2$, as well as allows for changing what is to be fit (Fit) and what it is to be fit to (Using). The error statistics will immediately update.

**Orbital Energies**

Selecting **Orbital Energies** leads to the display of an orbital energy diagram (this assumes that a wave function is available). This comprises up to twelve occupied molecular orbitals and two unoccupied molecular orbitals, the highest-occupied (HOMO) and lowest-unoccupied (LUMO) being explicitly designated.

*Clicking* on an energy level in the diagram leads to display of the corresponding molecular orbital. This may be manipulated in the usual way and the display style altered (from the menu at the bottom right of the screen). After one energy level has been selected and the associated orbital displayed, moving the mouse up or down over the diagram while holding down the left button (“swiping”) then releasing the button selects the next higher or lower energy level.

Moving a finger up or down over the diagram then lifting selects the next higher or lower energy level.
Surfaces (糌)

This accesses the same dialog already described in Chapter 8.

Spectra ( fName )

*Spartan Student* displays calculated IR and NMR spectra. Spectra need to have been previously requested from the Calculations dialog (Calculations... under the Setup menu; Chapter 8). In addition, it provides on-line access and display of experimental IR and NMR spectra from public databases, allowing comparison with calculated spectra.

Selecting Spectra from the Display menu leads to an empty display pane at the bottom of the screen.

The only accessible control (in a bar at the top of the pane) is + (add a spectrum). Clicking on this leads to a palette.

The right hand column lists the types of spectra for which calculations are available: IR, proton NMR with and without three-bond HH coupling, and $^{13}$C NMR. The entry is “red” if a calculation has actually been performed and the corresponding spectrum is available. The left hand column lists the types of spectra for which experimental spectra may be available (from on-line public databases): IR, proton NMR,
and $^{13}$C NMR. These are shown in blue.

The procedure for displaying either a calculated or experimental spectrum (or both) is independent of the type of spectrum. For the purpose of illustration, we use the IR spectrum of methyl trans-cinnamate. A calculated spectrum is displayed by clicking on the appropriated (red highlighted) entry, following which the palette is dismissed. Clicking on IR results in an IR spectrum.

Moving the mouse while holding down the left button moves the cursor (unfilled markers at the top and bottom of the spectrum) over the spectrum. When positioned directly over a special line, the markers are darkened and connected by a vertical yellow line, and a numerical value for the line is provided at the bottom of the spectrum. In the case of an IR spectrum, this is a frequency in cm$^{-1}$ and corresponds to a particular vibration of the atoms in the molecule. The molecular model (above the spectrum) vibrates to show this motion. For methyl trans-cinnamate, the line at 1645 cm$^{-1}$ corresponds to the C=C stretch while the line at 1739 cm$^{-1}$ corresponds to the C=O stretch.

Moving the mouse while holding down the right button slides the viewable scale from 4000 cm$^{-1}$ to 500 cm$^{-1}$ but does not change the overall range (of 3500 cm$^{-1}$). The range is changed by using the scroll wheel. The original settings may be restored by clicking on in the
bar at the top of the spectra pane.

Move one finger over the spectrum to position the cursor, move two fingers to slide the viewable scale and pinch two fingers to change the range.

In the case of IR (only) two buttons appear at the left of the spectrum, (i) and (i). Clicking on (i) leads to a scrollable panel at the left of the spectrum.

This contains a listing of calculated infrared frequencies and intensities. Checking the box to the left of an individual frequency moves the cursor on the spectrum over this line and animates the vibrational motion.

With a frequency selected, clicking on ( ) leads to a new panel.

This is used to make a list of structures centering around the minimum (or maximum in the case of a transition state) with control over the
amplitude of vibration (maximum displacement in Å) and number of steps. *Clicking* on **Make List** leads to a separate document.

If available, an experimental spectrum from one of the public on-line databases may be superimposed on top of the calculated spectrum. The IR spectrum of methyl trans-cinnamate is available. *Click* on and select **Experimental** from the palette.

![Image of spectra view](image)

You can if you wish **only** display the experimental spectrum. If a calculated is already displayed, *click* on and re-select (the control operates in toggle mode).

Additional spectra may be requested by *clicking* on in the bar above the spectra pane and then *clicking* on the appropriate entry in the resulting palette. Each new spectrum adds a tab to the bar, although calculated and experimental spectra share the tab. Switching between tabs changes the display. A spectrum can be deleted by *clicking* on in the bar above the spectra pane. If both calculated and experimental spectra were displayed, both will be deleted.

Controls at the top right of the spectra pane allow saving the spectrum as a PNG, JPEG or Bitmap image file ( ), printing the file ( ), detaching the spectrum pane from the main window ( ) and closing the pane ( ).

**Spreadsheet ( )**

Associated with each *Spartan Student* document (including documents with only a single molecule) is a spreadsheet. This may be displayed by selecting **Spreadsheet** from the **Display** menu.
The spreadsheet comprises a series of rows (corresponding to different molecules in the document) and columns (corresponding to different properties). Together, a row and column define a “cell”. The spreadsheet may be expanded or contracted by positioning the cursor at one of the corners, pressing the left mouse button and dragging the mouse.

Only one molecule from one document may be selected (although several molecules may be simultaneously displayed). Molecule selection follows either by clicking on the spreadsheet cell containing the molecule label or identifier (leftmost column), or by using the \[ \] and \[ \] buttons or the scroll bar at the bottom left of the screen. Molecules may be animated (stepped through in succession) using the \[ \] button at the bottom left of the screen. Animation speed may be adjusted from the Settings tab (Preferences under the Options menu; Chapter 10). Selection of a new molecule in the document results in deselection of the previously selected molecule. A molecule may be designated for permanent display by checking the box to the left of its identifier (Label) in the spreadsheet. The molecules in a document may either be translated and rotated in concert or manipulated independently. This is controlled by Coupled under the Model menu (Chapter 5). By default (Coupled checked) molecules move in concert. Uncheck Coupled to move them independently.

Upon initial entry, all columns of the spreadsheet except the leftmost column, are blank. The leftmost column contains a label that may be
changed either by directly typing a new label into the spreadsheet or into the Label box in the Molecule Properties dialog (see discussion earlier in this chapter). Additionally, default identifiers (M0001, ...) can be replaced by chemical names if the molecule has been retrieved from the Spartan Spectra and Properties Database (SSPD).

Information may be added to the spreadsheet in several ways:

**From the Add Dialog**

A selection of molecular properties may be entered into the spreadsheet by first clicking on the header cell of an empty column, and then clicking on Add... at the bottom of the spreadsheet. Alternatively, right click inside the header cell and then select Add... from the menu that results.

This leads to the Add dialog which comprises three tabs. The Columns tab requests information about the properties of individual molecules, the Summaries tab provides summaries of the properties for all molecules and the Linear Regression tab attempts to find relationships among properties of the molecules. Clicking on the Columns tab leads to the Add Columns dialog.
<table>
<thead>
<tr>
<th>Name</th>
<th>molecule name as it appears in SSPD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>molecular formula</td>
</tr>
<tr>
<td>E</td>
<td>energy (heat of formation, strain energy)</td>
</tr>
<tr>
<td>E\textsubscript{aq}</td>
<td>aqueous energy (heat of formation, strain energy) based on the SM5.4 model</td>
</tr>
<tr>
<td>rel. E</td>
<td>energy (heat of formation, strain energy) relative to selected molecule</td>
</tr>
<tr>
<td>rel. E\textsubscript{aq}</td>
<td>aqueous energy (heat of formation, strain energy) relative to selected molecule based on the SM5.4 model</td>
</tr>
<tr>
<td>E\textsubscript{HOMO}</td>
<td>energy of highest-occupied molecular orbital</td>
</tr>
<tr>
<td>E\textsubscript{LUMO}</td>
<td>energy of lowest-occupied molecular orbital</td>
</tr>
<tr>
<td>Dipole</td>
<td>dipole moment (in debyes)</td>
</tr>
<tr>
<td>Boltzmann Distribution</td>
<td>Boltzmann distribution based on energy</td>
</tr>
<tr>
<td>Boltzmann Distribution (aq)</td>
<td>Boltzmann distribution based on aqueous energy as estimated from SM5.4 model</td>
</tr>
<tr>
<td>Cumulative Boltzmann Distribution</td>
<td>Sum of the Boltzmann weights for the selected molecule and all molecules with lower energy than the selected molecule</td>
</tr>
<tr>
<td>Cumulative Boltzmann Distribution (aq)</td>
<td>Sum of the Boltzmann weights for the selected molecule and all molecules with lower energy than the selected molecule based on aqueous energy as estimated by the SM5.4 model</td>
</tr>
<tr>
<td>Alignment Score</td>
<td>(1 - \frac{R^2}{N}), where (R^2) is the root mean square distance and (N) is the number of alignment centers. 1 is a perfect score</td>
</tr>
</tbody>
</table>
One or more properties may be added to the spreadsheet by clicking on their entries, and where appropriate specifying units from the Energy menu, varying temperature from the Temp menu (which affects the Boltzmann and cumulative Boltzmann distributions), and finally clicking on OK or Apply. In the former case, the dialog is dismissed and in the latter it is left on screen. Clicking on Cancel or removes the dialog.

Column totals, averages and Boltzmann-weighted averages may be accessed by clicking on the Summaries tab. Alternatively, click on an empty row header (instead of an empty column header) inside the spreadsheet prior to clicking on Add.... This leads to Add Summaries dialog.

<table>
<thead>
<tr>
<th>Totals</th>
<th>sum of column values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Averages</td>
<td>average of column values</td>
</tr>
<tr>
<td>Boltzmann Averages</td>
<td>Boltzmann weighted average of column values</td>
</tr>
<tr>
<td>Boltzmann Averages (aq)</td>
<td>Boltzmann weighted average of column values using energies corrected for aqueous environment based on the SM5.4 model</td>
</tr>
</tbody>
</table>

Clicking on one or more of these followed by clicking on OK or Apply, leads to the requested summaries as rows at the bottom of the spreadsheet, identified as Totals, Averages, etc. (one row for each).
Finally, a linear regression analysis may be performed on the data in the spreadsheet. Clicking on the Linear Regression tab leads to the Add Linear Regression dialog. Select one entry from the Fit menu and one or more entries from the list under Using. Clicking on OK or Apply performs the linear regression analysis and places the results in a row at the bottom of the spreadsheet identified by Fit. As many regression analyses as desired may be performed on the data in the spreadsheet. The individual results will be entered as separate rows in the spreadsheet, with names Fit1, Fit2, etc.

From Post (P) Buttons

Post buttons (P) found in a number of properties dialogs provide an alternative method to the Add dialog for entering calculated properties into the spreadsheet. Note that some properties may require user specification. These include individual bond distances, angles and dihedral angles (available from Measure Distance, Measure Angle and Measure Dihedral under the Geometry menu; Chapter 6), bond distance, angle and dihedral angle constraints (available from Constrain Distance, Constrain Angle and Constrain Dihedral under the Geometry menu; see discussion in Chapter 6), atomic charges, chemical shifts (available from the Atom Properties dialog; this chapter), the accessible area of an electron density surface, the polar area of an electrostatic potential map, minimum and maximum property values on a map and the value of the property at a specific location on a property map (available from the Surfaces Properties dialog; this chapter). With the exception of the property value
on a map, post generates an entire column. Where atom labels are involved, for example, in defining a specific distance, post can be expected to yield consistent results for all molecules in a document only where the molecules are closely related, or where labels have been explicitly reassigned*.

The property value on a map is posted only for the selected molecule. Post buttons are also available for CAS numbers, for heats of formation from the T1 thermochemical recipe and (where available) for experimental heats of formation contained in Spartan Student’s internal database.

Copy/Paste

Properties of one or more molecules in a document may be copied and then pasted into individual or multiple spreadsheet cells. These include (but are not restricted to) bond distances, angles and dihedral angles (Measure Distance, Measure Angle and Measure Dihedral under the Geometry menu), bond distance, angle and dihedral angle constraints (Constrain Distance, Constrain Angle and Constrain Dihedral under the Geometry menu), atomic charges and chemical shifts (Atom Properties dialog), infrared frequencies and chemical shifts (IR Spectra and NMR Spectra dialogs, respectively) and the value of a property on a property map (Surface Properties dialog). To copy the spreadsheet, first highlight the numerical value of the property in the appropriate screen location (distances, etc.) or dialog (charges, etc.), then select Copy from the Edit menu, then click on the appropriate (destination) cell in the spreadsheet, and finally select Paste from the Edit menu.

Numerical Data

Numerical data may be entered by typing directly into the spreadsheet. A column header first needs to be specified. Double click on an empty column header cell, type in a name and press the Enter key (return key on Mac). Then, type the data into individual cells of the new column (press the Enter or return

* This may be done using the Atom Properties dialog (see discussion earlier in this chapter).
User-Defined Expressions

An expression may be entered either into a header cell (in which case it refers to all entries in a column) or into an individual cell (in which case it refers only to a single entry). Expressions in the column header take the form \texttt{name=formula}, where \texttt{formula} may involve arithmetic operations, specialty functions, calculated quantities, conversion factors and constants in addition to numerical values. References to specialty functions, molecular mechanics and quantum chemical quantities and conversion factors and constants must be preceded by @. For example, \texttt{mu = @DIPOLE} typed into a header cell gives the dipole moment. Some functions have arguments, for example, \texttt{c1 and c2} in the expression \texttt{c12 = @DISTANCE (c1,c2)} refer to atoms \texttt{c1} and \texttt{c2}, while \texttt{3} in the expression \texttt{orbitalE=@HOMO (-3)} designates the energy of the molecular orbital three orbitals below the HOMO. It is necessary to press the \texttt{Enter} key (\texttt{return} key on Mac) following entry of the expression into a cell. The leading \texttt{name=} is optional for entries in an individual (non-header) cell.

<table>
<thead>
<tr>
<th>Arithmetic Operations</th>
<th>Boolean Operations</th>
</tr>
</thead>
<tbody>
<tr>
<td>+</td>
<td>greater than</td>
</tr>
<tr>
<td>-</td>
<td>&gt;= greater than or equal to</td>
</tr>
<tr>
<td>*</td>
<td>&lt; less than</td>
</tr>
<tr>
<td>/</td>
<td>&lt;= less than or equal to</td>
</tr>
<tr>
<td>^</td>
<td>== equal to</td>
</tr>
<tr>
<td></td>
<td>!= not equal to</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>&amp; and</td>
</tr>
</tbody>
</table>

Mathematical Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABS(x)</td>
<td>absolute value</td>
<td>LN(x)</td>
<td>natural logarithm</td>
</tr>
<tr>
<td>ACOS(x)</td>
<td>inverse cosine</td>
<td>LOG(x)</td>
<td>log (base 10)</td>
</tr>
<tr>
<td>ASIN(x)</td>
<td>inverse sine</td>
<td>SIN(x)</td>
<td>sine</td>
</tr>
<tr>
<td>ATAN(x)</td>
<td>inverse tangent</td>
<td>SQRT(x)</td>
<td>square root</td>
</tr>
<tr>
<td>COS(x)</td>
<td>cosine</td>
<td>TAN(x)</td>
<td>tangent</td>
</tr>
<tr>
<td>EXP(x)</td>
<td>exponential</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Specialty Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AVG (column name)</td>
<td>average of values in column</td>
</tr>
<tr>
<td>FITVAL (fit name)</td>
<td>column of fit values from regression analysis</td>
</tr>
<tr>
<td>MIN (column name)</td>
<td>minimum of values in column</td>
</tr>
<tr>
<td>MAX (column name)</td>
<td>maximum of values in column</td>
</tr>
<tr>
<td>NUM (column name)</td>
<td>number of defined entries in column</td>
</tr>
<tr>
<td>ROW</td>
<td>the number of the row in the spreadsheet</td>
</tr>
<tr>
<td>ROW(molecule name)</td>
<td>the number of the row of molecule</td>
</tr>
<tr>
<td>REF(i, x)</td>
<td>the value of the x referenced to row i</td>
</tr>
<tr>
<td>STDEV (column name)</td>
<td>standard deviation of values in column</td>
</tr>
<tr>
<td>SUM (column name)</td>
<td>sum of values in column</td>
</tr>
</tbody>
</table>

### Calculated Quantities

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANGLE(i, j, k)</td>
<td>angle involving atoms i, j, k (degrees)</td>
</tr>
<tr>
<td>AREA</td>
<td>area of a user-defined plane (Å$^2$)</td>
</tr>
<tr>
<td>DIHEDRAL(i, j, k, l)</td>
<td>dihedral angle involving atoms i, j, k, l (degrees)</td>
</tr>
<tr>
<td>DISTANCE(i, j)</td>
<td>distance involving atoms i, j (Å)</td>
</tr>
<tr>
<td>ELECTROSTATIC (i)</td>
<td>electrostatic charge on atom i (electrons)</td>
</tr>
<tr>
<td>HOMOev(-n)</td>
<td>energy of n$^{th}$ orbital below the HOMO (eV)</td>
</tr>
<tr>
<td>HOMOBETAev(-n)</td>
<td>energy of the n$^{th}$ orbital below the β HOMO (eV)</td>
</tr>
<tr>
<td>INTERTIA(i)</td>
<td>principle movements of inertia from largest (i=1) to smallest (i=3)</td>
</tr>
<tr>
<td>ISOTOPE(i)</td>
<td>mass number of atom i</td>
</tr>
<tr>
<td>LENGTH (i)</td>
<td>length of bond i (Å)</td>
</tr>
<tr>
<td>LUMOev(+n)</td>
<td>energy of the n$^{th}$ orbital above the LUMO (eV)</td>
</tr>
<tr>
<td>LUMOBETAev(+n)</td>
<td>energy of the n$^{th}$ orbital above the β LUMO (eV)</td>
</tr>
<tr>
<td>ZPE</td>
<td>zero point energy</td>
</tr>
<tr>
<td>HØ</td>
<td>absolute enthalpy at 298K</td>
</tr>
<tr>
<td>CV</td>
<td>constant volume heat capacity at 298K</td>
</tr>
<tr>
<td>SØ</td>
<td>absolute entropy at 298K</td>
</tr>
<tr>
<td>GO</td>
<td>Gibbs energy at 298K</td>
</tr>
</tbody>
</table>
Conversion Factors and Constants

<table>
<thead>
<tr>
<th>Conversion</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANGS2AU</td>
<td>Ångstroms to atomic units</td>
</tr>
<tr>
<td>AU2ANGS</td>
<td>Atomic units to Ångstroms</td>
</tr>
<tr>
<td>EV2HART</td>
<td>eV to atomic units (hartrees)</td>
</tr>
<tr>
<td>EV2KCAL</td>
<td>eV to kcal/mol</td>
</tr>
<tr>
<td>EV2KJ</td>
<td>eV to kJ/mol</td>
</tr>
<tr>
<td>HART2KCAL</td>
<td>Atomic units (hartrees) to kcal/mol</td>
</tr>
<tr>
<td>HART2EV</td>
<td>Atomic units (hartrees) to eV</td>
</tr>
<tr>
<td>HART2KJ</td>
<td>Atomic units (hartrees) to kJ/mol</td>
</tr>
<tr>
<td>KCAL2EV</td>
<td>kcal/mol to eV</td>
</tr>
<tr>
<td>KCAL2HART</td>
<td>kcal/mol to atomic units (hartrees)</td>
</tr>
<tr>
<td>KCAL2KJ</td>
<td>kcal/mol to kJ/mol</td>
</tr>
<tr>
<td>KJ2EV</td>
<td>kJ/mol to eV</td>
</tr>
<tr>
<td>KJ2HART</td>
<td>kJ/mol to atomic units (hartrees)</td>
</tr>
<tr>
<td>KJ2KCAL</td>
<td>kJ/mol to kcal/mol</td>
</tr>
<tr>
<td>PI</td>
<td>(\pi)</td>
</tr>
</tbody>
</table>

Table 9-5: Examples of User Defined Expressions

<table>
<thead>
<tr>
<th>Expression</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>E/area = @ENERGY/@AREA</td>
<td>Energy divided by surface area</td>
</tr>
<tr>
<td>RelE = @ENERGY-@REF (6,@ENERGY)</td>
<td>Energy relative to energy of molecule in row 6</td>
</tr>
<tr>
<td>Eq = @EXP (-@ENERGY/592.1)</td>
<td>Equilibrium constant at room temperature</td>
</tr>
<tr>
<td>EnergyFilter = @ENERGY&lt;-99.43</td>
<td>&quot;true&quot; (≠0) for all energies &lt; -99.43</td>
</tr>
<tr>
<td>RowFilter = @ROW&gt;10</td>
<td>&quot;true&quot; (≠0) all entries past row 10</td>
</tr>
</tbody>
</table>

Each row in a spreadsheet corresponds to a molecule in a document, and new rows are automatically added in response to adding new molecules to the document. New molecules are added by building (New Molecule under the File menu; Chapter 3), by appending one or more existing documents each containing one or more molecules using either Append Molecule(s)... under the File menu (Chapter 3), or by right clicking inside the header cell of the first available
row and selecting Append from the menu that appears, by pasting from the clipboard, or by dragging from the file system. To copy a molecule into the clipboard, first select (click on) it, and then select Copy from the Edit menu, or click on its identifier (left most column) in its spreadsheet, and then select Copy from the Edit menu. Alternatively right click either on the molecule or on its identifier in the spreadsheet and select Copy from the menu that appears. Use of the clipboard permits several molecules to be selected (and copied) at once using the Shift and Ctrl keys in the usual manner. To copy the contents of the clipboard to its destination, click on an empty row header in the spreadsheet (for the destination document), and then select Paste from the Edit menu. An alternative to the two-step Copy-Paste procedure is to drag the molecule or set of molecules from one spreadsheet to another.

A row (molecule) may be deleted from a spreadsheet, either by first selecting the molecule and then selecting Delete Molecule from the File menu, or by first clicking on its identifier in the spreadsheet (leftmost column) and then either clicking on the Delete button at the bottom of the spreadsheet, or by right clicking on its identifier in the spreadsheet and then selecting Delete Selected from the menu that appears. In all cases, a warning is provided prior to deletion. An entire column in the spreadsheet may be deleted by first clicking inside its header cell and then clicking on the Delete button (or Delete Selected from the menu).

Rows in the spreadsheet may be sorted according to the numerical values in any column either by first clicking inside the header cell and then clicking on the Sort button at the bottom of the spreadsheet or by right clicking inside the header cell and selecting Sort from the menu that appears. The rows are placed in ascending order, the smallest (least positive) value of the selected property at the top, largest (most positive) value at the bottom. To sort in descending order, hold down the Shift key before clicking on the Sort button or selecting Sort from the menu.

Information in one or more columns of the spreadsheet may be formatted by right clicking inside the header cell(s) and selecting
Format Selected from the menu that appears.

Format as desired and click on OK to remove the dialog. The full contents of the spreadsheet may be formatted by right clicking inside the header cell for the left most column and then selecting Format Selected from the menu.

A button at the bottom right of the spreadsheet toggles between numerical representation of data, f(x), and formula presentation, =?.

The spreadsheet may be printed by right clicking in the spreadsheet and selecting Print.

As many spreadsheets as desired (corresponding to the same or to different documents) may be open on screen. A spreadsheet is removed when the associated document is closed and may also be removed by clicking on $\times$.

The contents of the spreadsheet may be brought into Excel™ using the clipboard. Select whatever cells are to be copied, select Copy from the Edit menu. Alternatively, right click with the proper cells selected and select Copy from the menu that appears. Paste into Excel.

The contents of an Excel spreadsheet may be brought into Spartan Student. Copy whatever information is to be transferred from Excel, move into Spartan Student, click on the appropriate cell and select Paste from the Edit menu (or right click on the appropriate cell and select Paste from the menu that appears). Note, that information on the clipboard that goes beyond the number of rows in Spartan Student’s spreadsheet will be ignored.

Plots ( đề thám )

Plots may be constructed from data in a spreadsheet and a variety of simple curves fit to these data. Selecting Plots from the Display menu leads to an empty display pane at the right of the screen.
Clicking on + (add plot) in the bar at the top of the plots pane leads to a dialog.

You need to select an item from the X Axis menu and one or more items from the Y Axes list, and then click on the Add button at the bottom of the dialog. A plot appears in the plot pane and the Add Plot dialog is dismissed.
By default, the scales for both horizontal and vertical axes are set to bound the data trying to provide limits and increments that are “rounded”. Moving the mouse left and right while holding down the right button slides the horizontal scale but does not change the range. Similarly, moving the mouse up and down while holding down the right button slides the vertical scale. The horizontal range may be changed by moving the mouse left and right while holding down both the right button and shift key, and the vertical range changed by moving the mouse up and down while holding down both the right button and the shift key. The scroll wheel may be used to simultaneously change both horizontal and vertical ranges. The original settings may be restored by clicking on \( \times \) in the bar at the top of the plots pane.

Move two fingers left and right and up and down to slide the viewable horizontal and vertical scales, respectively. Pinch two fingers left and right and up and down to change the horizontal and vertical scales, respectively.

The plot ranges may also be changed by clicking on \( \text{Edit Plot} \) in the bar at the top of the plots pane.

The resulting dialog also allows axis labels to be altered (from their initial values designated in the spreadsheet) the number of “tics” of horizontal and vertical axes to be changed and a plot title to be added. Finally, the default “curve” (a least-squares fit) can be changed or eliminated altogether.
Additional plots may be added by clicking on \textcolor{red}{+} in the bar at the top of the plots pane. Each plot is given a tab. Only one plot may be displayed at a time as controlled by which tab is selected. The selected (and displayed) plot may be deleted by clicking on \textcolor{red}{-}.

\textbf{Reactions... ( }}

Data in a \textit{Spartan Student} document or in SSPD may be used to calculate reaction energies (including activation energies).

\[ \Delta E = N_{P1} E_{\text{product1}} + N_{P2} E_{\text{product2}} - N_{R1} E_{\text{reactant1}} + N_{R2} E_{\text{reactant2}} \]

$N_{P1}$ and $N_{P2}$ are the numbers of product molecules 1 and 2 and $N_{R1}$ and $N_{R2}$ are the numbers of reactant molecules 1 and 2. Selection of \textbf{Reactions...} from the \textbf{Display} menu leads to the \textbf{Reactions...} dialog.
Two sets of menus under **Reactants:** and two sets of menus under **Products:** specify the number of each reactant and product and identify them. The latter correspond to the labels (identifiers) of the molecules in the document, plus a null entry `<none>`. The overall reaction needs to be mass balanced.

The **Use** menu identifies the source of the energies to be used in the reaction energy calculation.

**SSPD** refers to heats of formation drawn from the T1 data provided in the Spartan Spectra and Properties Database, **Current Document** refers to energies in document and **Current Document (aq)** refers to energies in the document that have been empirically corrected for aqueous solvent using the SM5.4 model.

A reaction energy (in kJ/mol) is computed by clicking on **Compute Energies** at the bottom left of the dialog.

The results of a reaction energy calculation may be printed by right clicking inside the display area of the **Reactions** dialog and selecting **Print** from the menu that results.

The **Reactions** dialog is closed by either clicking on **OK** or **X**.
Chapter 10
The Options Menu

Functions under the **Options** menu* set default colors, fonts, user preferences and van der Waals radii, provide addresses for on-line databases, set icon displays and identify/change URL’s for on-line accesses. They also allow for changing default colors and fonts and for monitoring executing jobs.

![Preferences](image)

**Preferences**

This sets up preferences relating to the graphical user interface (**Settings**), and to molecule displays (**Molecule**). It permits changes to default van der Waals radii used for space-filling models as well as for calculating molecular surface areas and volumes (**VDW Radii**). It also specifies the locations of on-line databases (**Databases**), specifies miscellaneous features (**Miscellaneous**), specifies which icons are to be displayed (**Icons**) and specifies URLs (**URLs**) for on-line connections. Selection results in one of seven dialogs, depending on which tab has been selected in the previous entry. *Clicking* on a tab brings up the associated dialog. To exit a **Preferences** dialog *click* on **OK**. *Clicking* on **Cancel** or **exit** exits the dialog without instituting any changes.

---

* **Preferences** is found under the **Spartan Student** menu in the Macintosh version.
Settings

(i) **View: Orthogonal/Perspective**
Controls the view of structural models and graphics.

(ii) **Menus: Classic List/Button Pad**
Controls presentation of menus either as lists or as button pads (icon palettes). The latter is likely to be better suited to touch screen computers and tablets.

(iii) **Icons: Small/Medium/Large/Extra Large/Jumbo**
Controls size of the icons.

(iv) **Sketch Pad: Small/Medium/Large**
Controls the size of the sketch pad (palette of sketch tools) for Spartan’s 2D builder.

(v) **Stereo: Off/Red-Cyan**
Turns stereographic display on and off.

(vi) **Global Rotate: Screen Centered/Molecule Centered**
- **Screen Centered** rotates all molecules about a common center; while **Molecule Centered** rotates each molecule about its own center.
(vii) **Animation Speed**
A slider bar controls the maximum speed for animations. This has become an important control as the performance of graphics cards has increased.

(viii) **Pin New Documents**
If *checked*, defaults to display of any new documents (from building or brought in from the File menu) irrespective of whether or not they are selected. Does not affect the status of existing documents. **Pin New Documents** has no meaning unless **Show Document Tabs** (see discussion following) is *checked*.

(ix) **Show Document Tabs**
If *checked*, this displays a tab at the bottom of the screen for each open document. Only if the box to the left of the tab is *checked* will the molecule display (if it is not the selected document). If **Show Document Tabs** is not *checked*, the display corresponds to previous versions of **Spartan Student**.

(x) **Split-Tubes**
If *checked*, the tubes in tube and ball-and-spoke models are split to designate multiple bonds.

(xi) **On-Screen Keyboard**
If *checked*, makes the on-screen (virtual) keyboard on Windows 7 and 8 touch-screen computers and tablets accessible. Should not be checked for non touch-screen devices or for touch-screen computers where the physical keyboard is to be used.

(xii) **ChemDraw Interface**
If *checked*, displays **ChemDraw** in the menu of model kits available to **Spartan Student**. **Uncheck** if **ChemDraw** is not installed.

(xiii) **Auto-Gen Graphics**
If *checked*, graphics calculations will be performed in the interface (without having to submit the job if a wave function is available). Does not pertain to **Orbital Energies** under
the **Display** menu. Note, however, that graphics calculations on documents containing more than 25 molecules will not be performed in the interface irrespective of this setting.

**(xiv) Tumble**

If *checked*, allows automatic tumbling of molecule. To tumble a molecule, select it, *press* the left mouse button, move the mouse and release the button. To stop tumbling, *left click*.

**(xv) Keep Verbose**

If *checked*, keeps extended (verbose) output. Normally discarded upon successful completion, this may be useful for identifying the source of problems for calculations that have not successfully completed or have led to suspicious results. (Verbose output is automatically kept for a job that has abnormally terminated.) Note that keeping verbose output significantly increases the size of the *Spartan Student* document.

**(xvi) Polar Area Range**

Set potential (in kJ/mol) for calculating polar area from electrostatic potential map. Values > | range | contribute to polar area. Default is 100 kJ/mol.

**(xvii) Accessible Area Radius**

Set sphere radius (in Å) for determining accessible area. Default is 1.0.
This specifies default settings for model appearance. These settings may be overridden for a specific molecule (or list of molecules) using entries under the **Model** menu.

(i) **Model: Wire/Ball and Wire/Tube/Ball/Spoke/Space Filling**
Controls default model style.

(ii) **Surface Style**
If **Bands** is *checked*, specifies that graphical surfaces, for example, electrostatic potential maps, are to be displayed in terms of a series of color bands, rather than as a continuous spectrum. The number of bands is selected from the menu to the right.

(iii) **Show: Constraints/Frozens/Points/Planes/Reactions**
If *checked*, constraints and frozen markers, points and planes and reaction arrows will always be shown as part of the model. Otherwise, they will be shown only in the appropriate mode.
(iv) **Atom Labeling**: Label/Element/Mass Number/Electrostatic Charge/Strand: Residue/Label/R/S/Exposed Area/Chem Shift
Controls default label type.

(v) **Bond Labels**
If *checked*, bond labels will be shown.

(vi) **Point Labels**
If *checked*, point labels will be shown.

(vii) **Plane Labels**
If *checked*, plane labels will be shown.

(viii) **Constraint Labels**
If *checked*, constraint labels will be shown.

(ix) **Residue Labels**
If *checked*, residue labels will be shown.

(x) **Reaction Labels**
If *checked*, reaction arrow labels will be shown.
VDW Radii

This provides a list of van der Waals radii

To order the list by element name click on **Element**, and by atomic radius click on **VDW Radius**. Individual entries may be changed from default values by first clicking on the entry and then entering a new value. The currently selected entry may be returned to its default radius by clicking on **Reset Selected** at the bottom of the dialog, and the full set of radii may be returned to their default values by clicking on **Reset All** at the bottom of the dialog.
Databases

This allows setting up of paths for SSPD and SRD.

*Spartan Student* is provided with a ~6,000 molecule subset of SSPD. The full database is available for license.
Miscellaneous

Items here refer to cross-platform applications and should not be of concern to users of a single platform.

(i) **Output/Spreadsheet Window**
Toggles between allowing the output window and the spreadsheet to be **Free** (able to move outside the main window) or **Confined** (restricted to move inside the main window).

(ii) **Builder Selection Method**
Toggles among **Buttons on top**, **Tabs on side** and **Menu** to control selection of the model kits in the 3D builder. The second and third choices conserve vertical space on small screen laptops and tablets.

(iii) **Builder Style**
**Use Alternative Builder** provides a different presentation of the model kits in the 3D builder. Try both and see which one you like.
Checking Expert at the bottom right brings up an extended dialog, which contains two additional controls that may be needed in exceptional circumstances.

(iv) **Use HTTP Proxy**
Allows setting up of an alternative path for access to external websites, for example, experimental spectra databases. Rarely needed.

(v) **Pick System**
Toggles between **OpenGL**, **Color** and **Hybrid** picking models. **OpenGL** is the standard but causes problems for Intel HD4000 graphics (very common), where either **Color** or **Hybrid** should be used. Graphics chip is automatically detected at installation and this control should be properly set.

**Icons**

Icons for all menu entries are listed (you may need to use the horizontal slider bar to see them all). If *checked*, the icon will appear at the top of the *Spartan Student* screen.
Icon display is limited to one “permanent” row. Approximately 20 medium size icons will fit on screen.

**URLs**

Lists URLs for access to experimental structural and spectral databases and to Wikipedia.

```
NMR: mrshtclb servlet?mrshtclbaction=exportcmlbyinchi&inchi=%inchi&spectrunttype=%type
IR: http://webbook.nist.gov/cgi/cbook.cgi/nist.jdx2/CAMP=C%&cas&index=0&type=%type
PDB: /www.rcsb.org/pdb/cgi/export.cgi?%s.pdb?format=PD8&pdbld=%s&compression=None
```

**Colors (🎨)**

This alters default colors. Selection leads to the Colors dialog.
After selecting an object, its color may be set by choosing from the palette, moving the cursor inside the window of colors, or by selecting either a set of hue, saturation and values, or red, green and blue settings. The default color may be reset by clicking on **Restore Default Color**. Color selection applies to all objects of the same type, for example, all carbon atoms, and not just to the selected carbon. Further control of colors is available from Utilities/Style dialogs associated with Properties dialogs (Properties under the Display menu; Chapter 21). Clicking on \(\text{ Restore Default Color }\) removes the dialog.

**Fonts/Graphics Fonts**  
This selects fonts, style and size of labels attached to molecules (Labels and Configure... under the Model menu; Chapter 5), and plots (Plots... under the Display menu; Chapter 9). Selection leads to the Fonts dialog.

![Fonts dialog](image)

Selections are made from the Font, Font Style and Size menus. Clicking on OK dismisses the dialog with selections kept. Clicking on Cancel or on \(\text{ Cancel }\) dismisses the dialog but selections are lost.
Monitor ( )

This provides a listing of all executing/queued jobs and their status. To see accumulated output for an executing job, click on its name. A ball-and-spoke model of the selected (executing) job will be displayed in a window to the right of the dialog. It can be manipulated using the usual mouse commands (you need to position the cursor inside the window). Touch-screen commands are presently limited to rotation (move one finger). Model style cannot be changed. Note that (except for molecular mechanics and semi-empirical calculations) the structure is updated throughout an equilibrium geometry of transition state optimization, and bond lengths, angles and dihedral angles can be queried.

To kill a job, click on its name, and then select Terminate from the Actions menu at the top of the dialog (or right click on its name and select Terminate from the menu that appears). To start a queued job (irrespective of the imposed queue limits; see previous discussions under Jobs), click on its name and select Start from the Actions menu (or right click on its name and select Start from the menu that appears).

The Monitor may be removed either by selecting Exit from the File menu or by clicking on at the top of the dialog.
Calculator (计算器)
Selection brings up a Calculator.

This functions the same way as a normal pocket calculator. The Calculator is removed by clicking on .

Icons (图标)
Toggles the set of icons that appear above the menus on and off.
Chapter 11

The Activities Menu

The Activities menu permits on-screen display of the full set of Spartan Student tutorials and a series of topics of practical relevance to molecular modeling. It also allows a Wikipedia page to be brought up (external to Spartan Student).

Tutorials/Topics

Selection of Tutorials or Topics brings up an HTML page (Tutorials shown).

Clicking on an entry (link) brings up the computer’s PDF reader alongside of Spartan Student. This allows you to access the materials while working with the program.
Note that the full User’s Guide is available as a PDF under the Help menu (see next chapter).

**Look Up in Wikipedia...**

Selection results in a dialog.

![Look Up in Wikipedia dialog](image)

Entering a query followed by *clicking* on **OK** leads to a Wikipedia page. This occupies a window that is external to *Spartan Student*. 
Chapter 12

The Help Menu

This chapter describes help.

Help

This provides information relating to application of computational methods available in Spartan Student, as well as technical details regarding the program’s operation. Help also provides a link to Wavefunction’s website. Help files are HTML documents.

Spartan Student Tutorials, Spartan Student Overview (this document) and a number of useful references are available from Help.

Overview

Opens a PDF file providing documentation on Spartan Student Edition menus and features.

About...*

Provides information about the user’s release of Spartan Student.

* About is located under the Spartan Student menu on the Macintosh version.
Spartan Student v6
Version 6.1.2
Nov 20 2013

Installed: C:\Users\Spartan\Desktop\Spartan Student v6.1.2

Copyright © 1991-2014 by Wavefunction Inc.
All rights reserved

Spartan Student v6 licensed with Local Sentinel SL
Key ID: 705433765546534408

SSPD Database licensed with Local Sentinel SL
Key ID: 705433765546534408

Machine ID: BBAC6FA353D8
Appendix A

Capabilities and Limitations

Molecular Mechanics Models

The MMFF molecular mechanics model is available for the calculation of energy (a combination of strain energy and intramolecular interaction energy), equilibrium geometries, equilibrium conformers and vibrational frequencies. Energies may be corrected for the effects of aqueous solvent. There are no atom limits for molecular mechanics calculations.

Semi-Empirical Models

The PM3 semi-empirical model is available for calculation of heats of formation, wave functions, equilibrium and transition-state geometries and vibrational frequencies. The elements H-Ne, Mg-Ar, Ca, Ti-Br, Zr, Mo-Pd, Cd-I, Hf-Pt and Hg-Bi and Gd are supported. PM3 calculations are limited to 75 atoms.

Hartree-Fock Models

Hartree-Fock models are available for calculation of energies and wave functions, equilibrium and transition-state geometries and vibrational frequencies with STO-3G, 3-21G, 6-31G* and 6-311+G** basis sets. Hartree-Fock calculations are limited to 30 atoms.

Density Functional Models

B3LYP and EDF2 density functional models are available for calculation of energies and wave functions, equilibrium and transition-state geometries and vibrational frequencies with both 6-31G* and 6-311+G** basis sets. NMR chemical shifts are available for the B3LYP/6-31G* and EDF2/6-31G* models only. Density functional calculations are limited to 30 atoms.
**MP2 Møller-Plesset Models**

The MP2 Møller-Plesset model is available for calculation of energies and wave functions and equilibrium and transition-state geometries with 6-31G* and 6-311+G** basis sets. Vibrational frequencies are also available, but are very costly in terms of computation. MP2 calculations are limited to 20 atoms.

**Solvent Models**

*Spartan Student* supports the SM5.0R\(^4\) (for molecular mechanics calculations) and SM5.4\(^5\) (for quantum chemical calculations) empirical solvation models to estimate the aqueous solvation energy. Both methods are parameterized for H, C–F, S–Cl, Br and I. Solvation energies are added to gas phase energy calculations to provide an aqueous energy (Eaq).

**Properties and Spectra**

The properties module (that is automatically called from the molecular mechanics module or one of the quantum chemical modules) provides for text output printing, population analyses based on fits to electrostatic potentials, evaluation of thermodynamic quantities (enthalpy, entropy, free energy and heat capacity), and calculation of the dipole moment.

The properties module is also responsible for calculating quantities related to infrared spectra (vibrational frequencies and intensities), and NMR chemical shifts (\(^{13}\)C chemical shifts are corrected for local environment). IR spectra calculations may be carried out with molecular mechanics models, semi-empirical models, Hartree-Fock models, B3LYP, EDF2 and MP2 models. NMR spectra calculations may be carried out only with the B3LYP/6-31G* and EDF2/6-31G* models.

**Graphical Models**

The graphics module provides for data preparation associated with the display as surfaces, property maps and slices of molecular orbitals, electron densities, spin densities, electrostatic potentials and local ionization potentials. The sizes of electron density surfaces (and of
property maps based on electron density surfaces) may be chosen either using a specific value of the density or a value that encloses a specific percentage of the total number of electrons. Accessible and inaccessible regions may be distinguished for electron density surfaces and all property maps based on electron density surfaces.

Database

The database supported with Spartan Student is a subset of the Spartan Spectra and Properties Database (SSPD). It contains structures, energies, T1^6 heats of formation, IR and NMR spectra and diverse molecular properties for ~6,000 molecules obtained from EDF2/6-31G* calculations. In addition, it contains the wave function allowed on-the-fly calculation and display of the full variety of graphical surfaces and property maps. The full version of SSPD (currently 250,000 molecules) may be licensed separately.

1. For a general discussion and assessment of the techniques and methods available in Spartan Student, see: W.J. Hehre, A Guide to Molecular Mechanics and Quantum Chemical Calculations, Wavefunction, Inc., Irvine, CA 2003. This is available from Wavefunction’s website (www.wavefun.com).
# Appendix B

## Menus

### Spartan Student Screen

**File**

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>New Build</td>
<td>Brings up a model kit for 3D molecule building or substitution</td>
</tr>
<tr>
<td>New Sketch</td>
<td>Brings up the sketch pad for molecule sketching in 2D</td>
</tr>
<tr>
<td>Open...</td>
<td>Opens (imports) a molecule or multi-molecule document</td>
</tr>
<tr>
<td>Close</td>
<td>Closes a molecule or multi-molecule document</td>
</tr>
<tr>
<td>Save</td>
<td>Saves (exports) a molecule or multi-molecule document</td>
</tr>
<tr>
<td>Save As...</td>
<td>Saves a molecule as a document under a user-specified name</td>
</tr>
<tr>
<td>Save Image As</td>
<td>Saves molecule or graphical model as a JPEG, PNG or a BMP file of user-specified resolution</td>
</tr>
<tr>
<td>Build New Molecule</td>
<td>Adds a molecule to an existing document; brings up a model kit for molecule building</td>
</tr>
<tr>
<td>Sketch New Molecule</td>
<td>Adds a molecule to an existing document; brings up the sketch pad for molecule sketching in 2D</td>
</tr>
<tr>
<td>Delete Molecule</td>
<td>Deletes a molecule (or molecules) from a document</td>
</tr>
</tbody>
</table>
Append Molecule(s)...  
Appends molecules to an existing document

Access Database by Name  
Searches the *Spartan Student* database by name or partial name

Access PDB Online...  
Accesses the online Protein Data Bank (PDB)

Print...  
Prints on-screen display; also prints contents of output window and the *Spreadsheet*

Start/Stop QuickTime Recording  
Starts and stops QuickTime recording of contents of main *Spartan Student* screen (only)

Exit  
Exits *Spartan Student*

**Edit**

Undo  
Undoes previous operations

Cut  
Moves the current molecule or contents of the selection box to the clipboard

Copy  
Copies the current molecule or contents of the selection box to the clipboard

Paste  
Pastes contents of the clipboard to the screen

Select All  
Selects all atoms in the selected molecule

Find...  
Locates a text string in the output dialog or an on-screen molecular fragment

Find Next  
Locates next occurrence of a text string or molecular fragment

Center  
Centers the molecule on screen; applies to all molecules in a document

Clear  
Clears the selected molecule
**Model**

**Wire**
Displays structure as wire-frame model

**Ball and Wire**
Displays structure as ball-and-wire model

**Tube**
Displays structure as tube model

**Ball and Spoke**
Displays structure as ball-and-spoke model

**Space Filling**
Displays structure as space-filling model

**Hide**
Hides structure model from view

**Global Model**
Applies model type and labels of current molecule to all molecules in the document

**Coupled**
Couples motions of all molecules in the document

**Hydrogens**
Toggles hydrogens on and off

**Labels**
Toggles labels on and off

**Ribbons**
Toggles ribbons on and off

**Ramachandran Plot**
Display a Ramachandran plot for a protein that has been brought in from the Protein Data Bank (PDB)

**Hydrogen Bonds**
Toggles hydrogen bonds on and off

**Configure...**
Labels atoms, bonds, etc., provides information about polypeptides/polynucleotides residues and designates ribbon displays

**Geometry**

**Measure Distance**
Displays and/or sets bond distance

**Measure Angle**
Displays and/or sets bond angle

**Measure Dihedral**
Displays and/or sets dihedral angle
Constrain Distance  Constrain bond distance
Constrain Angle  Constrain bond angle
Constrain Dihedral  Constrain dihedral angle
Freeze Center  Freezes selected atomic positions
Define Point  Defines a point as a geometric mean of a set of atoms; defines ligand point as a position that is perpendicular to the centroid of a plane made by three or more atoms
Define Plane  Defines a plane made by three or more atoms
Align  Aligns molecules in a document

Build

View  Removes the model kit
Edit Build  Brings up a 3D model kit (organic, inorganic, peptide, nucleotide, or ChemDraw) with the presently selected molecule
Edit Sketch  Brings up the sketch pad with the presently selected molecule. This function is only available if the sketch has not been altered using any of the 3D model kits or has not been replaced by an entry in SSPD.
Delete  Deletes atoms, bonds, points, planes, etc. Also available at the bottom of the 3D model kits
Make Bond  Makes bonds between free valences or atoms. Also available at the bottom of the 3D model kits
Break Bond  Breaks a bond. Also available at the bottom of the 3D model kits
Minimize  Performs energy minimization using MMFF molecular mechanics. Also
available at the bottom of the 3D model kits

**Guess Transition State**

Provides transition-state guess based on reaction database or, lacking a database entry, based on linear synchronous transit

## Setup

<table>
<thead>
<tr>
<th><strong>Calculations...</strong></th>
<th>Sets up molecular mechanics and quantum chemical calculations and similarity analyses; specifies calculation of IR and NMR spectra</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Surfaces</strong></td>
<td>Sets up generation of and displays graphical surfaces</td>
</tr>
<tr>
<td><strong>Submit</strong></td>
<td>Submits job to the execution queue</td>
</tr>
</tbody>
</table>

## Display

<table>
<thead>
<tr>
<th><strong>Output</strong></th>
<th>Displays text output</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Properties</strong></td>
<td>Displays molecule, bond and atom properties as well as information about geometrical constraints, graphical surfaces and statistical analyses</td>
</tr>
<tr>
<td><strong>Orbital Energies</strong></td>
<td>Displays an orbital energy diagram and allows on-the-fly generation and display of molecular orbitals</td>
</tr>
<tr>
<td><strong>Surfaces</strong></td>
<td>Sets up generation of and displays graphical surfaces (same as entry in Setup menu)</td>
</tr>
<tr>
<td><strong>Spectra</strong></td>
<td>Displays IR and NMR spectra, animates vibrational modes (IR), and accesses online experimental spectral databases</td>
</tr>
<tr>
<td><strong>Spreadsheet</strong></td>
<td>Displays spreadsheet</td>
</tr>
<tr>
<td><strong>Plots...</strong></td>
<td>Creates 2D and 3D plots from the data in</td>
</tr>
</tbody>
</table>
Reactions

Calculates reaction (activation) energies using data either from current document or from the Spartan Spectra and Properties Database (SSPD)

Options

Preferences...
Sets various run-time and labeling preferences, icon displays, establishes url’s for on-line access

Colors
Sets screen and model colors

Fonts...
Sets fonts for labels and plot displays

Graphics Fonts...
Sets fonts for graphical displays

Monitor
Monitors and allows for killing jobs

Calculator
Pocket calculator

Activities

Tutorials
Brings up Spartan Student tutorials as PDF documents

Topics
Brings up selection of topics relevant to calculations performed in Spartan Student as PDF documents

Look up in Wikipedia
Brings up an html page pointing to a Wikipedia page

Help

Help
Provides information about the performance and timing of computational methods in Spartan Student; provides information about using graphical models in Spartan Student; bulletin board for FAQs about Spartan Student
Overview Opens a PDF file providing a guided tour through Spartan Student Edition menus

About... Provides program version information for citation and support

Contextual

Main Screen

Copy Copies selected molecule to the clipboard

Paste Pastes the contents of the clipboard into the selected document

Delete Selected Deletes selected molecule from document

Properties Brings up the Molecular Properties dialog

Spreadsheet

Copy Copies text of selected cell or cells to the clipboard. If leftmost cell (or cells) selected, copies molecule(s) to the clipboard

Paste Pastes the contents of the clipboard into selected cells. If leftmost cell (or cells) selected, either pastes text or molecule(s) depending on menu choice

Add Brings up the Add dialog (spreadsheet) for adding calculated quantities into the spreadsheet

Sort Sorts the column from low to high. Pressing the Shift key prior to menu selection sorts from high to low

Format Selected Formats selected cell(s), selected column(s) if selection is in a header cell,
or entire spreadsheet if selection is header cell of leftmost column

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Delete Selected</td>
<td>Deletes selected molecule(s) from document</td>
</tr>
<tr>
<td>Append</td>
<td>Appends the contents of <em>Spartan Student</em> document(s) to the spreadsheet</td>
</tr>
<tr>
<td>(corresponding to the selected document)</td>
<td></td>
</tr>
<tr>
<td>Rename Selected</td>
<td>Rename selected molecule(s) with names in the Spartan Spectra and Properties Database (SSPD)</td>
</tr>
<tr>
<td>Using SSPD</td>
<td></td>
</tr>
<tr>
<td>Properties</td>
<td>Brings up the <em>Molecular Properties</em> dialog</td>
</tr>
</tbody>
</table>

**Reactions**

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Copy</td>
<td>Copies selected text to the clipboard</td>
</tr>
<tr>
<td>Print</td>
<td>Prints selected text</td>
</tr>
</tbody>
</table>

**Output Window**

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Copy</td>
<td>Copies selected text to the clipboard</td>
</tr>
<tr>
<td>Print</td>
<td>Prints selected text</td>
</tr>
</tbody>
</table>
Appendix C

Units

Geometries

Cartesian coordinates are given in Ångstroms (Å), and in atomic units (au).

Bond distances are given in Å and in au. Bond angles and dihedral angles are given in degrees (°).

Surface areas, accessible surface areas and polar surface areas are available in Å² and volumes in Å³, and in au² (au³).

1 Å = 0.1 nm=1.889762 au

Energies, Heats of Formation and Strain Energies, Zero-Point Energies, Enthalpies and Gibbs Energies and Entropies

Total energies from Hartree-Fock calculations are available in au, kcal/mol, kJ/mol and electron volts (eV).

Experimental heats of formation as well as those from semi-empirical calculations and from thermochemical recipes are available in kJ/mol, au, kcal/mol and eV.

Strain energies from molecular mechanics calculations are available in kJ/mol, au, kcal/mol and eV.

Energies, heats of formation and strain energies corrected empirically for the effects of aqueous media are given in the same units as the corresponding gas-phase quantities.

Zero-point energies, enthalpies and Gibbs energies available in kJ/mol, kcal/mol and au/mol. Entropies are available in kJ/mol•degree, kcal/mol•degree and au/mol•degree.

Orbital Energies

Orbital energies are available in eV, kcal/mol, kJ/mol and au.
Energy Conversions

<table>
<thead>
<tr>
<th></th>
<th>au</th>
<th>kcal/mol</th>
<th>kJ/mol</th>
<th>eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 au</td>
<td>-</td>
<td>627.5</td>
<td>2625</td>
<td>27.21</td>
</tr>
<tr>
<td>1 kcal/mol</td>
<td>1.593 (-3)</td>
<td>-</td>
<td>4.184</td>
<td>4.337 (-2)</td>
</tr>
<tr>
<td>1 kJ/mol</td>
<td>3.809 (-4)</td>
<td>2.390 (-1)</td>
<td>-</td>
<td>1.036 (-2)</td>
</tr>
<tr>
<td>1 eV</td>
<td>3.675 (-2)</td>
<td>23.06</td>
<td>96.49</td>
<td>-</td>
</tr>
</tbody>
</table>

a) exponent follows in parenthesis, e.g., 1.593 (-3) = 1.593 x 10^{-3}

Electron Densities, Spin Densities, Dipole Moments, Charges, Electrostatic Potentials and Local Ionization Potentials

Electron densities and spin densities are given in electrons/au^3.

Dipole moments are given in debyes.

Atomic charges are given in electrons.

Electrostatic potentials are given in kJ/mol.

Local ionization potentials are given in eV.

Vibrational Frequencies

Vibrational frequencies are given in wavenumbers (cm^{-1}).

Chemical Shifts, Coupling Constants

Chemical shifts are given in parts-per-million (ppm) relative to the following standards: hydrogen, tetramethylsilane; carbon, tetramethylsilane; nitrogen, nitromethane; fluorine, fluorotrichloromethane; silicon, tetramethylsilane, phosphorous, phosphoric acid.

Coupling constants are in ppm.
Appendix D

Citation

The proper citation for *Spartan Student* is as follows:

*Spartan Student*
Wavefunction, Inc.
Irvine, CA

Appendix E

Accessing ChemDraw
(Windows Only)*

The ChemDraw program may be seamlessly accessed inside of Spartan Student** allowing chemical drawings to be produced in a familiar environment and then brought over as 3D structures***. The conversion is unambiguous as long as all stereochemical cues are in place in the 2D drawing. Note that the conformation implied by the 2D drawing may be ambiguous and need to be altered.

You need to check the box next to ChemDraw Interface in the Settings Preferences dialog under the Options menu (Chapter 10). This will add a ChemDraw button, tab or menu entry to the 3D builder.

To access ChemDraw, select ChemDraw from the buttons or menu at the top of the model kit, and click on Edit at the bottom of the panel that results. ChemDraw will appear. To return to Spartan Student, close ChemDraw. The 2D drawing will appear at the center of the panel and manipulatable 3D structure will appear at the top of the panel. Clicking on screen will move the 3D structure into Spartan Student’s main window.

* ChemDraw files (.cdx) may be read with all versions of Spartan.
** ChemDraw is not provided with Spartan but must be obtained from CambridgeSoft at http://www.cambridgesoft.com.
***Transfer is one directional only. 3D structures that have been altered may not be transferred back to ChemDraw.