MacSpartan Guide

Notes:

- A hardware key must be plugged into the keyboard for the program to load. This device is often found between the mouse and the keyboard.
- The version of MacSpartan that the Chemistry Department owns only models organic molecules.
- Page 7 of the manual shows the mouse commands that allow one to move the molecule in different ways.
- The MacSpartan manual provides quite a bit of background information on modeling, selecting different models, and graphing strategies (Sections 12-15).

Building Molecules

- If starting a new molecule, go to **New** under the **File** menu. This will bring you into the Builder Module where you can build your molecule.
- If you wish to call up a molecule which has already been built, select **Open** under the **File** menu. To edit this molecule, select **Edit Structure** under the **Build** menu.
- In the Builder module, most building is performed by selecting the different types of atoms (with different bonding environments), peptides, functional groups, or ring systems from the Model Kit visual menu that is usually found on the right side of the screen and either clicking on an empty portion of the screen or an empty valence (bond with no atom at the end).
    - ***Note*: The final 3-dimensional structure can greatly depend on the initial structure that you enter.**
    - Bonds or atoms can be added or deleted by using the keys below the atom/peptide/group/ring system menus.
    - Double- or triple-bonds can be formed between atoms by selecting **Make Bond** and selecting two empty valences.
    - The 3-dimensional orientation of the last bond added or selected (designated by a dashed line) can be modified by holding down the space bar and moving the mouse.
    - The menu often found on the left-hand side of the screen contains many of the commands that can be accessed under the **Edit** and **Geometry** menus.
    - If you want to change an element on a portion of the molecule that has already been built, select the atom and select **Change Element** under the **Edit** menu.
    - If valences are not filled, hydrogens are assumed.
- **Minimize** and **Save** the structure before leaving the Builder Module.

From the main MacSpartan window, the following actions can be performed under the following menu options.

File Menu

- All of the normal operations (**Open**, **Save**, **Print**, etc.) can be performed. You can also import and export different file formats. Of special interest is the **Export/Pict...** option which allows you to save graphics as .PICT files.

Edit Menu

- All of the normal operations that can be performed under the Edit menu on other Mac programs are found here.

Model Menu

- Selections under this menu allow you to show the molecule in different representations (ball and spoke, ribbon, space filling, wire, ball and wire, tube) along with hiding hydrogens and adding labels.

Geometry Menu

- Selections under this menu allow you to find the distance between atoms <bond lengths> (**Distance**), bond angles (**Angles**), and dihedrals (**Dihedral**). These options can also be selected on the graphical menu bar.

Build Menu

- Besides allowing you to go into the Builder Module, you can change the isotope of certain atoms in a structure.

Setup Menu

- Under **Calculations** you set up calculations of single-point energy, 3-dimensional geometry, transition state, and/or IR frequencies. The type of calculation is selected under **Task**. As you go down the **Task** menu, the calculation time increases. Under the **Level** menu, the type of calculation to be performed and the type of force field or basis set is selected (**SYBYL**: molecular mechanics; **AM1** or **AM1-SM2**: semi-empirical; **3-21G(*)** or **6-31G(*):** ab initio). Several other parameters can be selected. When the set up is completed, select SAVE.
    - Only single-point energy and 3-dimensional geometries can be calculated with molecular mechanics calculations.
    - In general the match between calculated values and experimental values increase as you go from molecular mechanics -> semi-empirical -> ab initio calculations. The time that it takes for the calculations to finish greatly increase in the same order.
- Under **Surfaces** you set up calculations of different types of surfaces and properties. You can select a number of different types of (iso)surfaces (**DENSITY, DENSITY (BOND), HOMO-, HOMO, LUMO, LUMO+, SOMO, SPIN, ELPOT**). The same options are available for properties that can be mapped on **DENSITY** and **DENSITY (BOND)** surfaces**.** For some of the **Surface** options you can select a value that determines which isosurface is plotted. When you finish selecting the combination of options that you wish, select the **ADD** button. You can select more than one combination of **Surface/Property** to calculate at a time.
- After you are finished setting up your **Calculations** and/or **Surfaces**, select **Submit**.

Display Menu

- Selecting **Output** provides a text file that provides information on the calculation.
- Selecting **Vibrations** brings up a window when a vibration calculation has been performed. From the vibration window, selecting a vibration value and checking **Display Vibration** will visually show where this vibration occurs on the molecule.
- Selecting **Surfaces** brings up a window that allows one to select which **Surface (and Properties)** you wish to view.

- Selecting **Properties** can be used to obtain values for a number of different properties. If a surface has been selected for which a property has been selected, the surfaces selection brings up a window that allows you to point to a place on the surface and obtain a value.

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