Instructions for Using the Spartan Molecular Modeling Program

The Spartan molecular modeling program allows you to build models of molecules and polyatomic ions, and to predict their geometric structures as well as a number of other properties, such as bond angles, bond lengths, and bond energies. To obtain meaningful results you need to know the connectivity of the atoms in the compound, the number of lone pairs, and the overall charge. If you give Spartan a flawed structure—a carbon with five bonds, for example—it will comply gladly and calculate the best geometry. It is incumbent upon you, therefore, to consider carefully the structure you enter into Spartan.

1. Restart your computer—the program is a bit buggy if it does not get a fresh crack at the memory—and launch the program from the dock at the bottom of the screen.
2. To build a molecule or ion, select **File: New Build** from the menu bar. Select the Inorganic Model Kit by clicking on the **Inorganic** tab in the **Model Kit** window.
3. Click on the pop-up menu below the default tetrahedral carbon; this brings up a periodic table from which you can choose the atom you wish to add. Next, choose the correct bonding geometry from the boxes below the atom you selected. Click in the main window and Spartan will add the atom to the window. To add additional atoms to the structure, select a new atom type and bonding geometry, and click on an open valence (the yellow sticks) on an atom already placed in the main window. After drawing the basic structure, you can change a single bond into a double bond with the double bond tool. To view the structure from different perspectives, click in the window and drag the mouse.
4. Spartan interprets an open valence—a stick without an atom at the end—as needing a hydrogen atom. Before you do a calculation you must delete any open valences using the **eraser** tool, which is found at the bottom of the **Model Kit** window. You can also use this tool to delete any atoms or bonds added in error. You can also access the eraser tool from the main menu using **Build: Delete**.
5. At this point you should save your file. Choose **File: Save as** from the main menu. Navigate to where you want to save the file and choose **Save** in the lower right hand corner.
6. To optimize the geometry and calculate the lowest energy configuration, you first must minimize the structure using the **energy minimization** tool found at the bottom of the **Model Kit** window. Energy minimization uses an idealized VSEPR structure and a database of known bond distances to create a starting point for subsequent calculations. You can also access this tool from the main menu using **Build: Minimize**.
7. To improve your structure further you need to complete a more detailed calculation. Spartan contains many computational algorithms for doing this, but, for consistency, we will use just one of these methods. To set-up a calculation:
    a. Select **Set Up: Calculations** from the main menu.
    b. In the **Calculate:** section choose **Equilibrium Geometry** in the top menu, select **Semi-Empirical** from the **with** menu, and select **PM3** for the type of calculation.
    c. In the **Compute** section be sure that nothing is selected.
    d. On the far right select the correct **Total Charge** for your molecule or ion.
    e. Leave the **Unpaired Electrons** as zero unless otherwise instructed.

f. In the section labeled **Print** check **Orbitals & Energies** as well as **Charges & Bond Orders**; these will give you additional information for comparing relative energies of structures and charges per atom.

g. Finally, make sure the **Global Calculations** box is checked.

h. Click **OK**. Now you are ready to actually do the calculation.

8. Select **Setup: Submit** from the main menu (you can also do this from the bottom of the dialog box under Calculations). The program will use pop up messages to let you know that the calculation is running and when the calculation is finished. If you do not get a message saying **Job "filename" has completed**, then something is wrong and your calculation was NOT completed and you will need to rebuild and resubmit the structure.

9. There are many things you can do with the results, including:

   a. Using the atom distance (**Geometry: Measure Distance**) and bond angle (**Geometry: Measure Angle**) tools to find structural information.

   b. Displaying selected properties of the molecule (such as its energy) by selecting **Display: Properties** from the main menu (Other information is available in the properties box if you click on individual atoms or bonds first.).

   c. Displaying the electrical charges or atom labels by selecting what you would like to display using **Model: Configure** from the main menu.

10. If you have multiple molecules or ions in a particular exercise, you can start a new one in the same file by selecting **File: New Molecule** from the main menu.

11. If you have too many molecules open on the page at the same time, select a molecule and close it until you see only the molecule you want on the screen.