Instructions for Using Spartan

Spartan molecular modeling program allows you to build models of molecules and polyatomic ions, and to predict their bond angles, bond lengths, and energies. To obtain meaningful results you need to know the connectivity and geometry 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 even if the result is meaningless. It is incumbent upon you, therefore, to consider carefully the structure you enter into Spartan.

1. Restart your computer—Spartan can be 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. Double-click in the main window and Spartan will add the atom to your workspace. The "sticks" attached to the atom called open valences, which are locations where Spartan expects to find an atom. To add additional atoms, select a new atom type and bonding geometry, and double-click on an open valence of an atom already placed in the main window. After drawing the basic structure, you can change a single bond into a double bond or triple bond by selecting the appropriate bond tool and double-clicking on the bond you wish to change. To view the structure from a different perspective, 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 all 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 that you added in error. You can also access the eraser tool from the main menu using Build: Delete.
5. 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 any subsequent calculations. You can also access this tool from the main menu using Build: Minimize.
6. To improve your structure further you need to complete a more detailed calculation. Spartan contains many computational algorithms for doing this, so be sure you select the correct method for the exercise on which you are working. 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 and the appropriate method for the exercise on which you are working.
    c. On the far right, select the correct Total Charge for your molecule or ion.
    d. Leave the Unpaired Electrons as zero unless otherwise instructed.
    e. Finally, make sure the Global Calculations box is checked.
    f. Click OK. Now you are ready to actually do the calculation.
7. 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 it 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.
8. 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.

d. Measure a molecular orbital's energy by selecting Display: Output from the main menu.

e. Examine the shape of molecular orbital by selecting Display: Surfaces from the main menu and adding in the orbital of interest.

9. You can delete a structure from your workspace by selecting File: Delete Molecule.