"Computer Lab; Jan 23 and 28"

Instruction for Spartan

Spartan 16 is a computational package that includes molecular mechanics methods, conformational searches, semiempirical methods, ab-initio Hartree-Fock, and correlated methods. Spartan is available on the PCs at the computer lab (Beury 220) and the TECH Center.

A Tutorial and User's guide for detailed information is accessed from the Help menu of Spartan. Here are some basic instructions to get you started:

The following instructions will build the **water (H_2O)** molecule, optimize its geometry, and display the results:

1- Login to your account by using your TUID and password.
2- Open Spartan by clicking on its icon on the desktop.
3- File > New Build (or click icon on upper left); at the right of the screen appears a menu that allows you to build molecules.
4- Select oxygen from panel and click anywhere in main window. It has two bonds. Now, select H atom and click on the bonds—one by one. Now you have made a water Molecule. You can repeat the procedure to make any molecule.
5- You can use the left mouse button to rotate the molecule and the right mouse button to translate it (On a Mac command+mouse for translation).
6- From the menu at the top of the page choose Setup, and then calculations. A box appears that has several options. **(a)** The first one specify the type of calculation you want to perform. The choices are: Single point energy, equilibrium geometry, transition state geometry, equilibrium conformer, conformer distribution, etc. For this example choose equilibrium geometry to perform a minimization. **(b)** The second choice is the level of theory, which can be molecular mechanics, semiempirical, Hartree-Fock, MP2 or DFT. For this example choose **Hartree-Fock**. Here, you can also choose the **basis set**. For this example choose **STO-3G**. **(c)** The other options do not need to be changed in the simple case of a neutral **closed shell (zero unpaired electrons)** molecule like water. You can also choose that you want to do calculation in Gas phase or solution. For this example choose Gas phase.
7- Check box for orbital and energy
8- Check box for charges and bond orders
9- Submit (it will ask you where to save the data, it is good to give them proper names and save them on Desktop). The calculation is running. Wait until calculation is done.
10- When the job is finished a message will appear indicating so.
11- From the menu at the top of the page choose DISPLAY.
12- Display > orbital energies
    Record approximate HOMO and LUMO energies.

13- Display > Surfaces:
   (a) Add HOMO, LUMO and Electrostatic potential map
   (b) Look at different shape of HOMO, LUMO and electrostatic potential map by clicking on boxes next to them (Do this one by one).Close this window.
14- Display > output:
   Record values for HOMO (eV), LUMO (eV), and total energy (Convert to eV from Hartree)

Let's try an O atom:

Select oxygen atom from panel and click anywhere in main window. It has two bonds. Remove the bonds by using delete tool (build > delete, or select eraser icon in the panel. You have to click it each time you want to delete an atom). Repeat all the steps (use Hartree-Fock method and STO-3G basis set); except in this case choose single point energy for the type of calculation—because it is just an atom and it does not need to be optimized (energy minimization). Repeat calculations for O atom using 3-21G and 6-31G* with these multiplicities: **Singlet** (choose 0 unpaired electrons) and **triplet** (choose 2 unpaired electrons). Remember, the oxygen's electronic configuration ($1s^2\, 2s^2\, 2p^4$). For singlet, the method treats electrons as indistinguishable (2 electrons in an orbital are not labeled). For triplet, the method labels α and β electrons to 2 electrons in an orbital (convention is to start from α as the lowest energy one)

About energies: 1 Hartree = 27.2 eV.

H$_2$O molecule:

Basis set	HOMO energy (eV)	LUMO energy (eV)	Total Energy (eV)
STO-3G			

Oxygen atom:

Basis set	Unpaired electrons	Multiplicity	HOMO energy (eV)	LUMO energy (eV)	Total Energy (eV)
STO-3G	0	singlet			
3-21G	0	singlet			
6-31G*	0	singlet			
STO-3G	2	triplet			
3-21G	2	triplet			
6-31G*	2	triplet			