Geometry optimization and calculation of MO diagram

Objectives: optimize geometry of a species, calculate its energy and MO diagram

Basic steps:

a) Draw your species (steps 1-5 below);
b) Set up a Molecular Orbital calculation (steps 6-7 below);
c) Optimize geometry / calculate energy (step 8 below);
d) Calculate (and visualize) molecular orbitals (step 9)

Detailed instructions:

Drawing a species

1) Run HyperChem program.
2) Double-click the **Draw** button (the left-most button, below **File**), the **Element table** will pop up. Choose necessary element by clicking on its symbol.
3) Draw necessary molecule in the program main window. When you click on the black window area, an atom of a selected element appears (you can change the appearance of atoms by choosing an appropriate **Rendering** option from **Display** menu). To draw a bond, point mouse cursor on the center of one of the atoms to be bound, left-click and drag the cursor to the center of another atom, then release the mouse button. To delete an atom or a bond, right-click on it center.
4) If error message appears because of exceeding regular valence, turn on **Allow arbitrary valence** in the **Edit** menu.
5) To beautify you drawing (set all bond lengths and angles to their regular values), choose **Add H & model build** from the **Build** menu;

Setting up a calculation

6) To set up an *ab initio* calculation, click **Setup** button, choose "**Ab Initio…"**. In the **Ab Initio Method** window which pops up, choose orbital **Basis Set** "**Large (6-31G****)**". Lager basis means higher precision AND slower rate of your calculation. If your species is charged and/or has a spin multiplicity greater than 1 (one or more unpaired electrons), choose "**Options …**" button in the same window. Enter appropriate value in the box **Total charge**. If spin multiplicity is greater than 1, choose **Spin Paring** "**UHF**" and then you will be able to change the multiplicity. Close the window **An ab initio and DFT options** by clicking **OK**.
7) Finally, click **Apply basis set** in the **Ab Initio Method** window and then **OK**.

Optimizing geometry / calculating energy

8) To optimize geometry of a species, choose **Compute** menu and then **Geometry optimization**. In the window **Ab Initio optimization** which will appear, click **OK**. Wait until the optimization is complete. Look at the message in the bottom of the HyperChem window; it should contain finally the word **YES**. In the beginning of this line you will find the energy of formation of your species from isolated nuclei and electrons **E=** … expressed in kcal/mol. Write down this value in your report.

Calculating molecular orbitals

9) To calculate MO's of a species, choose **Compute** menu and then **Single Point**. Wait until the calculation is complete. See the message in the bottom of the HyperChem window, it should say finally "**Energy= …**" and "**Symmetry = …**" providing you with information about the calculated energy and the symmetry of your species.
10) To get the MO diagram calculated, choose **Compute** menu and then **Orbitals**. Click on the **Orbitals** window and drag it so that the molecule in the main window will be visible.
11) Check **Labels** box so that you will see energy calculated for each of the levels in the black Pan.
12) To visualize and analyze MO's, select with your mouse a rectangular zone with orbitals of your interest. (It is worth to start from either the very bottom of the diagram or from HOMO/LUMO zone!). Click on the energy level of your interest, so that its line turns from green to red. In the grey box **Symmetry**, to the left from the Pan, see the orbital Mulliken label.
13) Click **Plot** to observe corresponding MO in the main HyperChem window.
14) Repeat steps 12-13 with other MO's of your interest.
15) If you close window **Orbitals**, the last orbital displayed in the main window will be available for such operations as "**Rotate …**", **Translate**, **Magnify/Shrink** etc.