Geometry optimization and visualization of IR and Raman active normal modes

Objectives: optimize geometry of a species, calculate its energy and normal modes, observe animation of IR and Raman active normal modes and analyze them

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 vibrations (step 9)
e) Observe and animate vibrations calculated (steps 10-11 below).
f) Fill in the table given in the text of the problem starting from the lowest energy vibration.

Detailed instructions:

Drawing a species

1) Run HyperChem Professional 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 vibrations

9) To calculate vibrations, choose "**Compute**" menu and then "**Vibrations**". The calculation will be over, when all menu buttons but "**Cancel**" will be in a black font.
10) To analyze and animate vibrations, choose "**Compute**" menu and then "**Vibrational spectrum**". In the window which appears check the "**Animate vibrations**" box. Then choose one of the green lines in the black window. The lines correspond to normal modes found. Read related information (Degeneracy, frequency, symmetry) in the bottom part of the window.
11) Click "**OK**" to animate the vibration selected. Figure out if it is a stretching or bending mode. Repeat with other normal modes calculated.