● Goals of this Exercise

Optimization of the H_2O molecule using B3LYP/6-31G* method.

Then we will measure the distances between the atoms and the HOH angle.

On the basis of the geometry optimized using B3LYP calculation, we will compute and draw the IR spectrum.

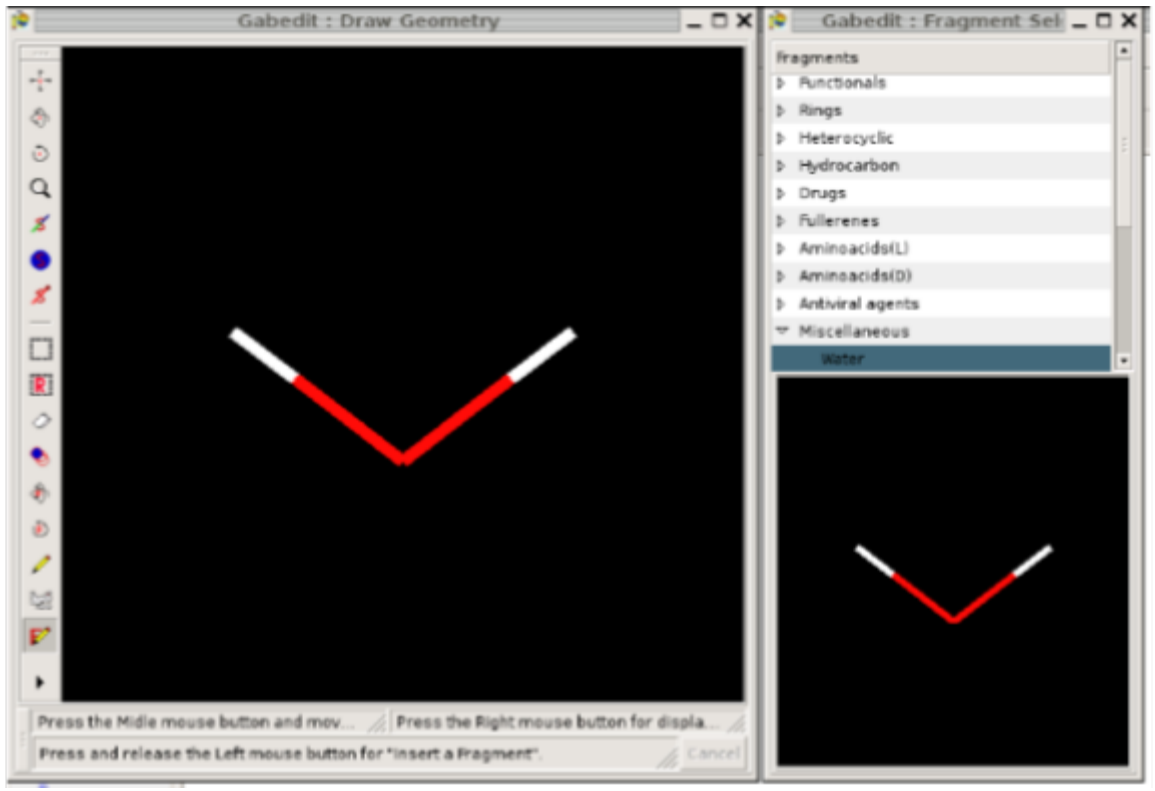
Then we will visualize the HOMO orbital, the laplacian of the electronic density

• Detailed Instructions

Building of the Molecule

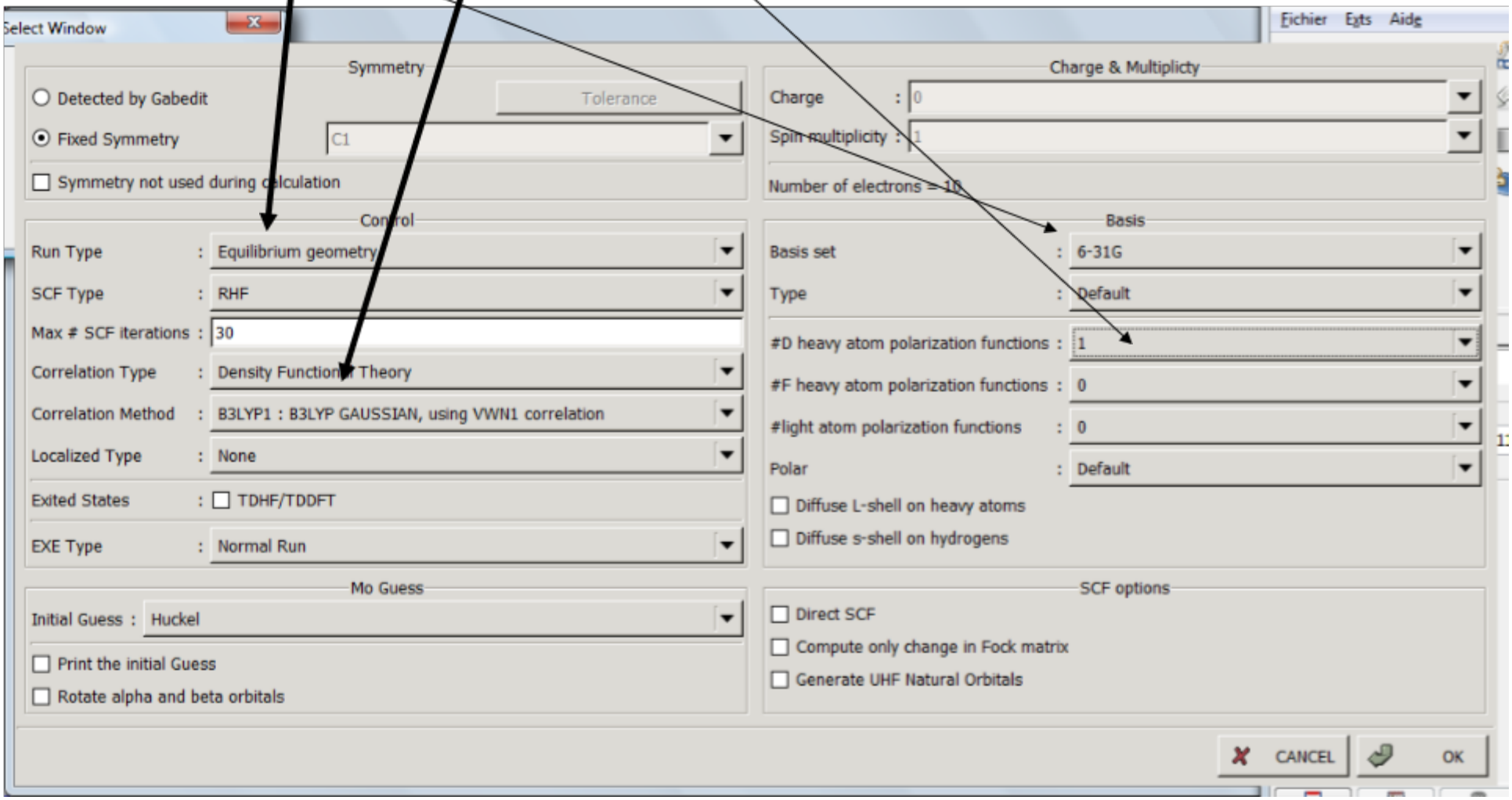
Click on Draw/Display Geometry icon

On Drawing Area click with right button of mouse and select Add/Fragment. Select Water molecule, and click to Drawing Area. You have successfully built the desired structure :



Optimizing the Molecule using B3LYP method

1) Close Geometry Windows.
2) Choose File/New PC Gamess input (or PC Gamess icon) from the principal Menu.
3) Select Equilibrium Geometry for Run Type.
4) Density functional theory for correlation type
5) Select 6-31G for basis and 1 for #D heavy..
6) Click OK button.

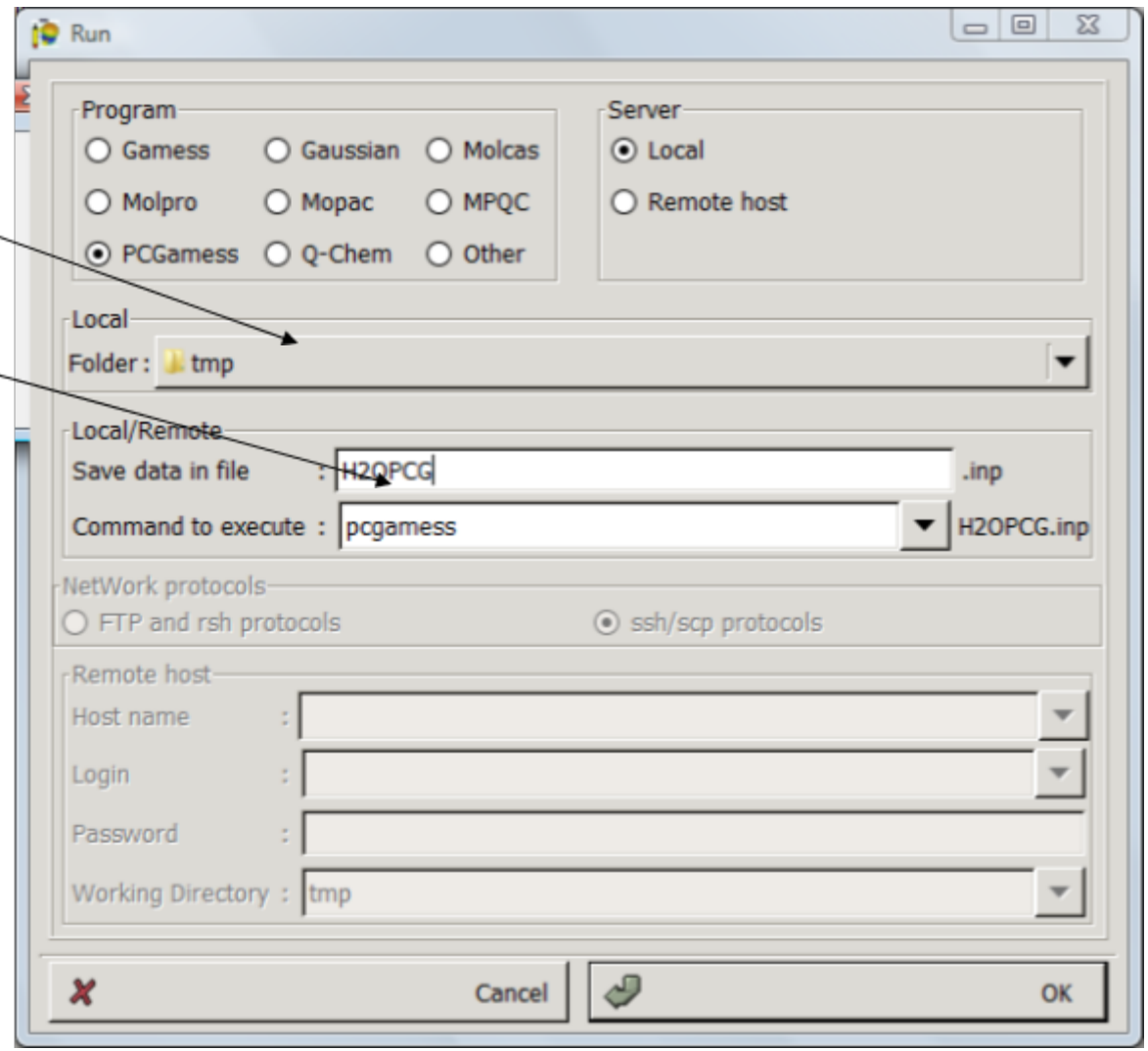


Optimizing the Molecule using B3LYP method

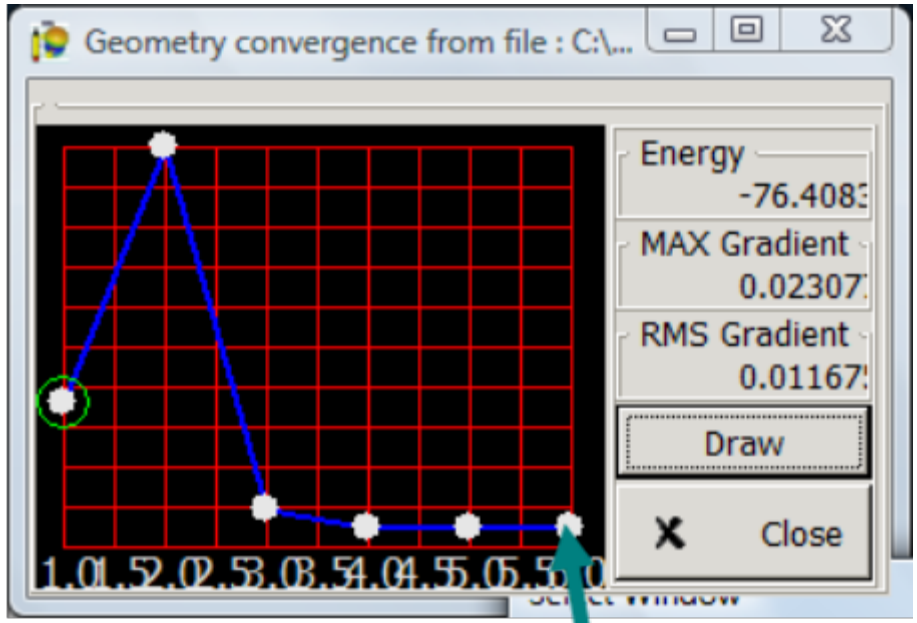
7) Click to Run icon (toolbar, top of window).

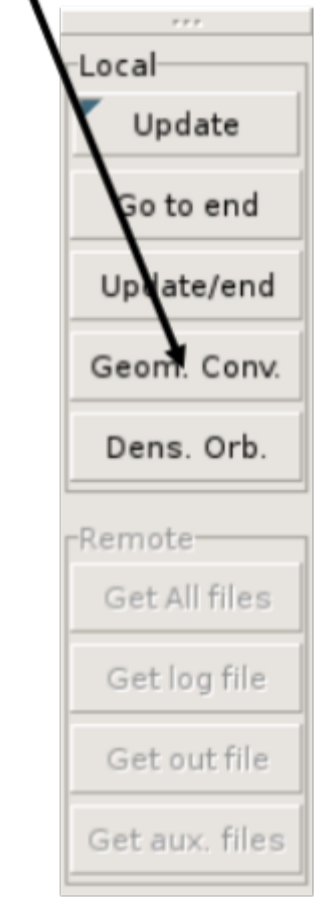
8) Select your folder

9) At save data file in text zone , type H2OPCG



10) Click to OK button.
11) PCGamess is now started at background job.
12) Select H2OPCG.log notebook.
13) Click to Update/End for reload the output file of PCGamess.
14) When the job completes (and this may take several minutes) : click to Geom. Conv.
15) click to Draw

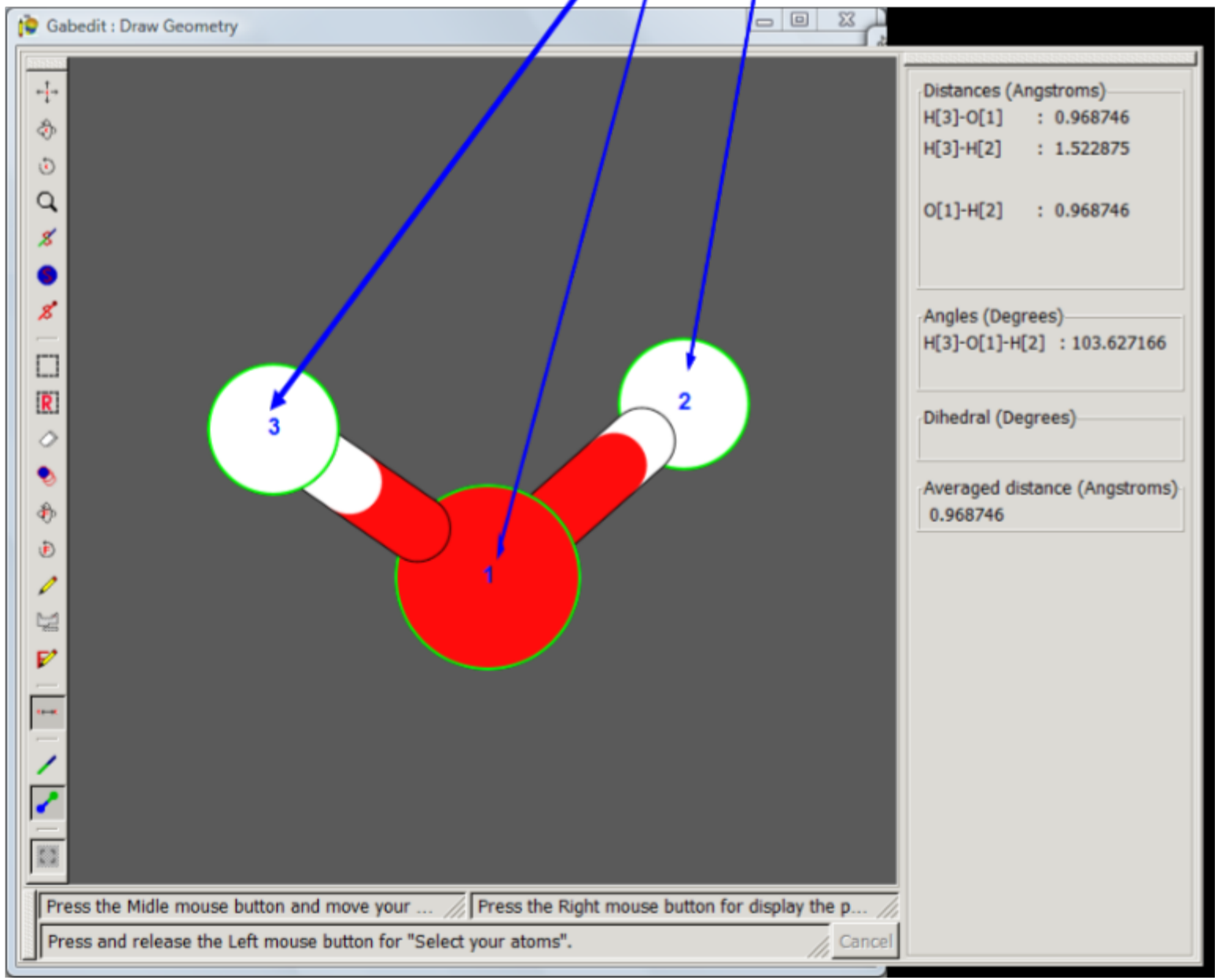




16) Discover various optimized values for this structure by selection of various value. Select the last value.

17) On Drawing Area of Geometry/Display window click with right button of mouse and select Label/Numbers.

18) Click to Mesure icon and select the H, O and H atoms respectively.



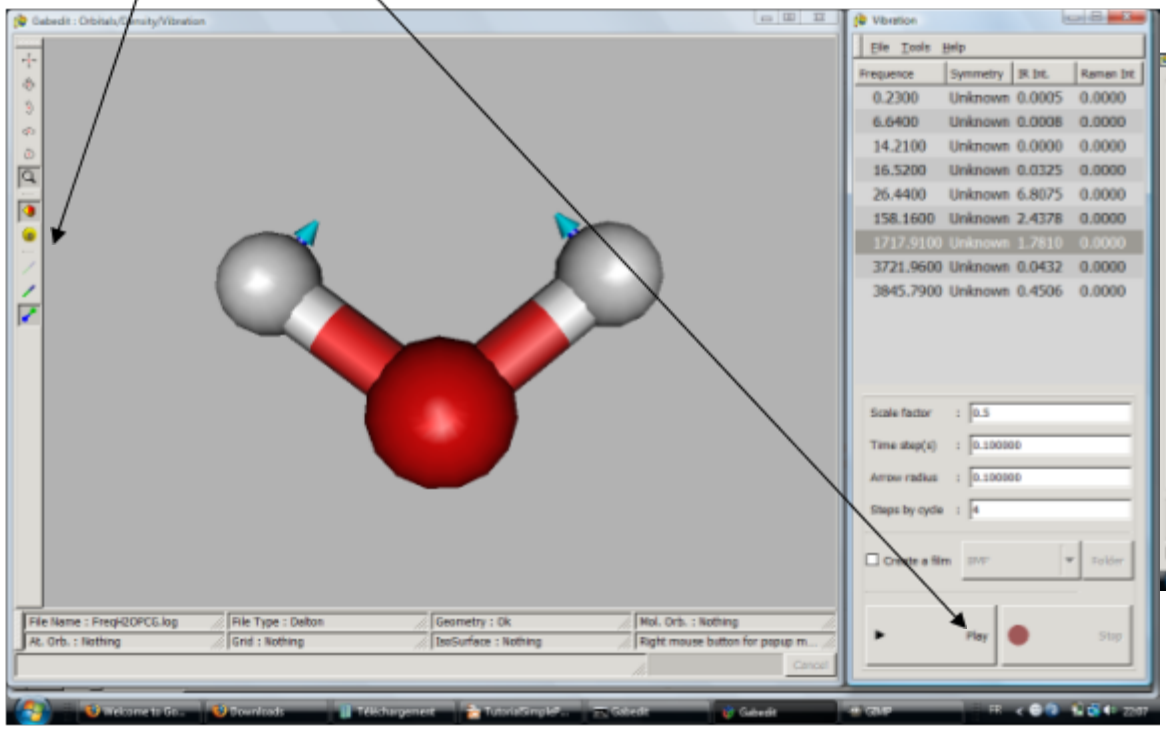
Compute and draw the IR spectrum of H2O molecule

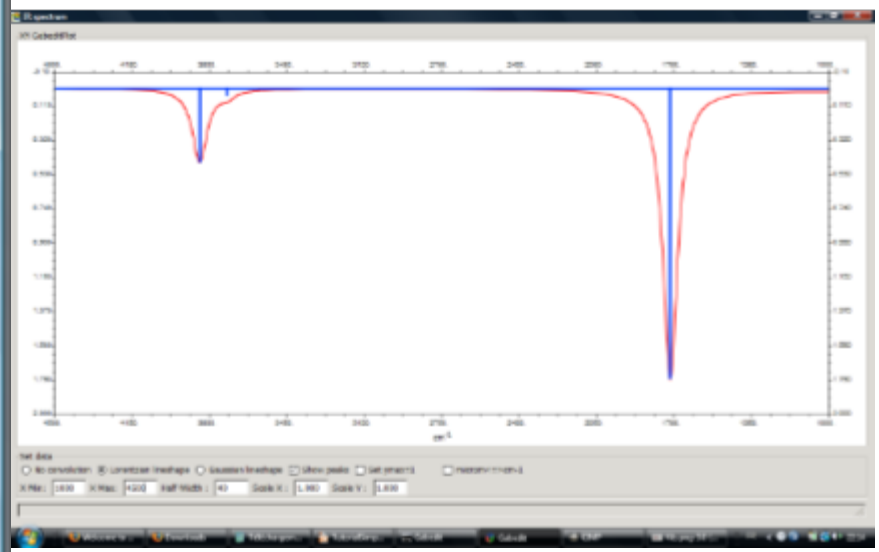
Close Geometry Windows.
Choose File/New PCGamess input (or PCGamess icon) from the principal Menu.
Select “Frequencies” for Run Type
Select « Density functional theory » for correlation type
Select 6-31G for basis and 1 for #D heavy..
Click to OK button.
Click to Run icon (toolbar, top of window).
At save data file in text zone , type FreqH2OPCG
Click to OK button.

PCGamess is now started at background job.
Select FreqH2OPCG.log notebook.
Click to Update/End for reload the output file of PCGamess.
When the job completes (and this may take several minutes) : click to “Dens. Orb.” button

Compute and draw the IR spectrum of H2O molecule

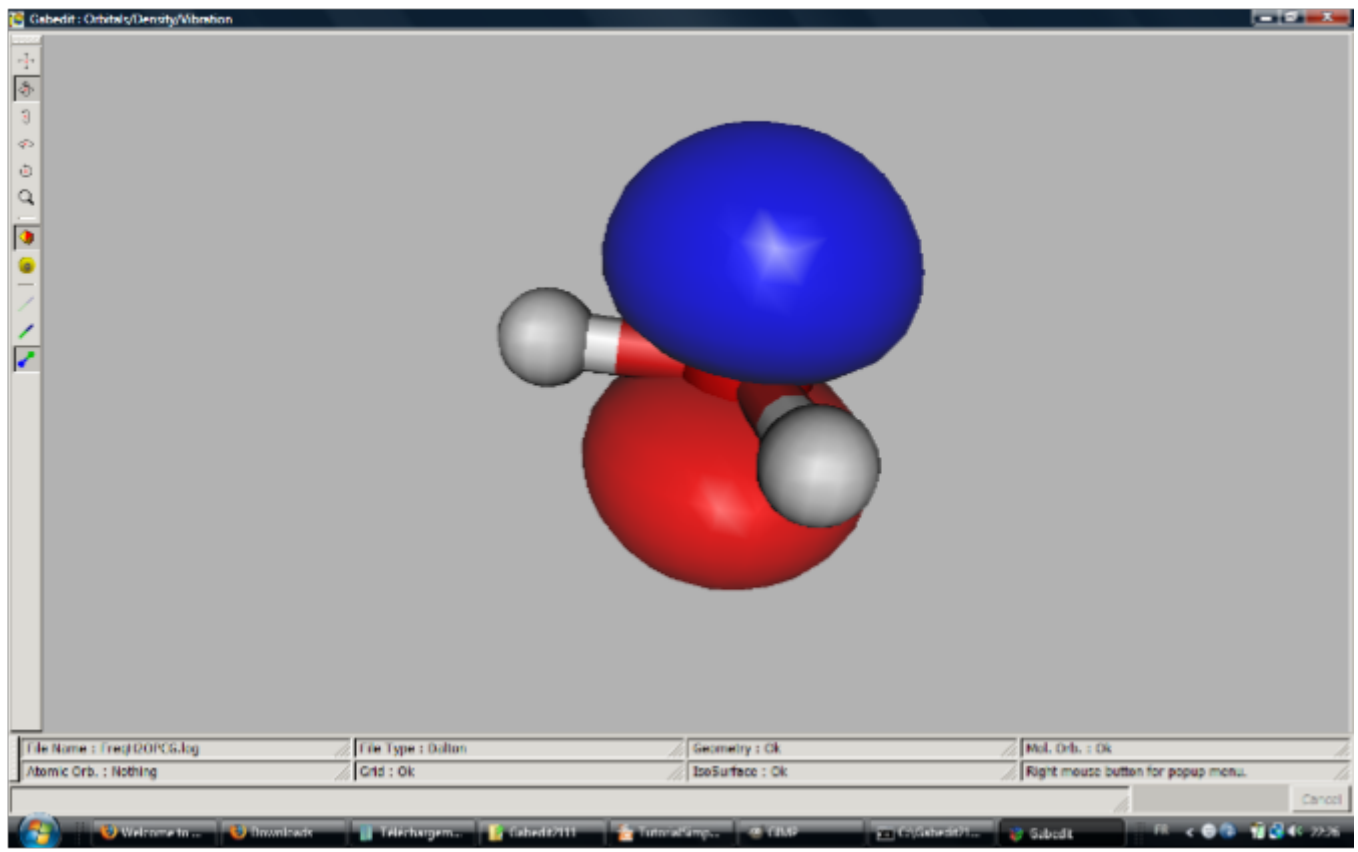
On Drawing Area of Geometry/Display window click with right button of mouse and select Animation/Vibration.
From the menu of the new window, select Read/PCGamess file and select FreqH2OPCG.log file
Click to “O” button (toolbar at the left of the Drawing window)
Click to Play (or Stop) for animate the vibration of your molecule.
From the menu of the new window, select Tools/draw IR spectrum.





Viewing of the HOMO Orbital and the electronic density

Close “**IR Spectrum**” and “Vibration” window
On Drawing Area of Geometry/Display window click with right button of mouse and select “” **Orbitals/Read PCGamess file**” and select FreqH2OPCG.log file
Click to Ok Button. (the HOMO Orbital is selected)
Set iso value to 0.1 and click to OK.
Click to “O” button
You can easily change the display type by selecting the type of rendering :
Render/Geometry and/Or Render/Surface



On Drawing Area of Display/Geometry window click with right button of mouse and select Surfaces/Delete all.
On Drawing Area of Display/Geometry window click with right button of mouse and select Density/Electronic.
Set xmin to -4 and Number of points to 65
Click to OK button
Click to cancel button on the isovalue window
With right button , select Cube/Laplacian
Choose 0 for the isovalue

For create a BMP image file, click with right button of mouse and select Screen Capture/BMP.