

● Goals of this Exercise

Optimization of the H₂O 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

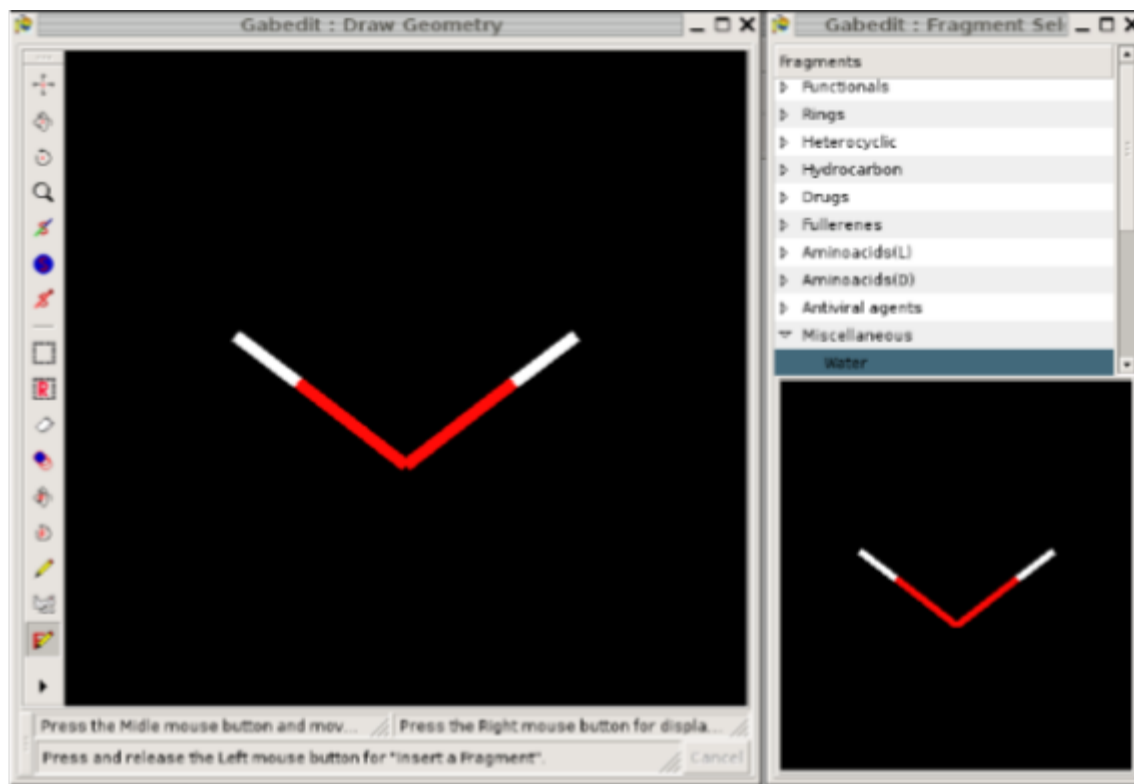
● Detailed Instructions

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.

The screenshot shows the 'Select Window' dialog box with the following settings:

- Symmetry:** ☐ Detected by Gabedit, ☒ Fixed Symmetry (C1), ☐ Symmetry not used during calculation.
- Control:** Run Type: Equilibrium geometry, SCF Type: RHF, Max # SCF iterations: 30, Correlation Type: Density Functional Theory, Correlation Method: B3LYP1 : B3LYP GAUSSIAN, using VWN1 correlation, Localized Type: None, Exited States: ☐ TDHF/TDDFT, EXE Type: Normal Run.
- Charge & Multiplicity:** Charge: 0, Spin multiplicity: 1, Number of electrons: 10.
- Basis:** Basis set: 6-31G, Type: Default, #D heavy atom polarization functions: 1, #F heavy atom polarization functions: 0, #light atom polarization functions: 0, Polar: Default, ☐ Diffuse L-shell on heavy atoms, ☐ Diffuse s-shell on hydrogens.
- Mo Guess:** Initial Guess: Huckel, ☐ Print the initial Guess, ☐ Rotate alpha and beta orbitals.
- SCF options:** ☐ Direct SCF, ☐ Compute only change in Fock matrix, ☐ Generate UHF Natural Orbitals.

Buttons: CANCEL, OK.

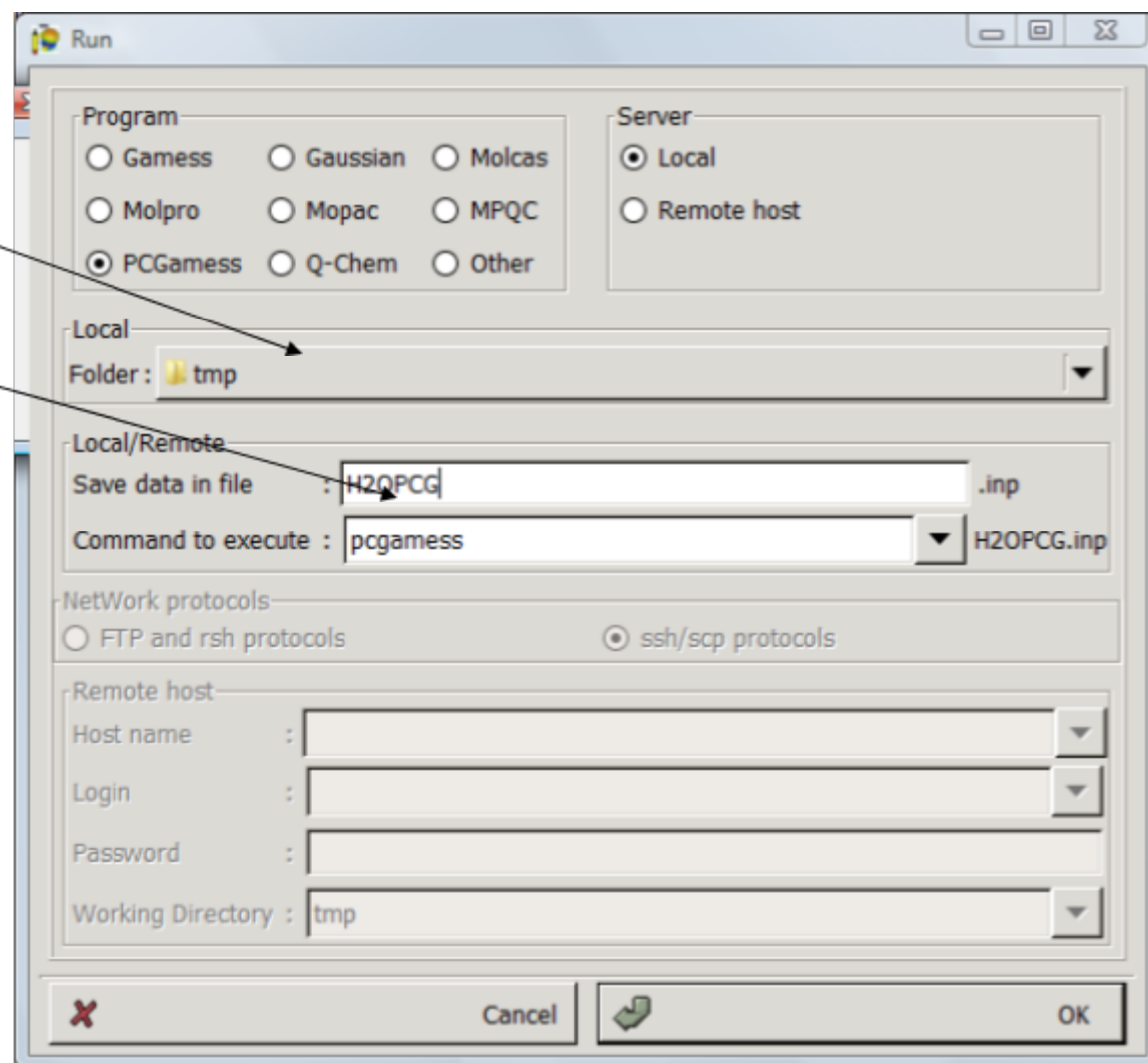
Optimizing the Molecule using B3LYP method

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

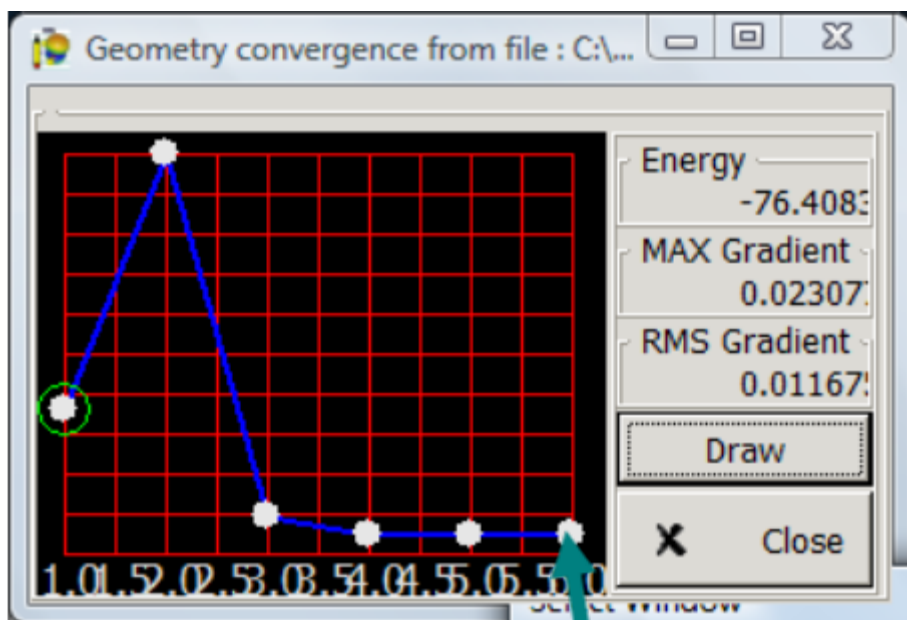


8) Select your folder

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



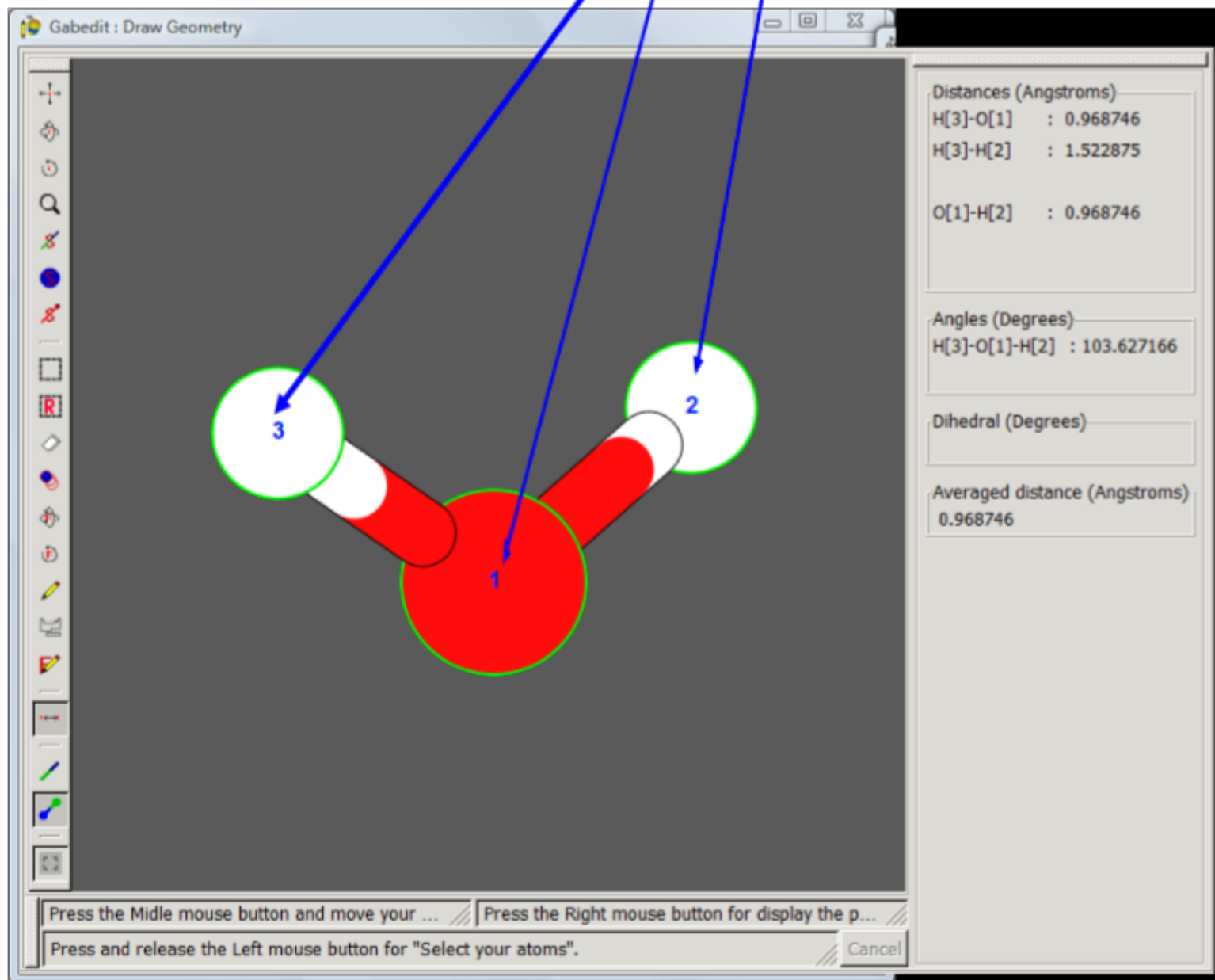
- 10) Click to OK button.
- 11) PCGmess is now started at background job.
- 12) Select H2OPCG.log notebook.
- 13) Click to Update/End for reload the output file of PCGmess.
- 14) When the job completes (and this may take several minutes) : click to Geom. Conv.
- 15) click to Draw



- 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 Measure 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

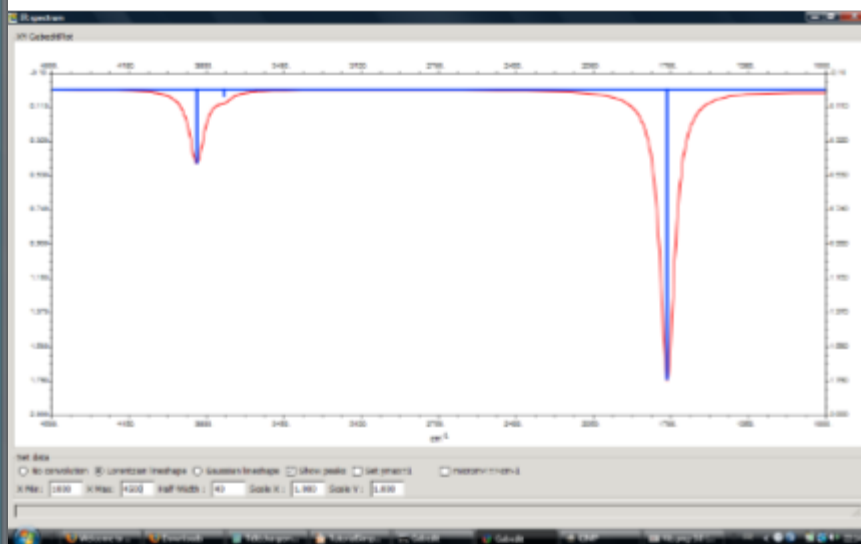
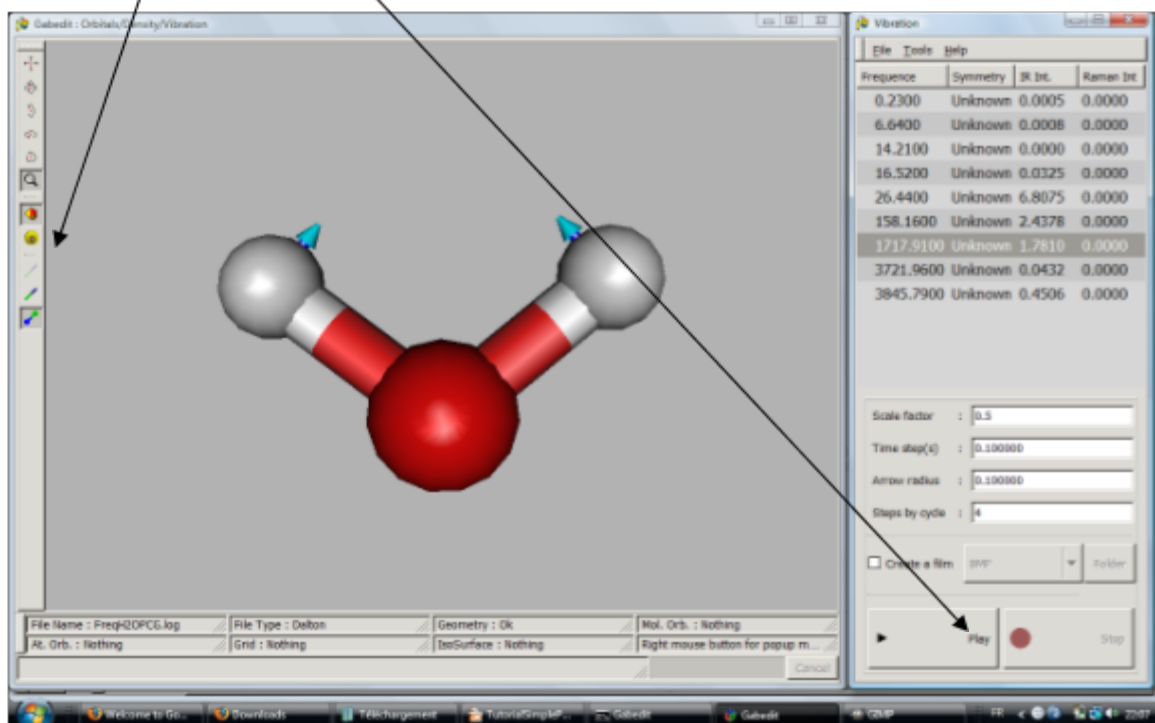
On Drawing Area of Geometry/Display window click with right button of mouse and select Animation/Vibration.

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

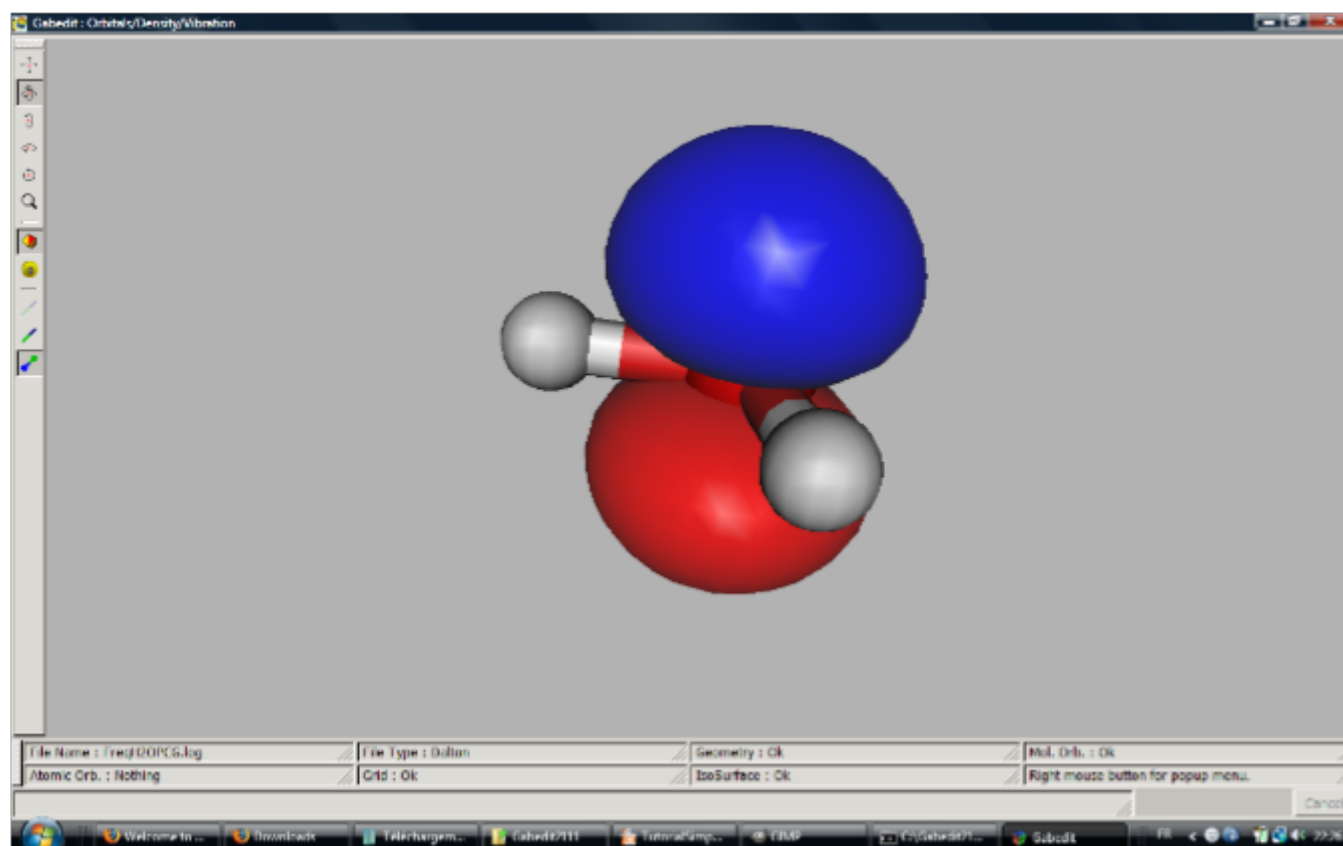
Click to Ok Button. (the HOMO Orbital is selected)

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.

