Goals of this Exercise

the Goals of this exercise are as follows:

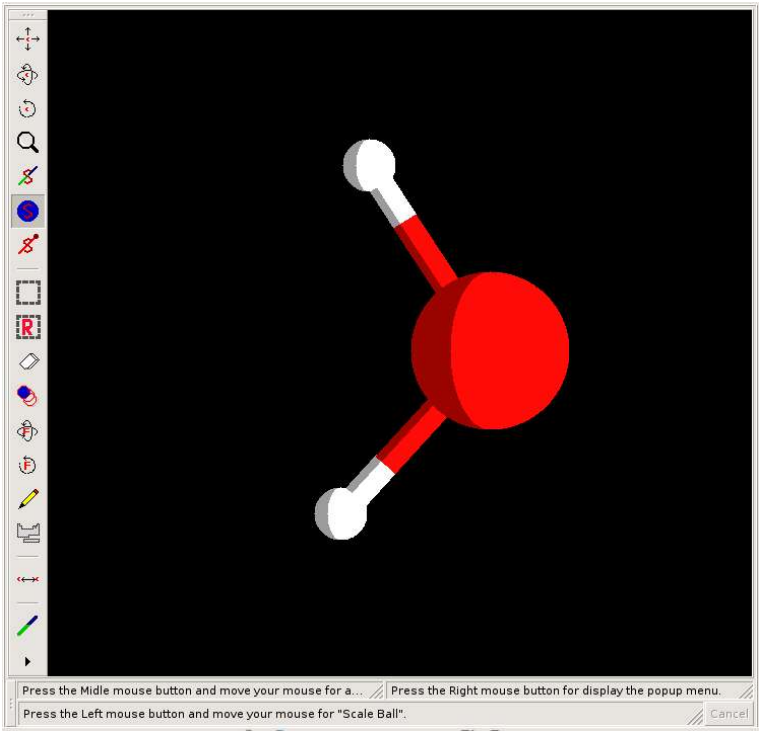
- Optimization of the H_2O molecule by a Hatree Fock calculation using the 6-31G basis.
- Then we will measure the distances between the atoms and the HOH angle.
- On the basis of the geometry optimized by a Hatree Fock calculation, we will optimize the geometry by a B3LYP calculation.
- Then we will measure the distances between the atoms and the HOH angle.
- Then we will visualize the HOMO orbital, the electronic density and the HOMO orbital colorcoded with electronic density.

Detailed Instructions

Building of the Molecule

1. Click on Draw/Display Geometry icon.

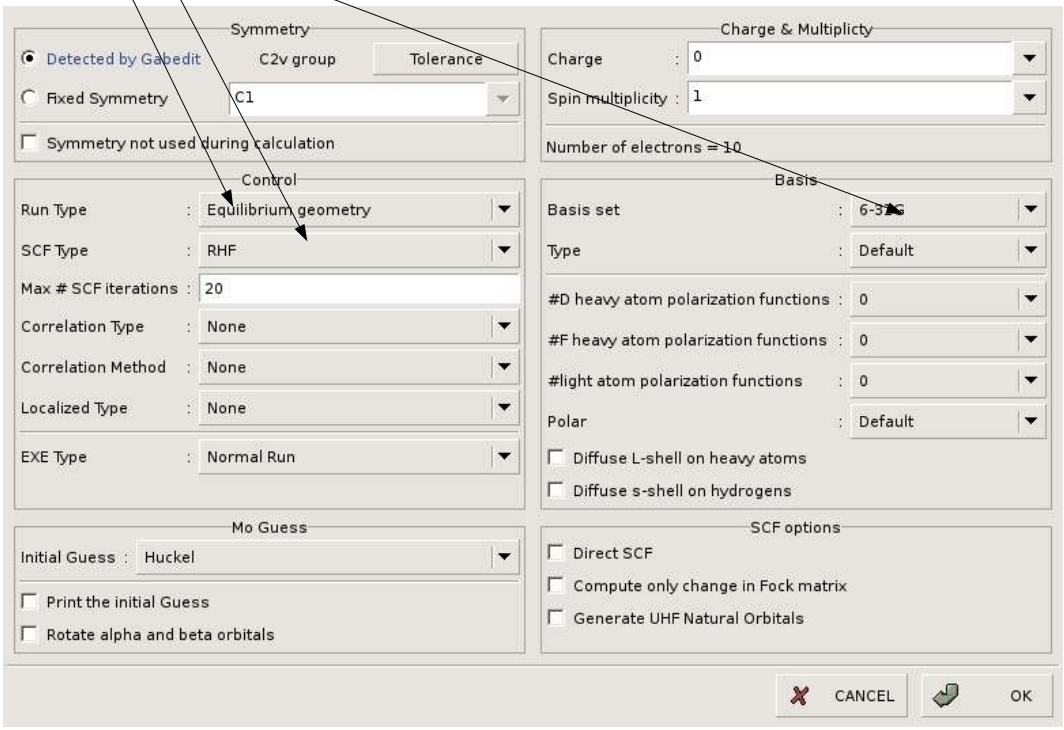
2. On Drawing Area click with right button of mouse and select Add/miscellaneous/Water, and click to Drawing Area. You have successfully built the desired structure :



Optimizing the Molecule by a HF Calculation

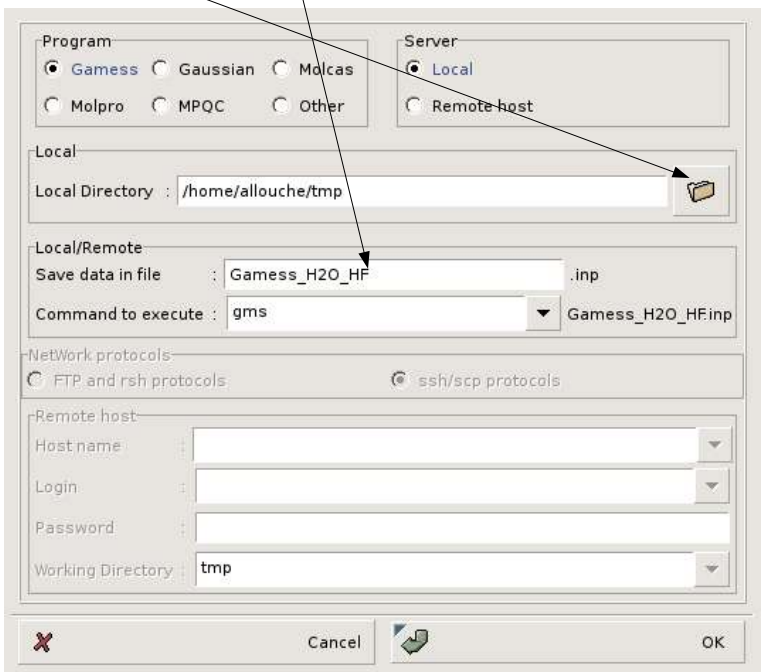
1. Close Geometry Windows.
2. Choose File/New Gamess input (or Gamess icon) from the principal Menu.

3. Select Equilibrium geometry for Run Type
4. Select RHF Method
5. Select 6-31G Basis.
6. Click OK button.



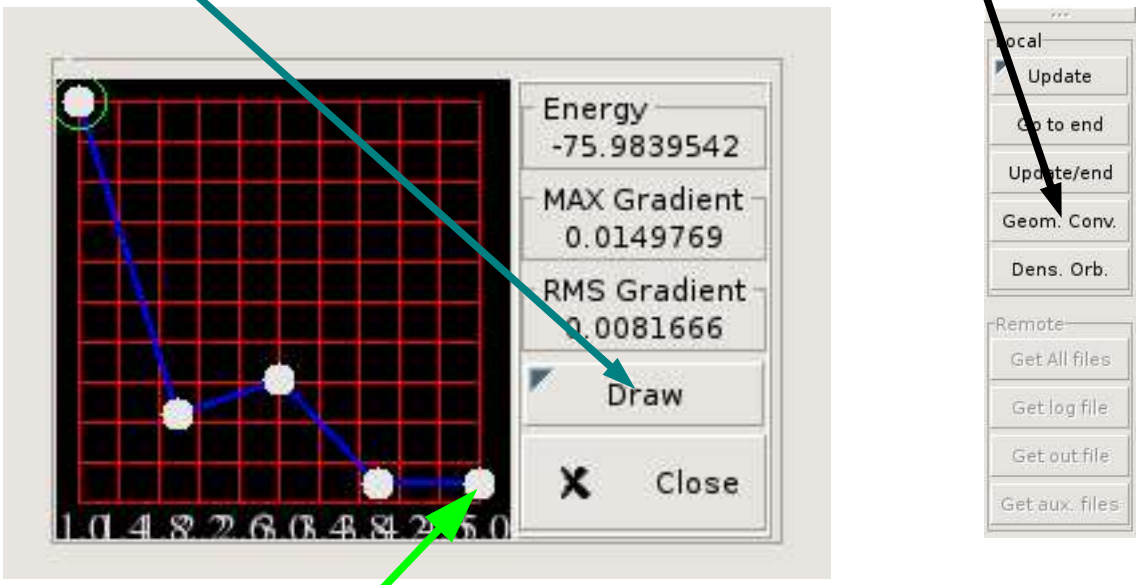
7. Click to Run icon (toolbar, top of window).

8. Select your folder
9. At save data file in text zone , type Gamess_H2O_HF

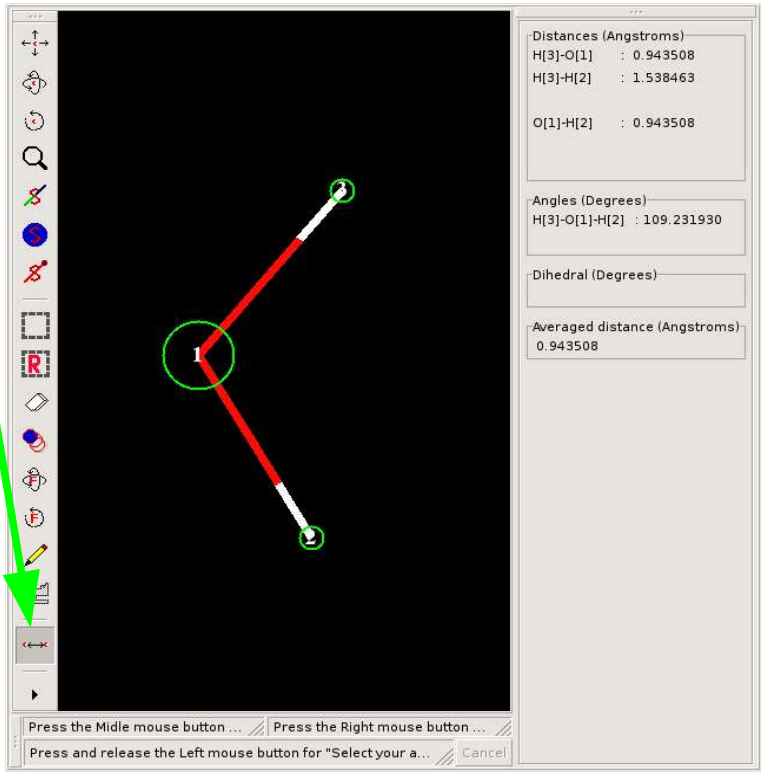


10. Click to OK button.
11. Gamess-US is now started at background job.

12.Select Gamess_H2O_HF.log notebook.
13.Click to Update/End for reload the output file of Gaussian.
14.When the job completes (and this may take several minutes) : click to Geom. Conv.
15.click to Draw



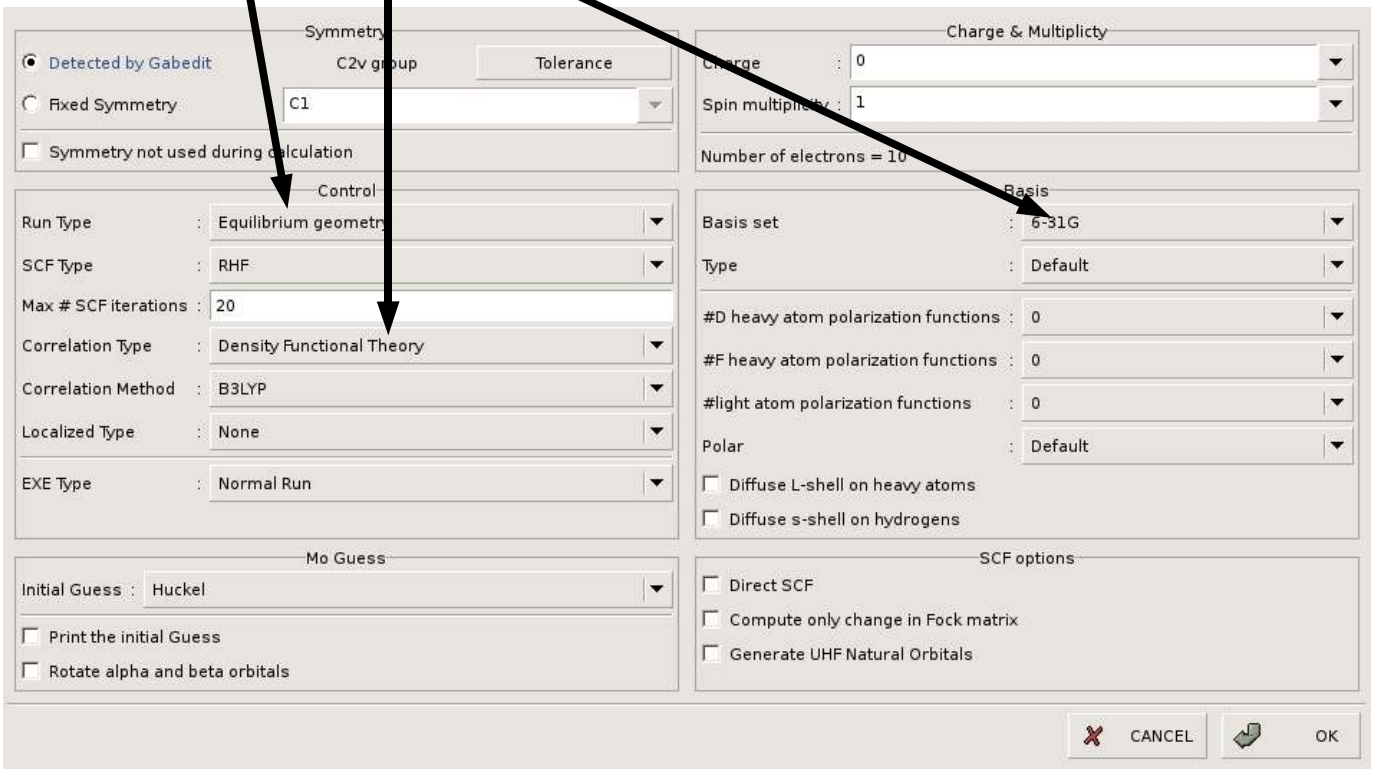
16. Discover various optimized values for this structure by selection of various value.
    Select the last value.
17. On Drawing Area of Geometry/Display window click with right button of mouse and select
    Label/Numbers.
18.Click to Mesure icon and select the H, O and H atoms respectively.



Optimizing the Molecule by a B3LYP Calculation

1. Close Geometry Windows.
2. Choose File/New Gamess input (or Gamess icon) from the principal Menu.

3. Select Select Equilibrium geometry for Run Type
4. Select Density Functional Theory for correlation type.
5. Select 6-31G at Basis Frame.
6. Click to OK button.



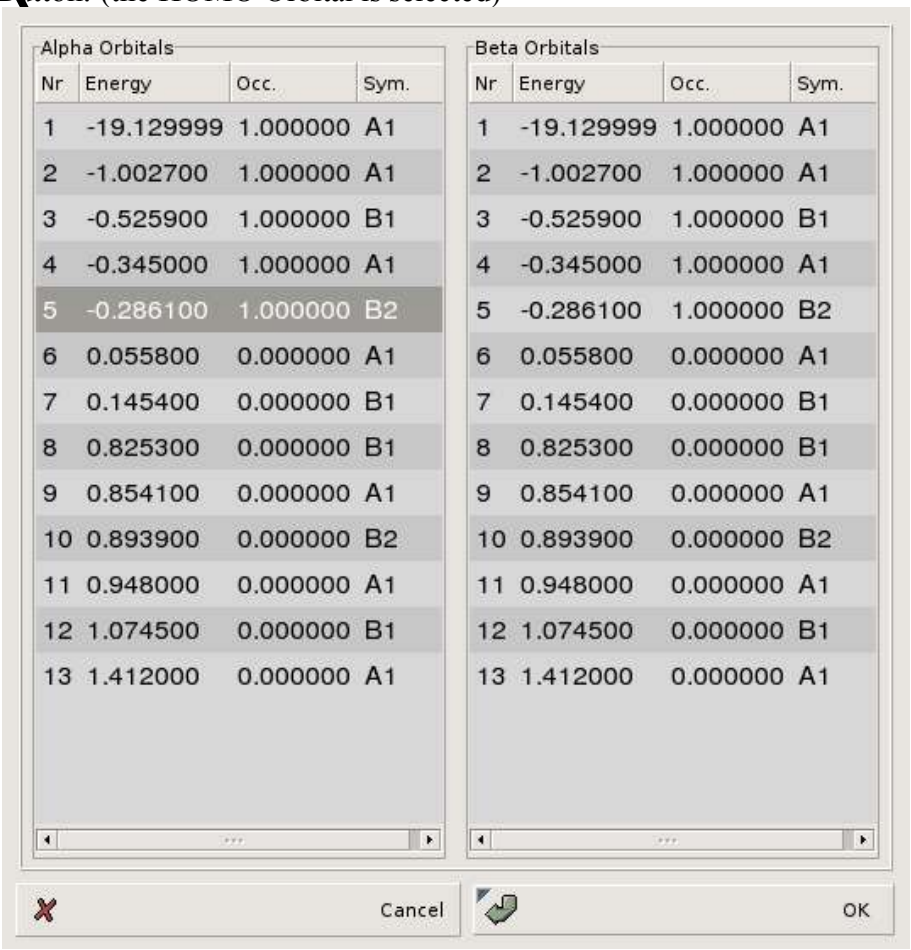
7. Click to Run icon (toolbar, top of window).

8. At save data file in text zone , type Gamess_H2O_B3LYP
9. Click to OK button.
10. Gamess-US is now started at background job.
11. Select Gamess_H2O_B3LYP.log notebook.
12. Click to Update/End for reload the output fileof Gamess.
13. When the job completes (and this may take several minutes) : click to Geom. Conv.
14. click to Draw
15. Discover various optimized values for this structure by selection of various value. Select the last value.

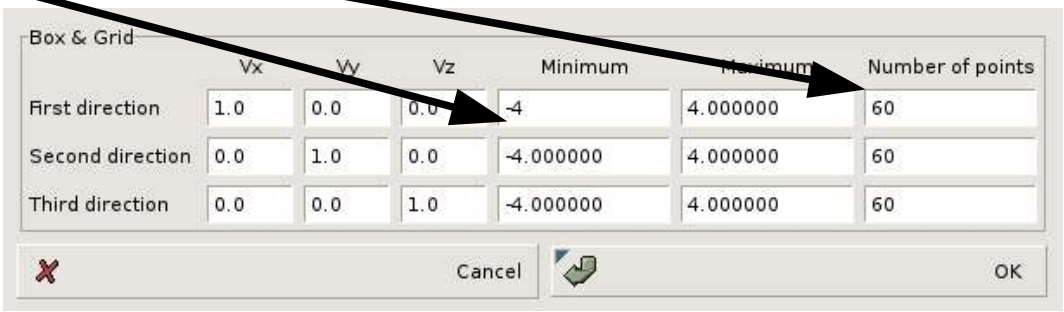
Viewing of the HOMO Orbital and the electronic density

1. Close Geometry Windows.
2. Click to Density/Orbital icon.

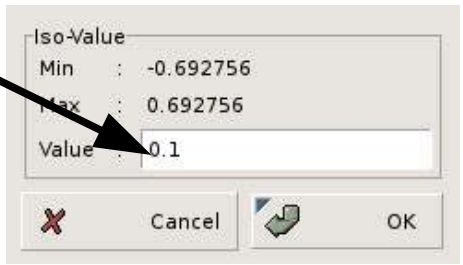
3. Click to Ok Button. (the HOMO Orbital is selected)



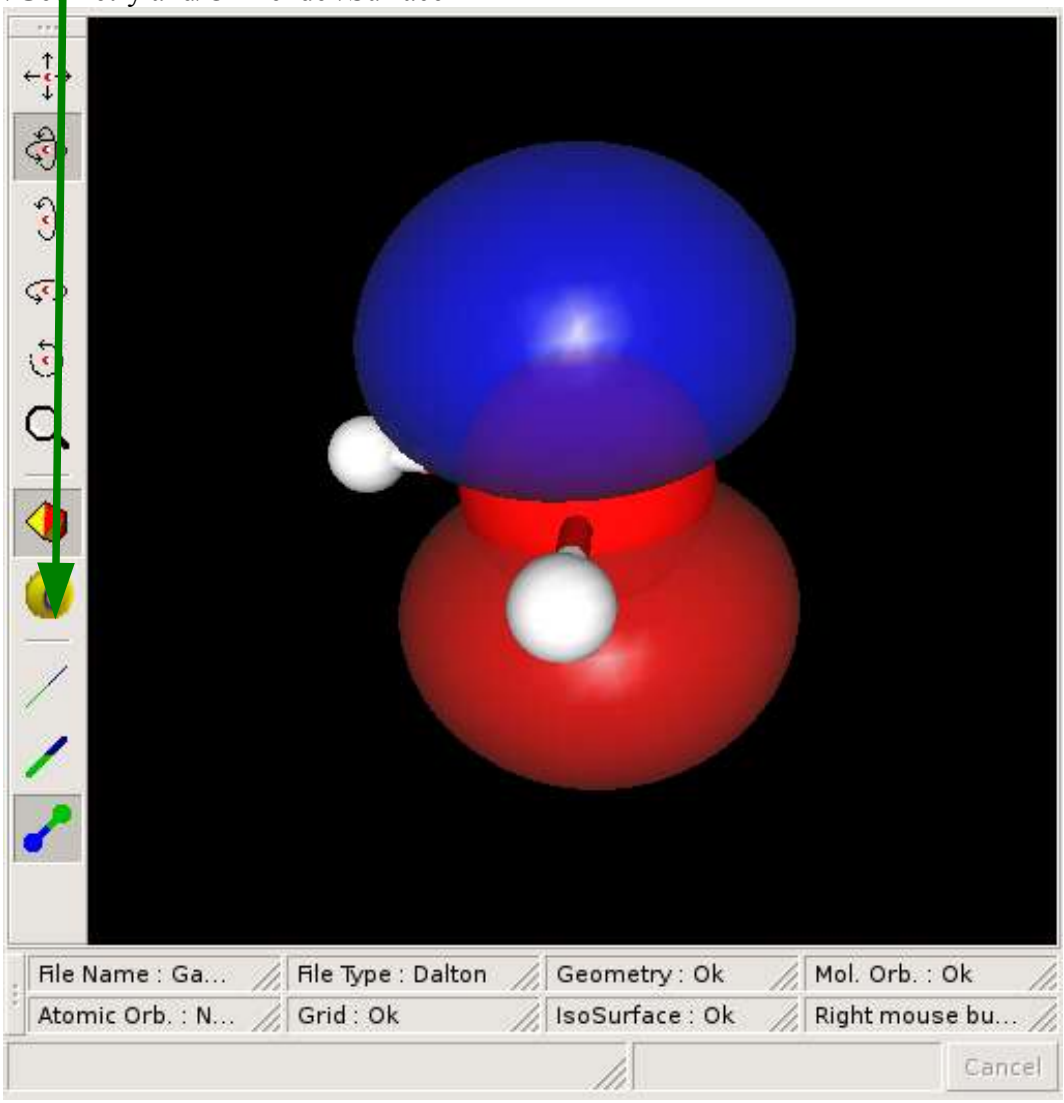
4. Set X Min to -4 and Nx to 60 and click to OK button



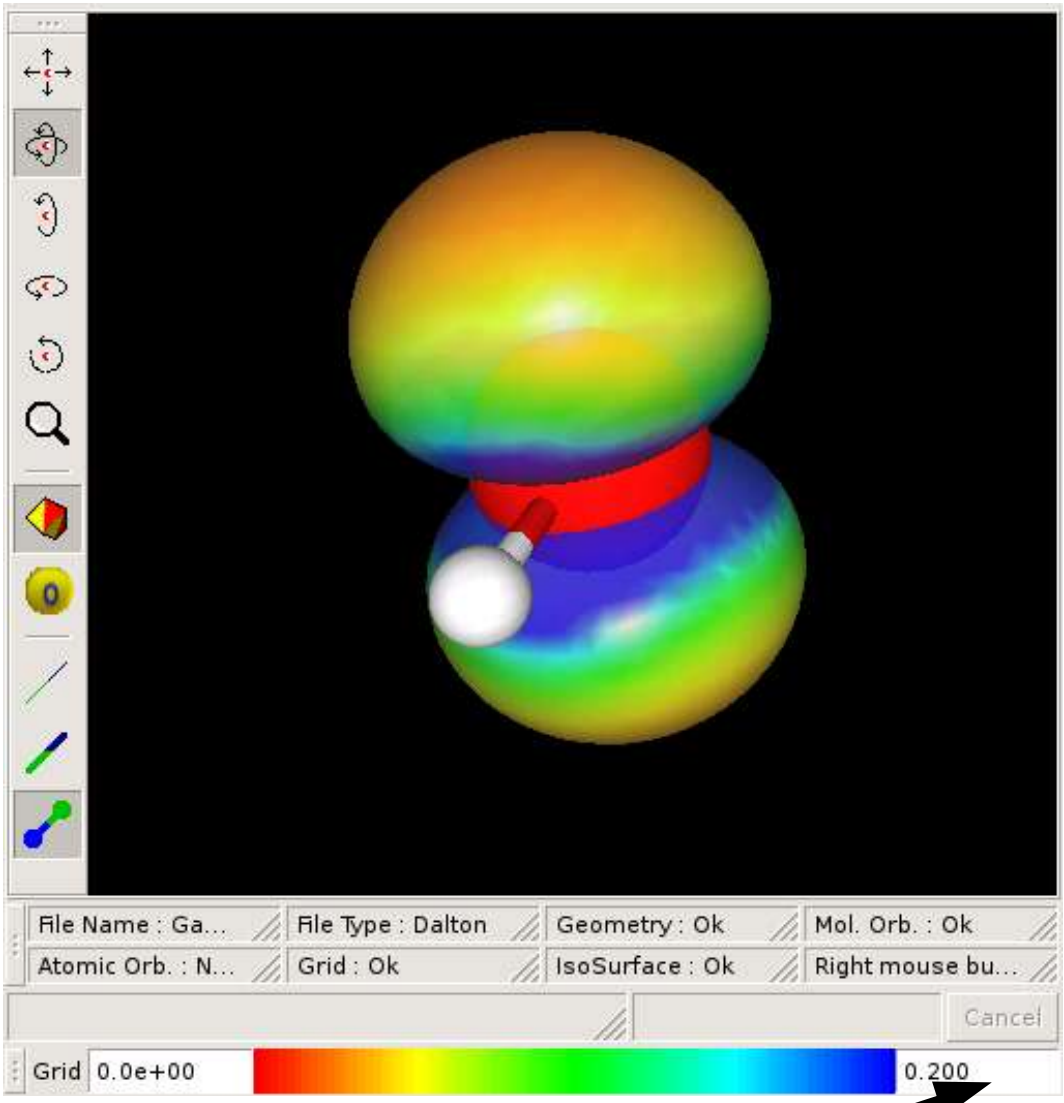
5. Set iso value to 0.1 and click to OK.



6. Click to “O” button
   You can easily change the display type by selecting the type of rendering :
   Render/Geometry and/Or Render/Surface



7. On Drawing Area of Geometry/Display window click with right button of mouse and select Density/Electronic. Click to OK button and choose 0.1 for the isovalue.
8. click with right button of mouse and select Cube/Save for save the electronic density grid at a **edensity.gcube** file.
9. click with right button of mouse and select Surfaces/delete all
10. click with right button of mouse and select Orbitals/Selection and click to OK button.
11. click with right button of mouse and select Cube/Color Mapping. Select the **edensity.gcube** file.
12. choose 0.1 for the value for the isosurface.



13. At the bottom of the window set the maximal value to 0.2.
14. For create a BMP image file, click with right button of mouse and select Screen Capture/BMP.