Gools of this Exercise

the Goals of this exercise are as follows:

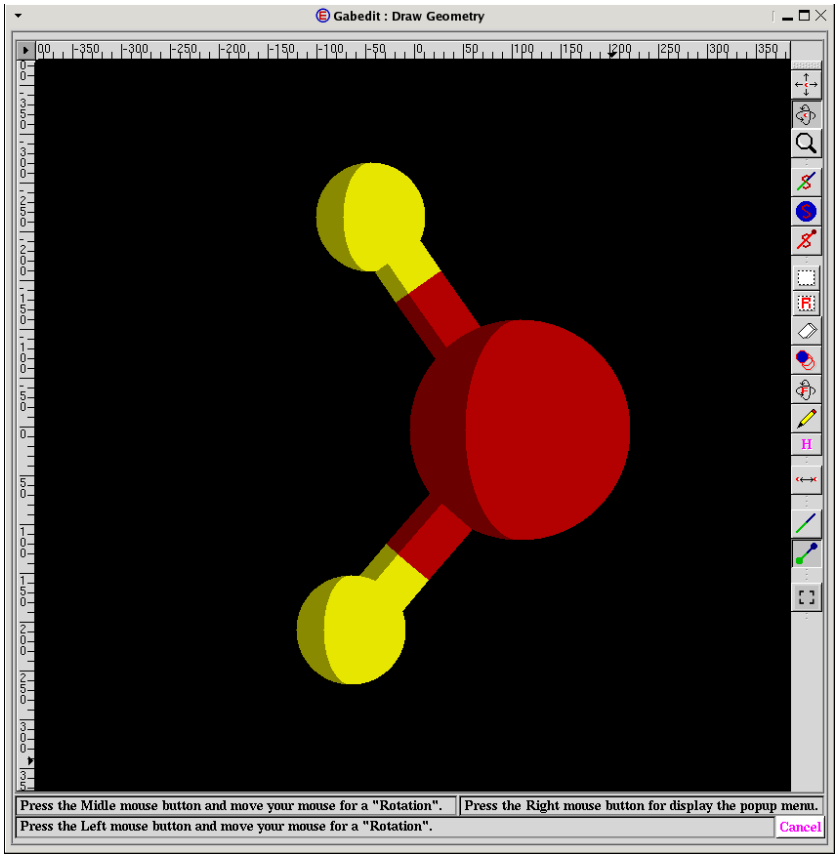
- Optimization of the H_2O molecule by a Hatree Fock calculation using the STO-3G basis.
- Then we will measure the distances between the atoms and the HOH angle.
- On the basis of the geometry optimized by a Hatree Fock calculation, we will optimize the geometry by a B3LYP calculation.
- Then we will 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. If Gabedit is not already running, go to a unix command window and type the command "gabedit".
2. Click on Draw/Display Geometry icon.

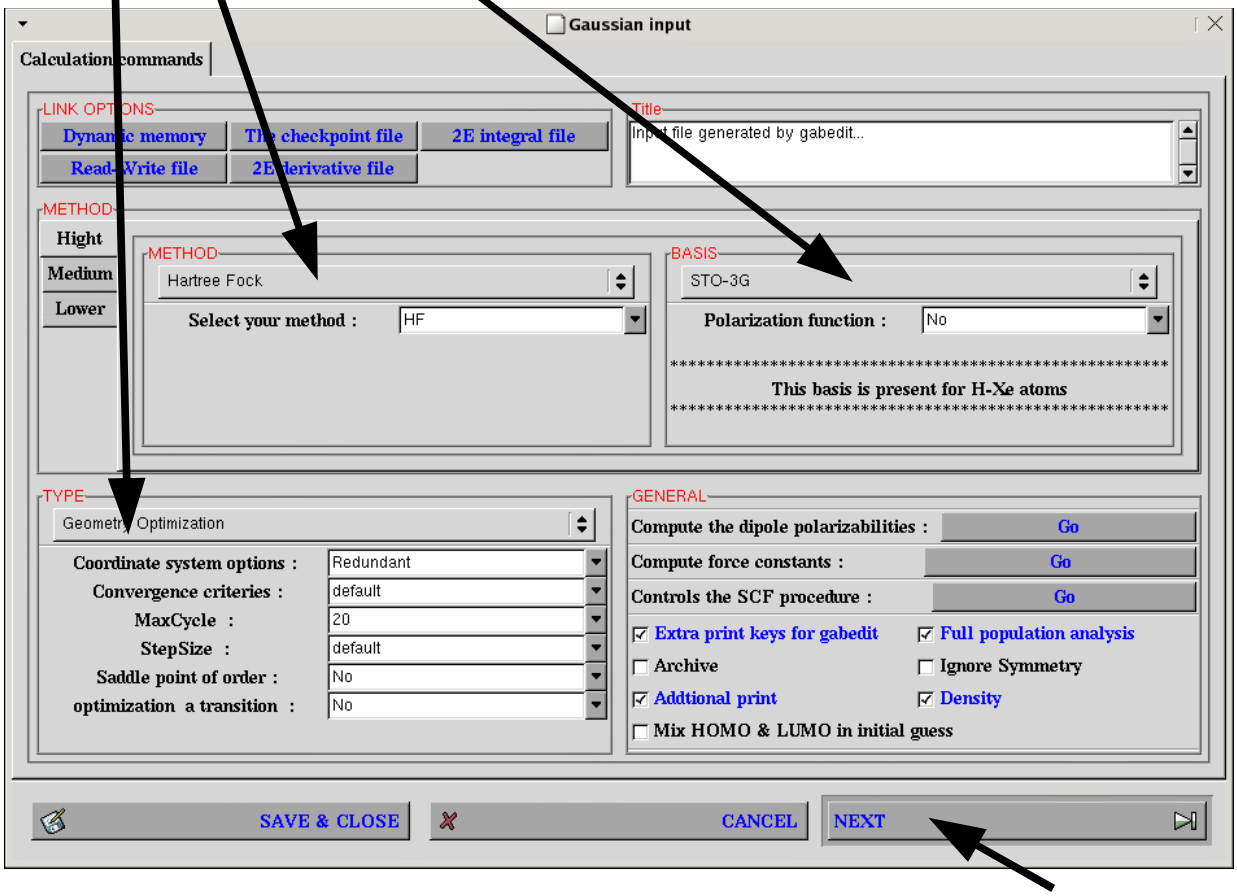
3. On Area zone click with right button of mouse and select Add/miscellaneous/Water, and click to Area zone. You have successfully built the desired structure :



Optimizing the Molecule by a HF Calculation

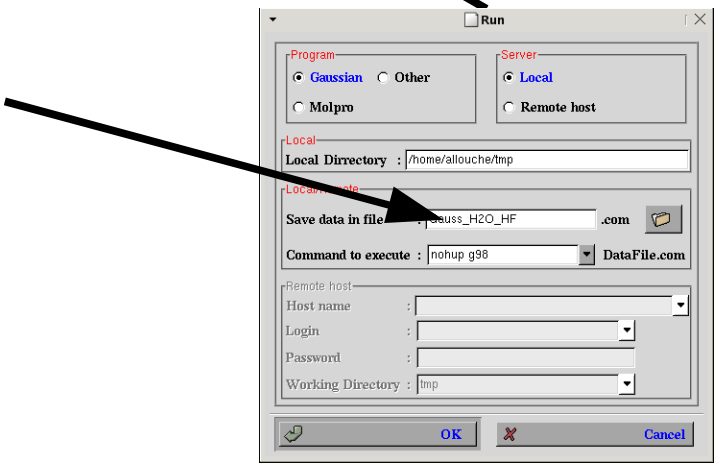
1. Close Geometry Windows.
2. Choose File/New Gaussian input (or Gaussian icon) from the principal Menu.

3. Select Hartree Fock at Method Frame.
4. Select STO-3G at Basis Frame.
5. Select Geometry Optimization at Type Frame.
6. Click to NEXT button.

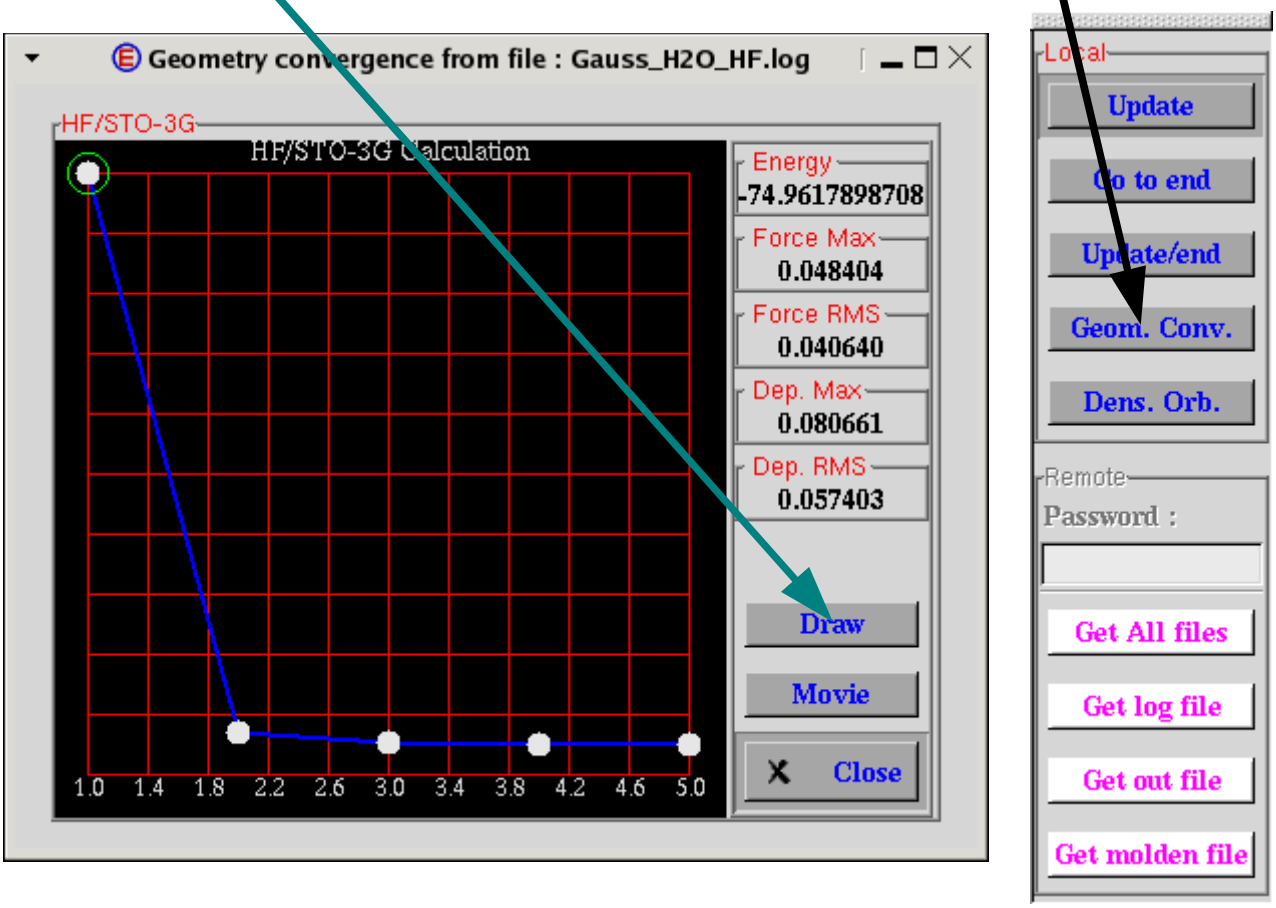


7. Click to FINISH button.
8. Click to Run molpro/Gaussian icon (toolbar, top of window).

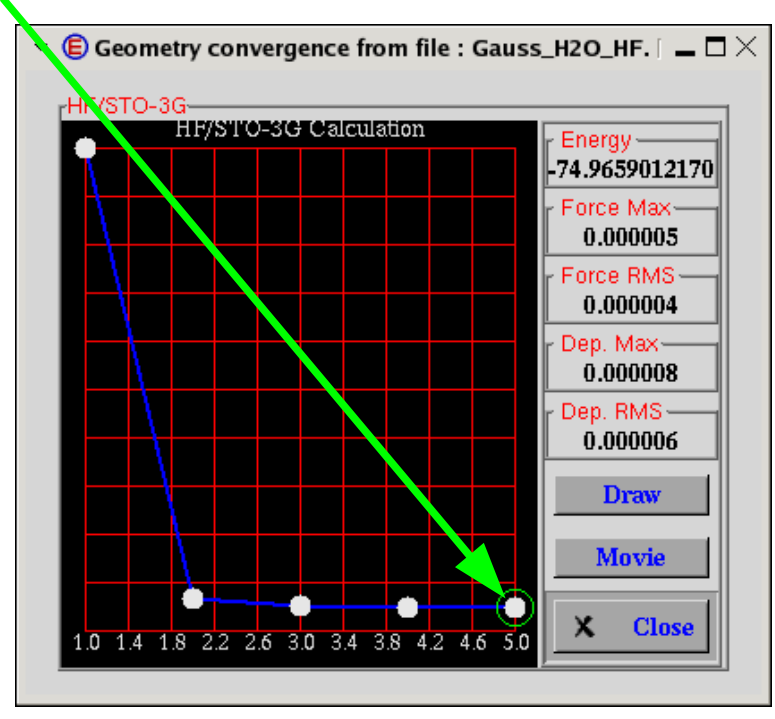
9. At save data file in text zone , type Gauss_H2O_HF



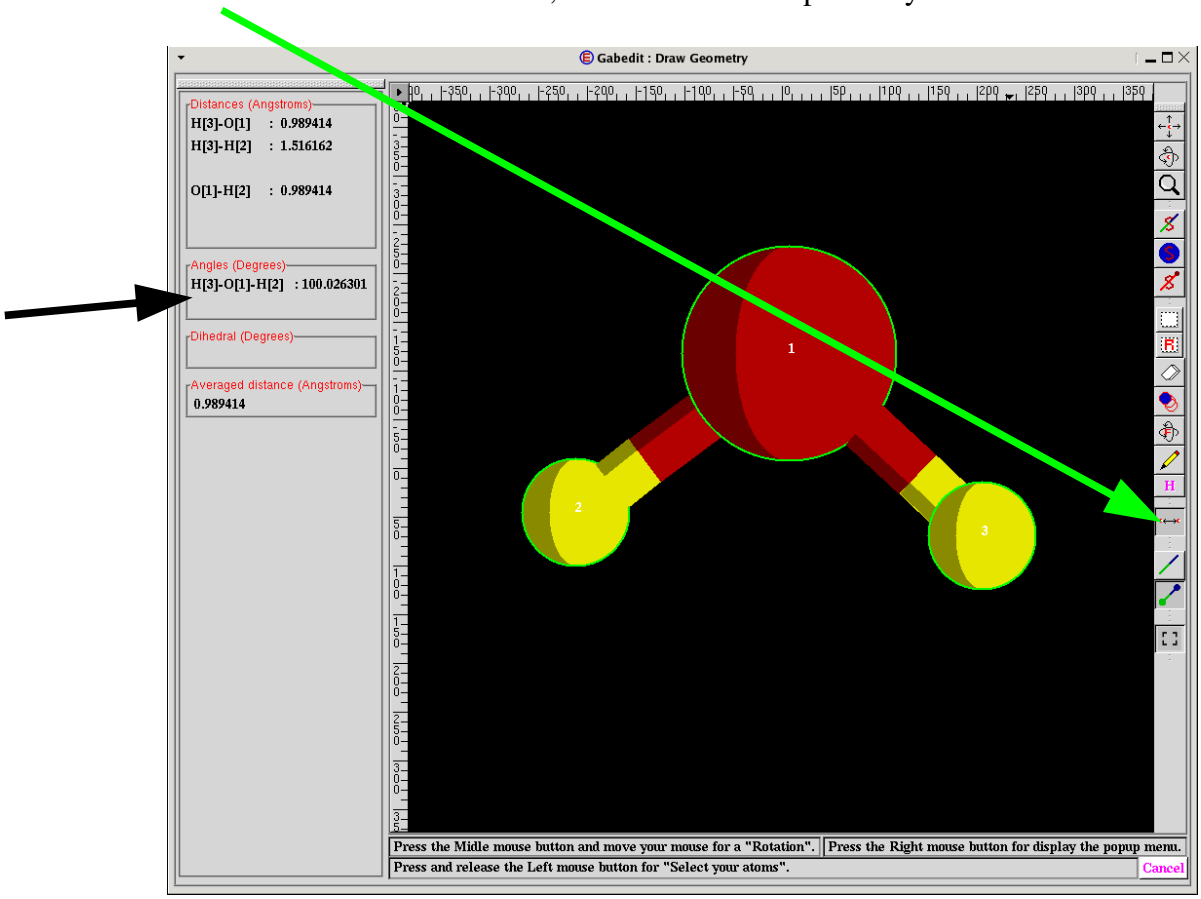
10.Click to OK button.
11.Gaussian is now started at background job.
12.Select Gauss_H2O_HF.log notebook.
13.Click to Update/End for reload the output file of Gaussian.
14.When the job completes (and this may take several minutes) : click to Geom. Conv.
15.click to Draw



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



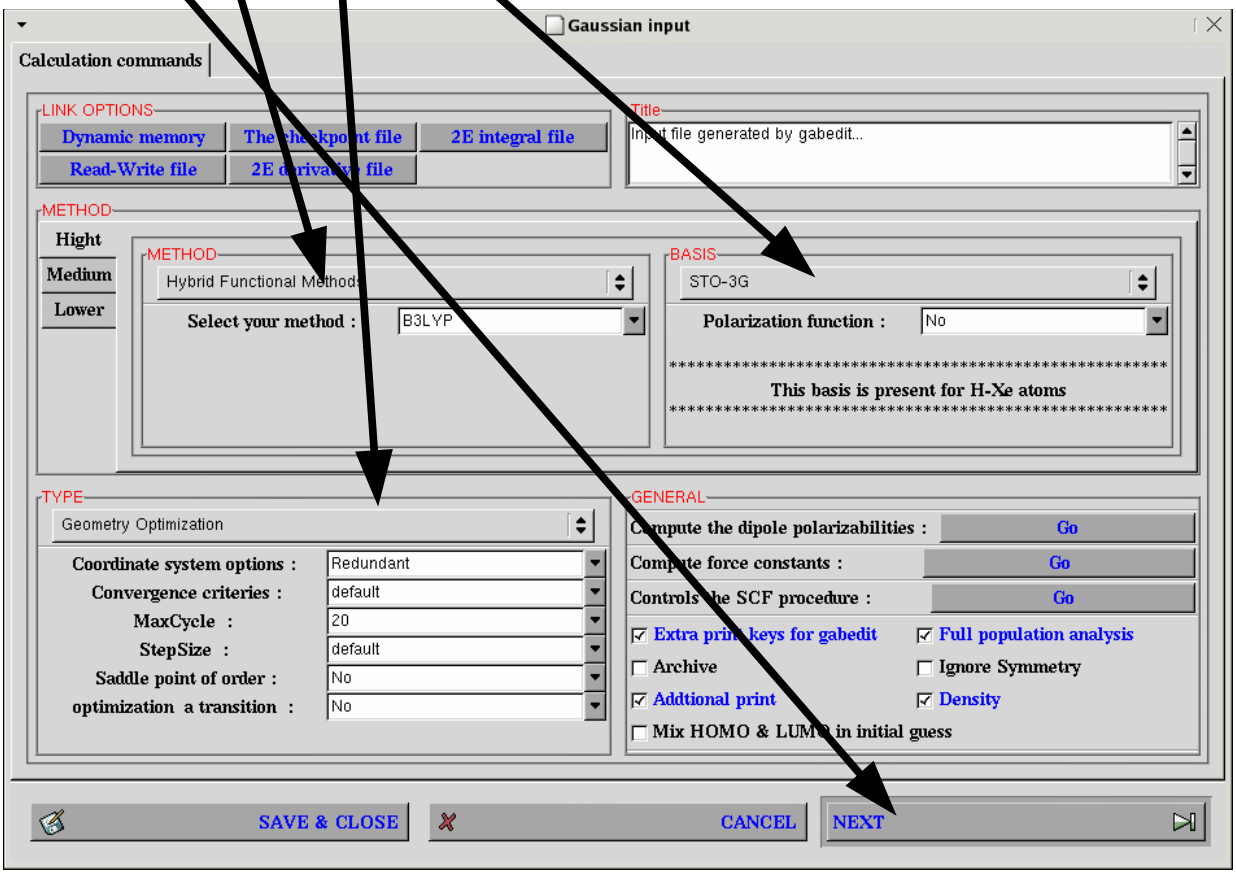
17. On Area zone of Geometry/Display window click with right button of mouse and select Label/Numbers.
18. Click to Mesure icon and select the H, O and H atoms respectively.



Optimizing the Molecule by a B3LYP Calculation

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

3. Select Hybrid functionals at Method Frame.
4. Select STO-3G at Basis Frame.
5. Select Geometry Optimization at Type Frame.
6. Click to NEXT button.

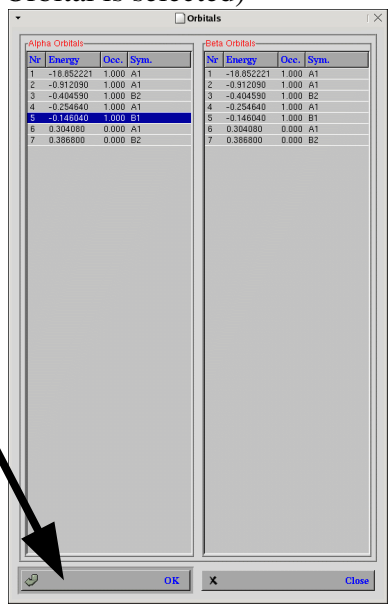


7. Click to FINISH button(Your first geometry at this calculation is the last geometry of HF calculation).
8. Click to Run molpro/Gaussian icon (toolbar, top of window).
9. At save data file in text zone , type Gauss_H2O_B3LYP
10. Click to OK button.
11. Gaussian is now started at background job.
12. Select Gauss_H2O_B3LYP.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.

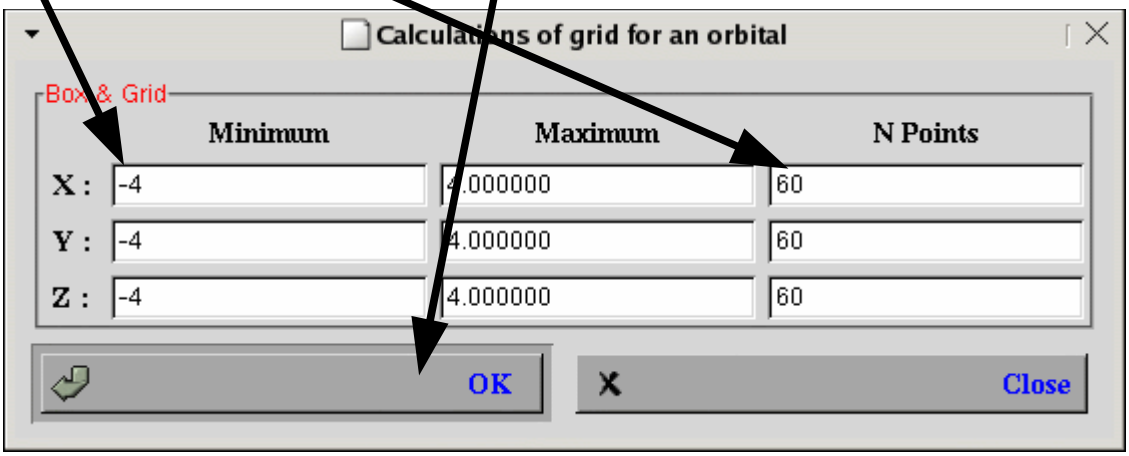
Viewing of the HOMO Orbital and the electronic density

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

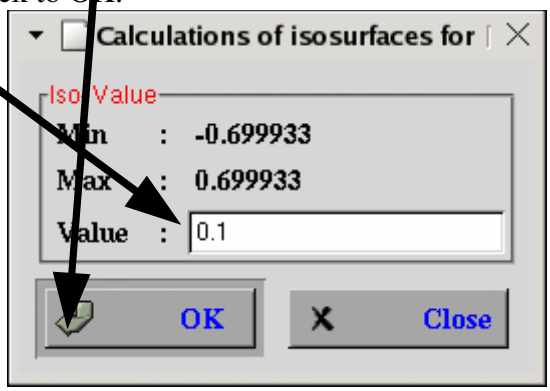
3. Click to Ok Button. (the HOMO Orbital is selected)



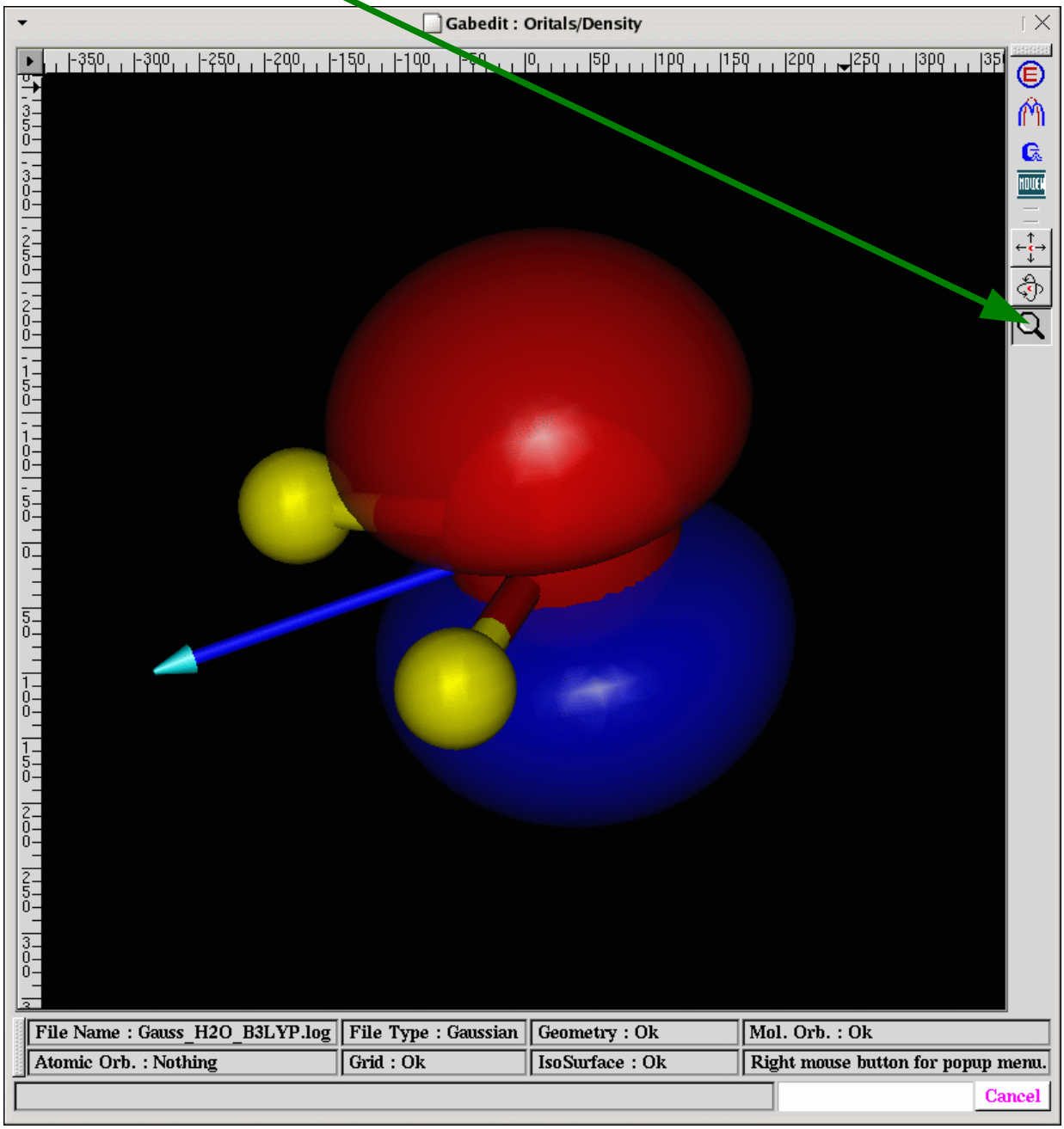
4. Set X Min to -4 and Nx to 60 and click to OK



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

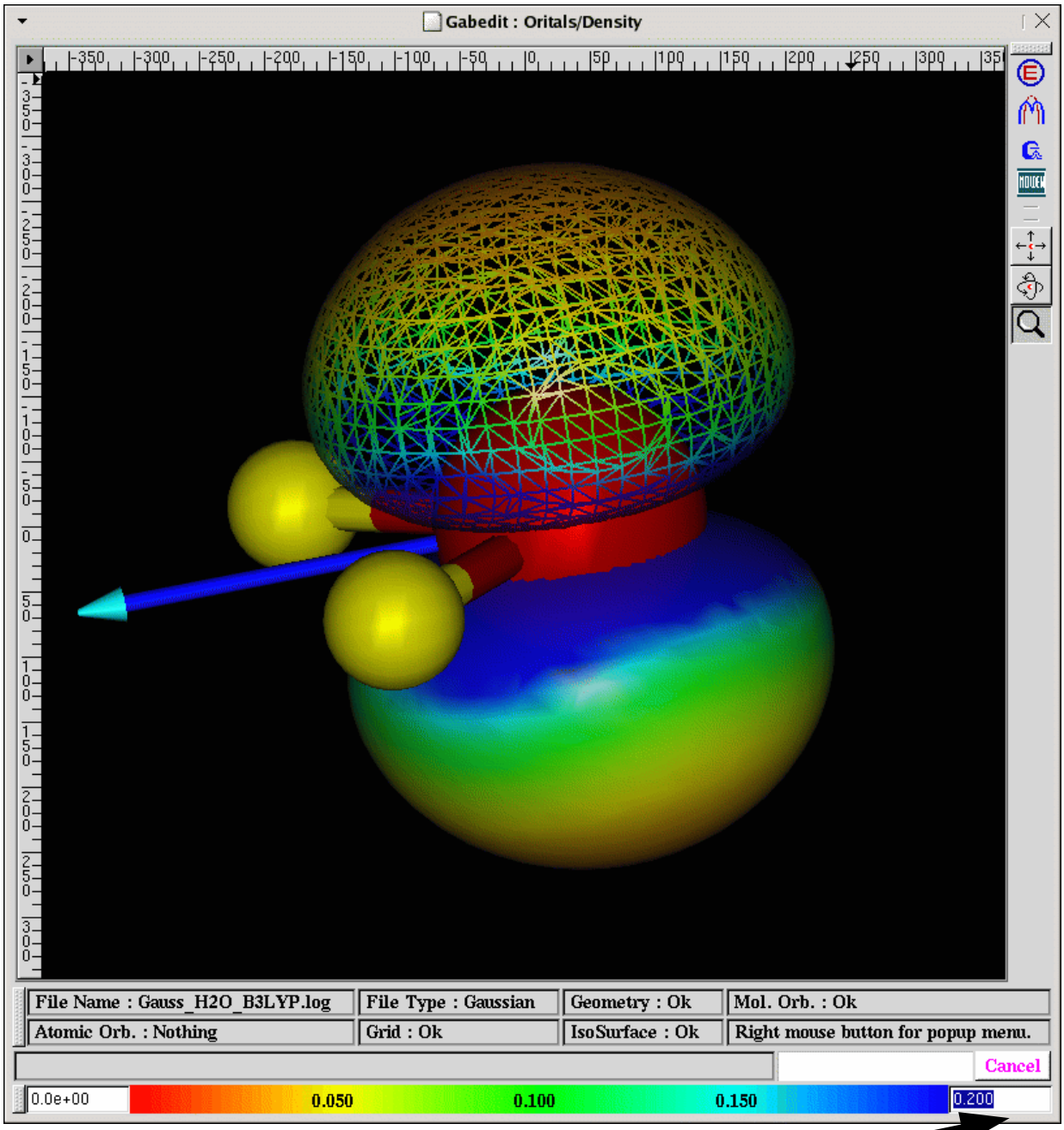


6. Select Zoom icon.
   Move the mouse while holding down the left button for obtain an optimal image.
   You can easily change the display type by selecting the type of rendering :
   Render/Geometry and/Or Render/Surface



7. On Area zone 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 Orbitals/Selection and click to OK button.
10. click with right button of mouse and select Cube/Color Mapping. Select the **edensity.gcube** file.

11.choose 0.1 for the value for the isosurface.



12.At the bottom of the window set the maximal value to 0.2.

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