

# Goals of this Exercise

the Goals of this exercise are as follows:

- Optimization of the H<sub>2</sub>O 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.

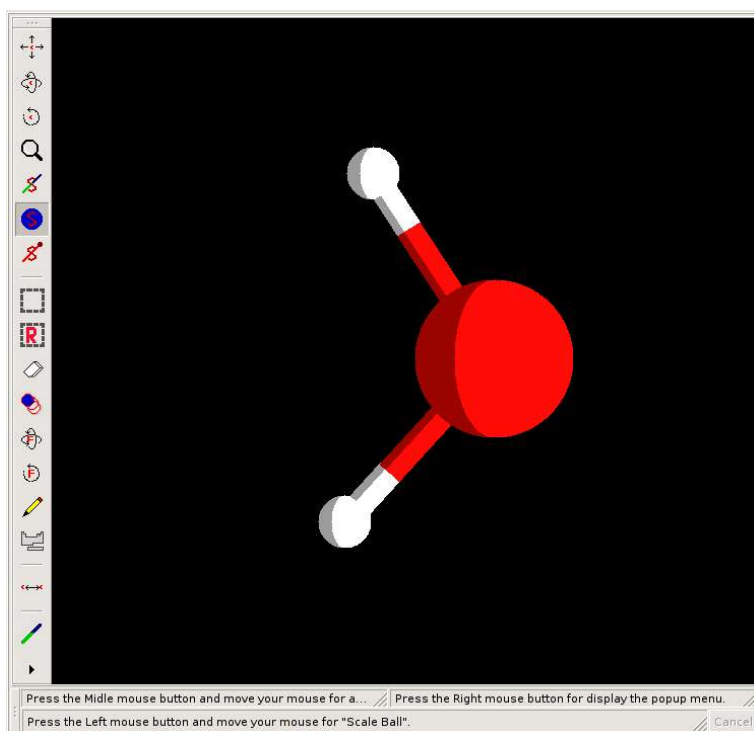
## Detailed Instructions

### 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.

The screenshot shows the Gamess-US input dialog box. The 'Symmetry' section has 'Detected by Gabedit' selected. The 'Control' section has 'Run Type' set to 'Equilibrium geometry', 'SCF Type' set to 'RHF', and 'Max # SCF iterations' set to '20'. The 'Basis' section has 'Basis set' set to '6-31G'. The 'SCF options' section has 'Direct SCF' checked. The 'Initial Guess' section has 'Huckel' selected. The 'OK' button is at the bottom right.

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

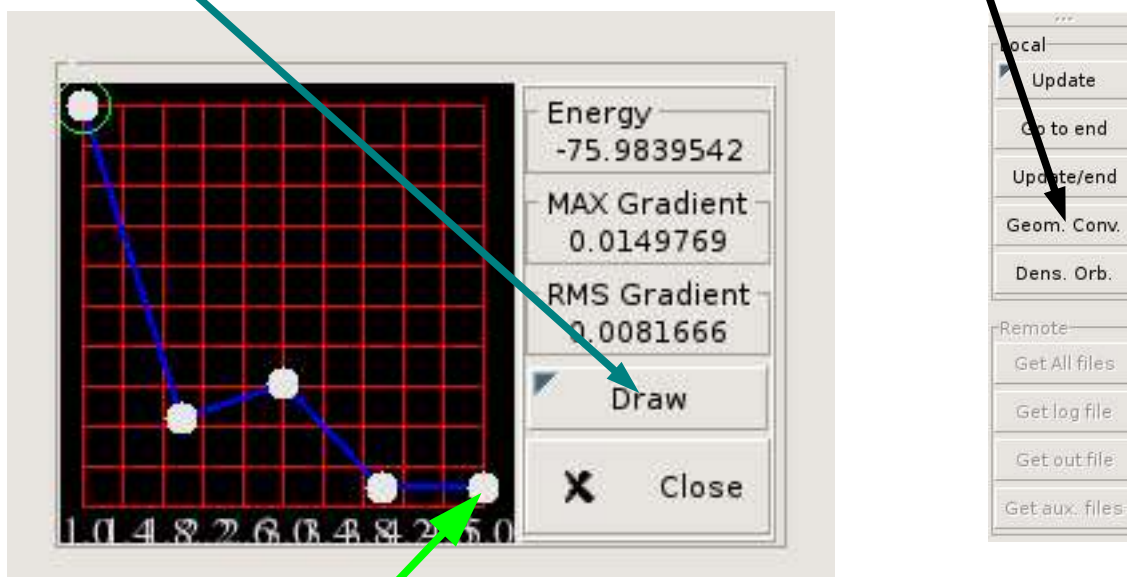


8. Select your folder
9. At save data file in text zone, type Gamess\_H2O\_HF

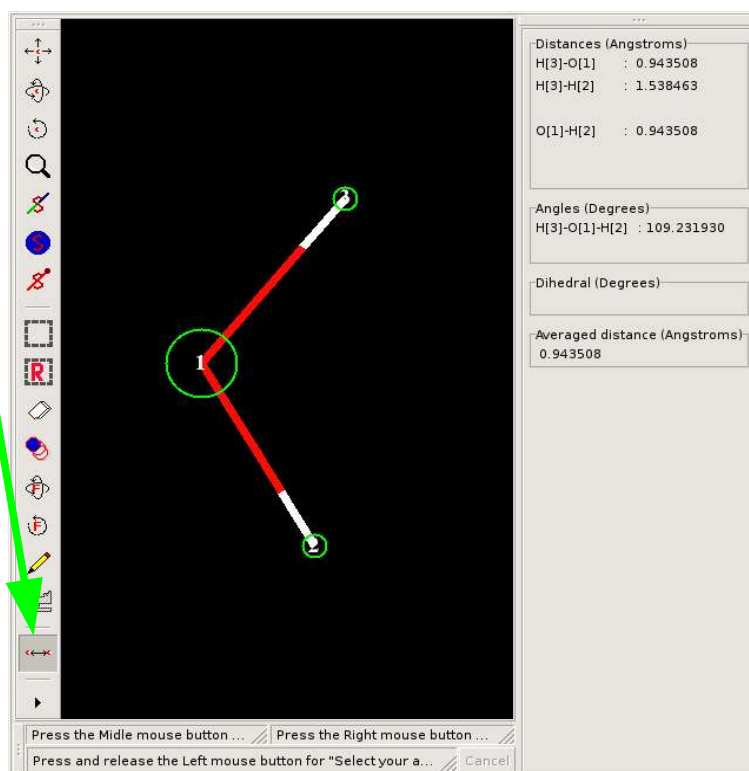
The screenshot shows the 'Local' dialog box in Gamess-US. The 'Local Directory' field is set to '/home/allouche/tmp'. The 'Save data in file' text box contains 'Gamess\_H2O\_HF'. The 'Command to execute' is set to 'gms'. The 'OK' button is at the bottom right.

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 Measure icon and select the H, O and H atoms respectively.

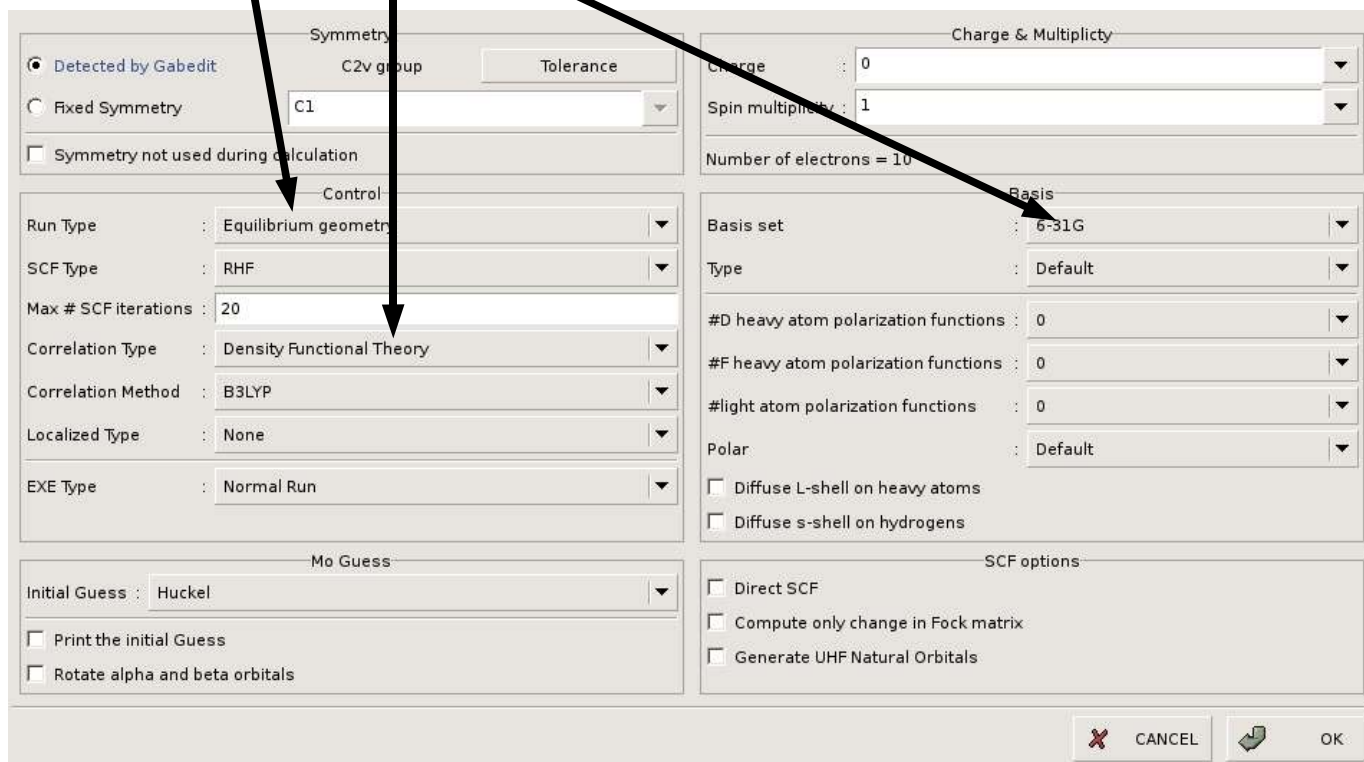


### Optimizing the Molecule by a B3LYP Calculation

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 as Basis Frame.
6. Click to OK button.



The dialog box contains the following settings:

- Symmetry:** Detected by Gabedit, C2v group, Tolerance.
- Charge & Multiplicity:** Charge: 0, Spin multiplicity: 1, Number of electrons = 10.
- Control:** Run Type: Equilibrium geometry, SCF Type: RHF, Max # SCF iterations: 20, Correlation Type: Density Functional Theory, Correlation Method: B3LYP, Localized Type: None, EXE Type: Normal Run.
- Basis:** Basis set: 6-31G, Type: Default, #D heavy atom polarization functions: 0, #F heavy atom polarization functions: 0, #light atom polarization functions: 0, Polar: Default.
- 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: ☐.

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 file of 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)

Alpha Orbitals				Beta Orbitals			
Nr	Energy	Occ.	Sym.	Nr	Energy	Occ.	Sym.
1	-19.129999	1.000000	A1	1	-19.129999	1.000000	A1
2	-1.002700	1.000000	A1	2	-1.002700	1.000000	A1
3	-0.525900	1.000000	B1	3	-0.525900	1.000000	B1
4	-0.345000	1.000000	A1	4	-0.345000	1.000000	A1
5	-0.286100	1.000000	B2	5	-0.286100	1.000000	B2
6	0.055800	0.000000	A1	6	0.055800	0.000000	A1
7	0.145400	0.000000	B1	7	0.145400	0.000000	B1
8	0.825300	0.000000	B1	8	0.825300	0.000000	B1
9	0.854100	0.000000	A1	9	0.854100	0.000000	A1
10	0.893900	0.000000	B2	10	0.893900	0.000000	B2
11	0.948000	0.000000	A1	11	0.948000	0.000000	A1
12	1.074500	0.000000	B1	12	1.074500	0.000000	B1
13	1.412000	0.000000	A1	13	1.412000	0.000000	A1

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

Box & Grid						
	Vx	Vy	Vz	Minimum	Maximum	Number of points
First direction	1.0	0.0	0.0	-4	4.000000	60
Second direction	0.0	1.0	0.0	-4.000000	4.000000	60
Third direction	0.0	0.0	1.0	-4.000000	4.000000	60

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

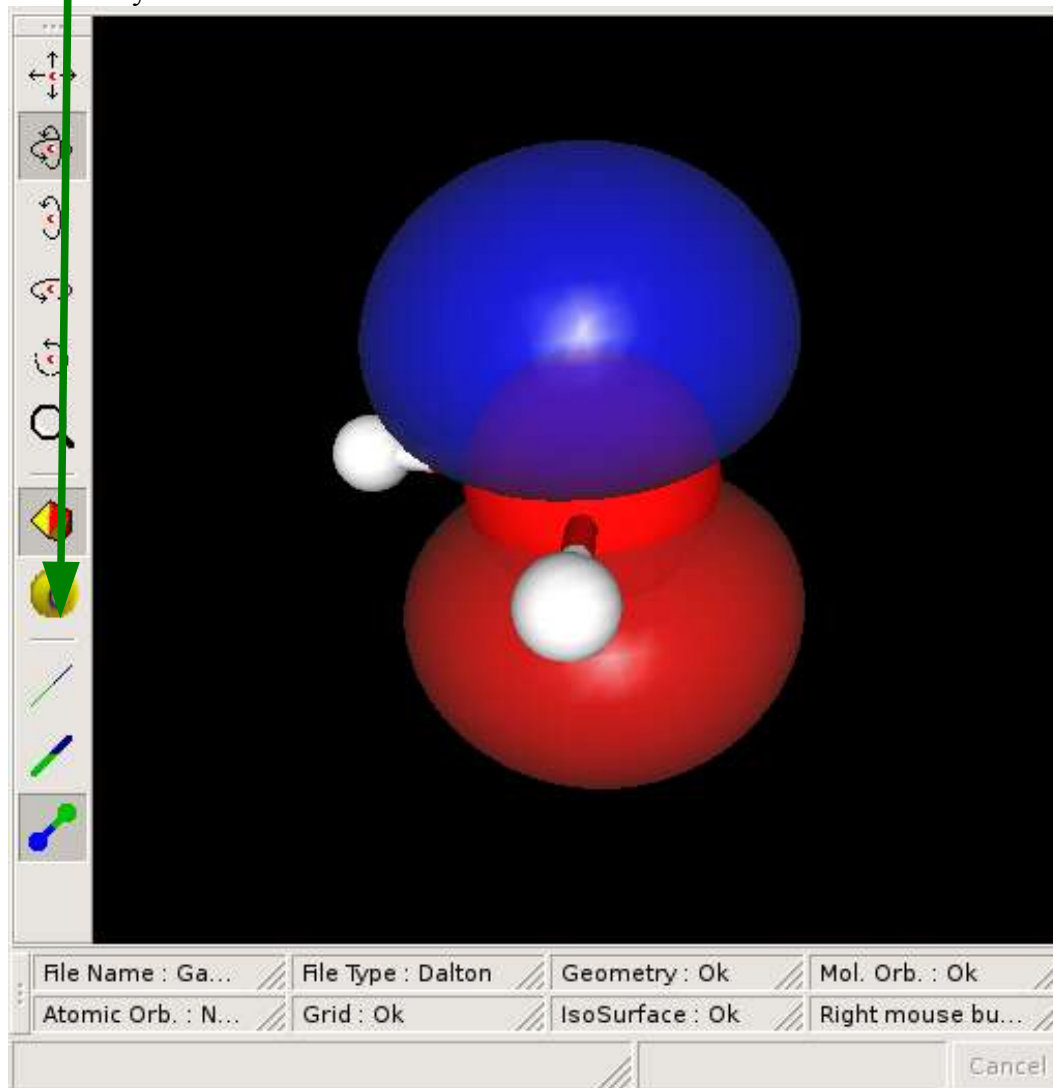
Iso-Value	
Min	-0.692756
Max	0.692756
Value	0.1



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.

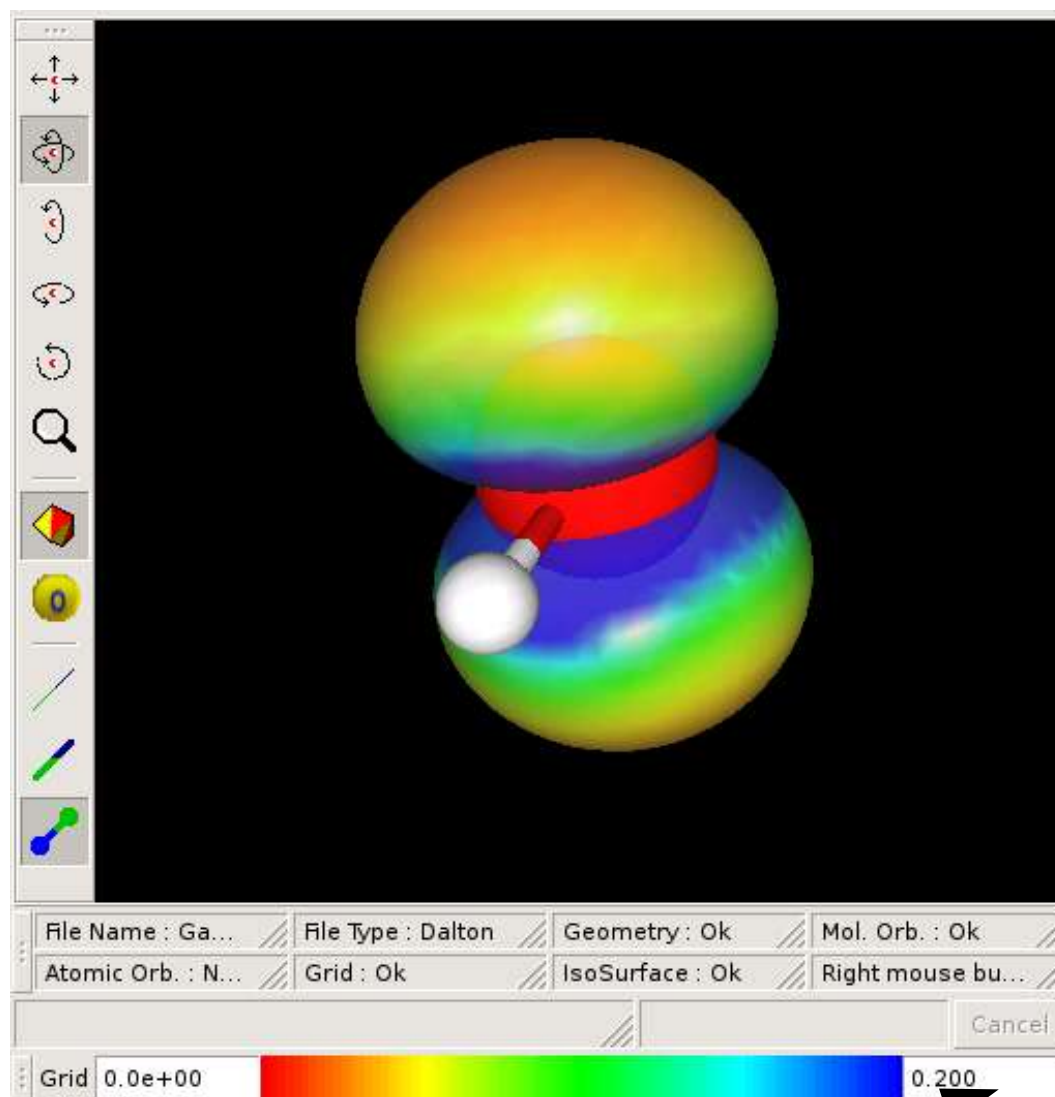
8. click with right button of mouse and select Cube/Save for save the electronic density grid at a **edensity.gcube** file.

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.