Goals of this Exercise

Optimization of the H_2O molecule using PM6 method.

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

On the basis of the geometry optimized using PM6 calculation, we will compute and draw the IR spectrum.

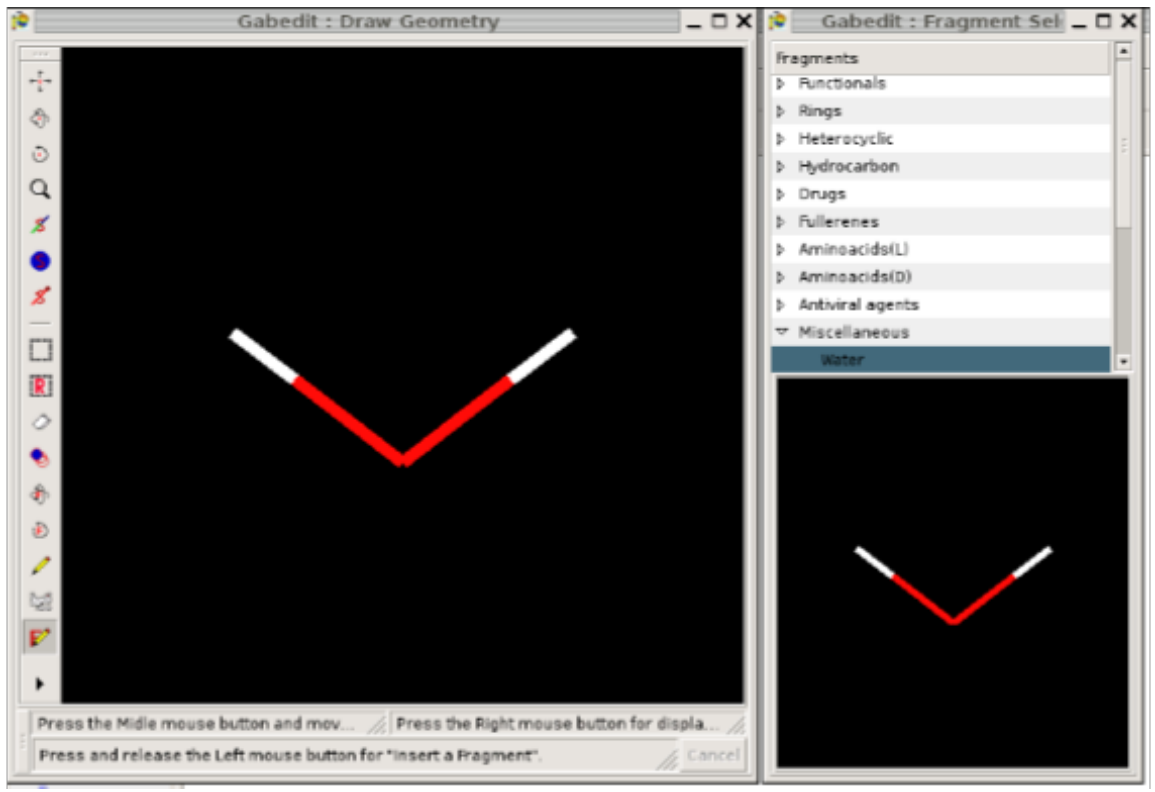
Then we will visualize the HOMO orbital, the electronic density and the HOMO orbital colorcoded with electronic density.

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 :

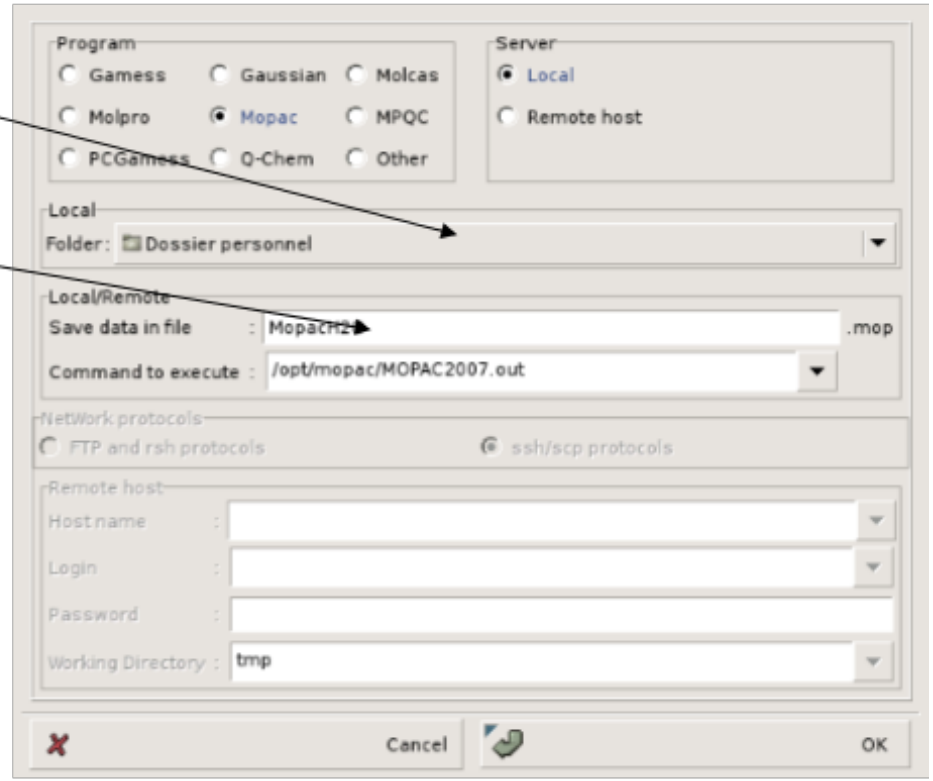


Optimizing the Molecule using PM6 method

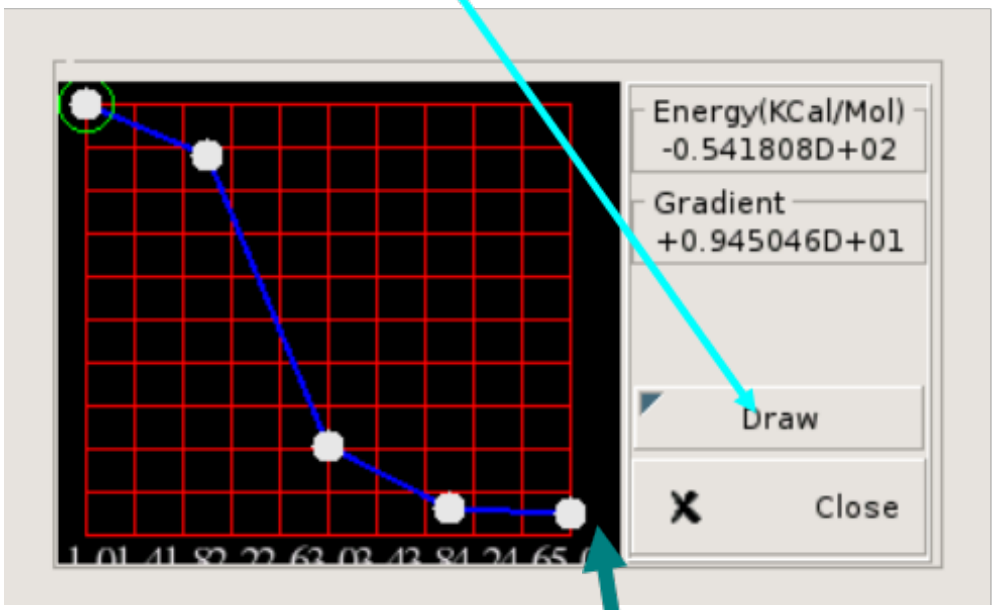
1) Close Geometry Windows.
2) Choose File/New Mopac input (or Mopac icon) from the principal Menu.
3) Select Equilibrium structure search.
4) Click OK button.
5) Click to Run icon (toolbar, top of window).

6) Select your folder

7) At save data file in text zone ,
type MopacH2O



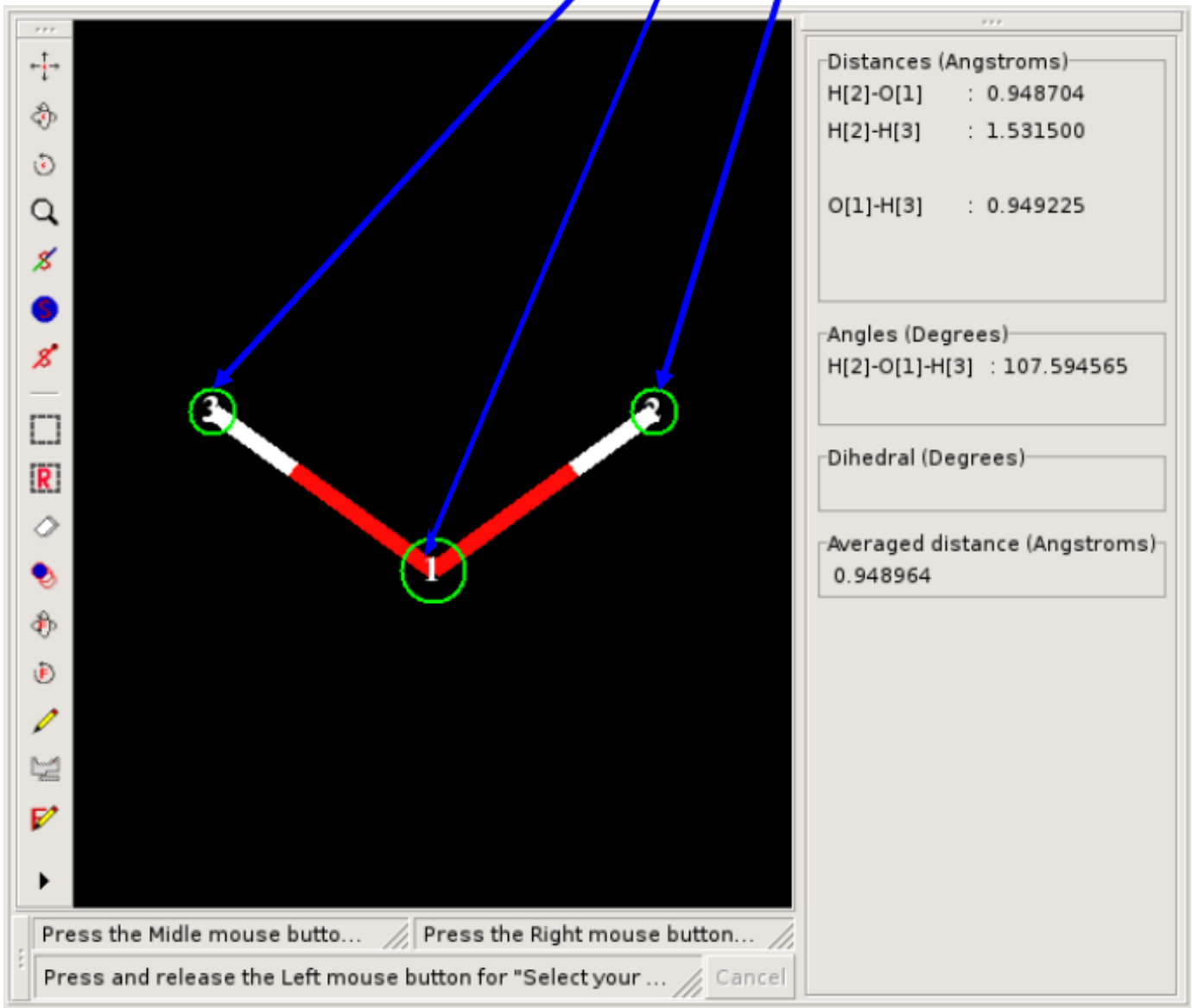
8) Click to OK button.
9) Mopac is now started at background job.
10) Select MopacH2O.out notebook.
11) Click to Update/End for reload the output file of Mopac.
12) When the job completes (and this may take several minutes) : click to Geom. Conv.
13) click to Draw



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

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

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

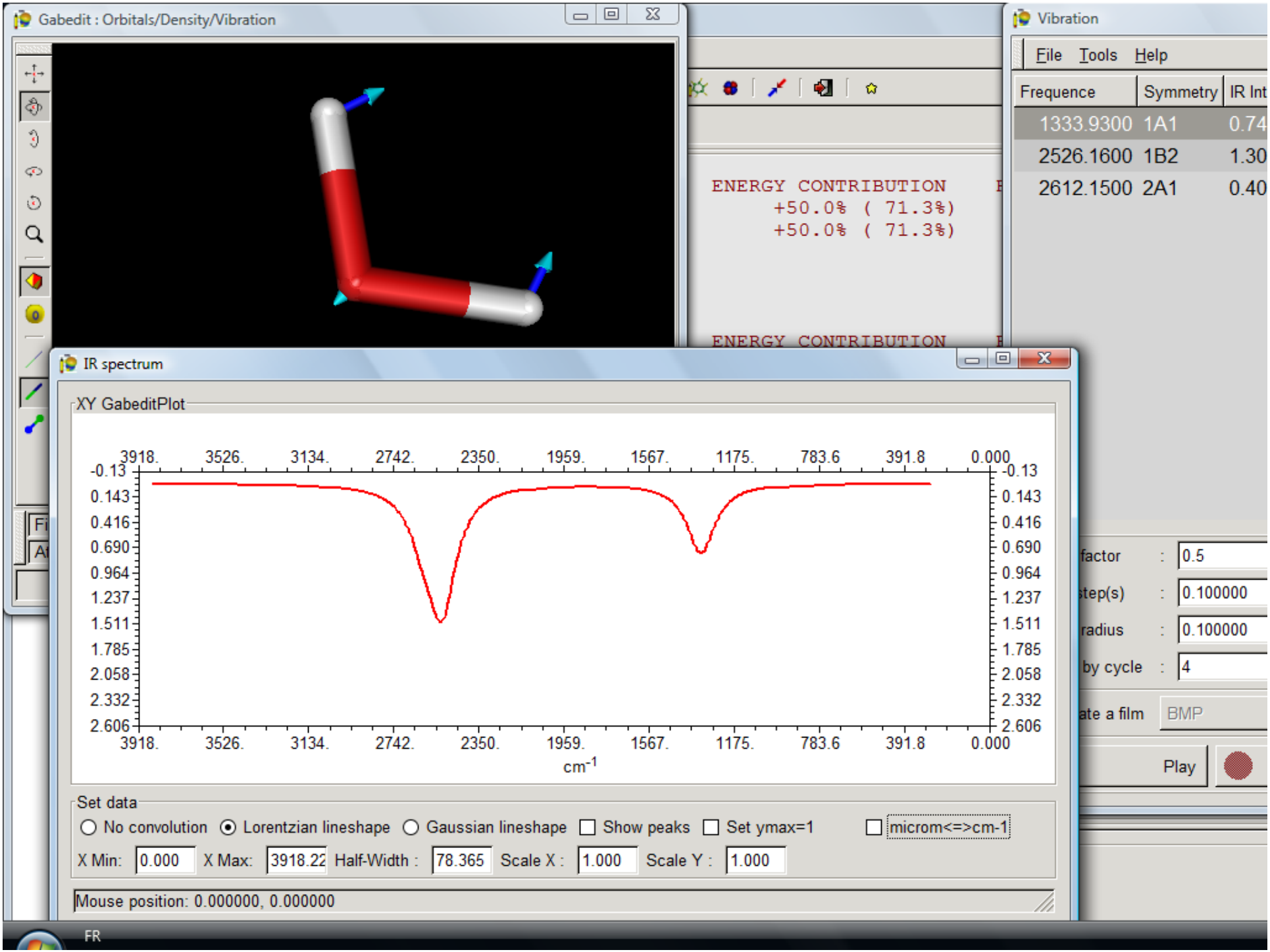


Compute and draw the IR spectrum of H2O molecule

Close Geometry Windows.
Choose File/New Mopac input (or Mopac icon) from the principal Menu.
Select “Frequencies” for Job Type
Click to OK button.
Click to Run icon (toolbar, top of window).
At save data file in text zone , type MopacH2OFreq
Click to OK button.

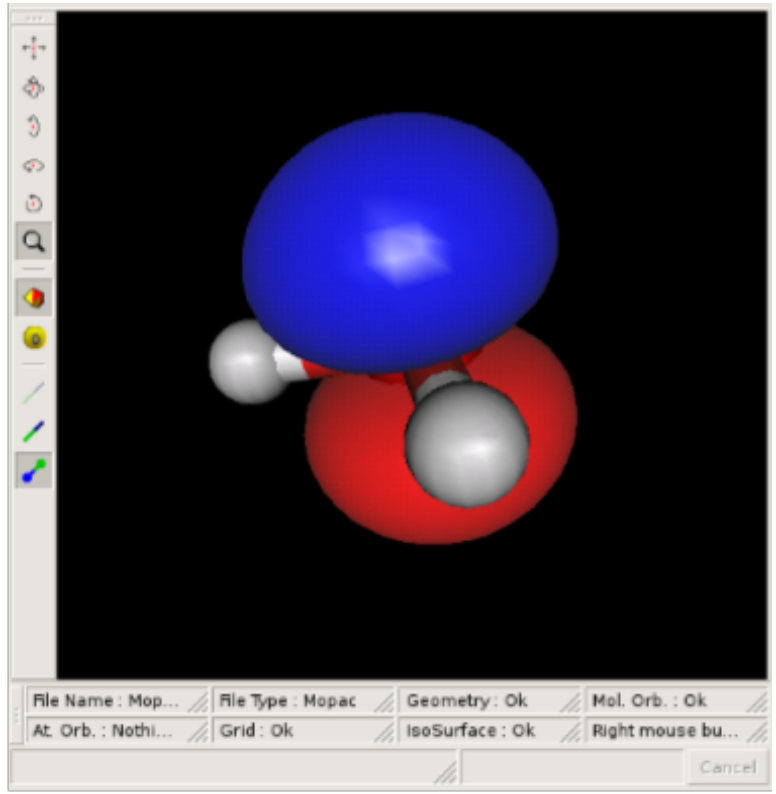
Mopac is now started at background job.
Select MopacH2OFreq.out notebook.
Click to Update/End for reload the output file of Mopac.
When the job completes (and this may take several minutes) : click to “Dens. Orb.” button

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/mopac aux file and select MopacH2OFreq.aux 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.


Gabedit : Orbitals/Density/Vibration
ENERGY CONTRIBUTION
+50.0% (71.3%)
+50.0% (71.3%)
ENERGY CONTRIBUTION
Vibration
File Tools Help
Frequence Symmetry IR Int
1333.9300 1A1 0.74
2526.1600 1B2 1.30
2612.1500 2A1 0.40
IR spectrum
XY GabeditPlot
3918. 3526. 3134. 2742. 2350. 1959. 1567. 1175. 783.6 391.8 0.000
-0.13 0.143 0.416 0.690 0.964 1.237 1.511 1.785 2.058 2.332 2.606
cm-1
Set data
No convolution
Lorentzian lineshape
Gaussian lineshape
Show peaks
Set ymax=1
microm<=>cm-1
X Min: 0.000 X Max: 3918.22 Half-Width : 78.365 Scale X : 1.000 Scale Y : 1.000
Mouse position: 0.000000, 0.000000
factor : 0.5
step(s) : 0.100000
radius : 0.100000
by cycle : 4
ate a film BMP
Play
FR

Viewing of the HOMO Orbital and the electronic density

Close “**IR Spectrum”**and “Vibration” window (It have a list of modes)
On Drawing Area of Geometry/Display window click with right button of mouse and select “”**Orbitals/Read Mopac aux file**” and select MopacH2OFreq.aux 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 Geometry/Display window click with right button of mouse and select Density/Electronic. Click to OK button and choose 0.1 for the isovalue.
click with right button of mouse and select Cube/Save for save the electronic density grid at a **edensity.gcube** file.
click with right button of mouse and select Surfaces/delete all
click with right button of mouse and select Orbitals/Selection and click to OK button.
click with right button of mouse and select Cube/Color Mapping. Select the **edensity.gcube** file.
choose 0.1 for the value for the isosurface.

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

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