● Configuration

On unix (linux, mac os x11, ...) OS : Make sure that your path variable contains a reference to the directory of orca binary files.

On Windows : Run gabedit. From the menu, select « Prefrences/Setting » and click to « Other » tab. Set the directory of orca binary files.

● Goals of this Exercise

Optimization of the C_2H_4 molecule using HF/6-31+G* method.

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

On the basis of the geometry optimized, we will compute and draw the IR spectrum, visualize the vibrational modes.

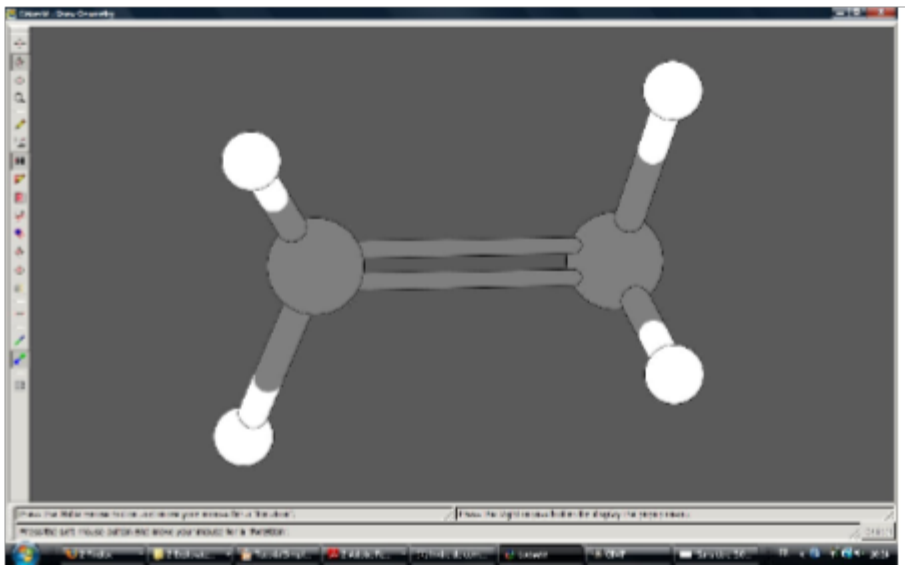
On the basis of the geometry optimized, we will compute and draw the UV spectrum using the CIS and ZINDO/S methods, we visualize the orbitals implicated on the principal transition.

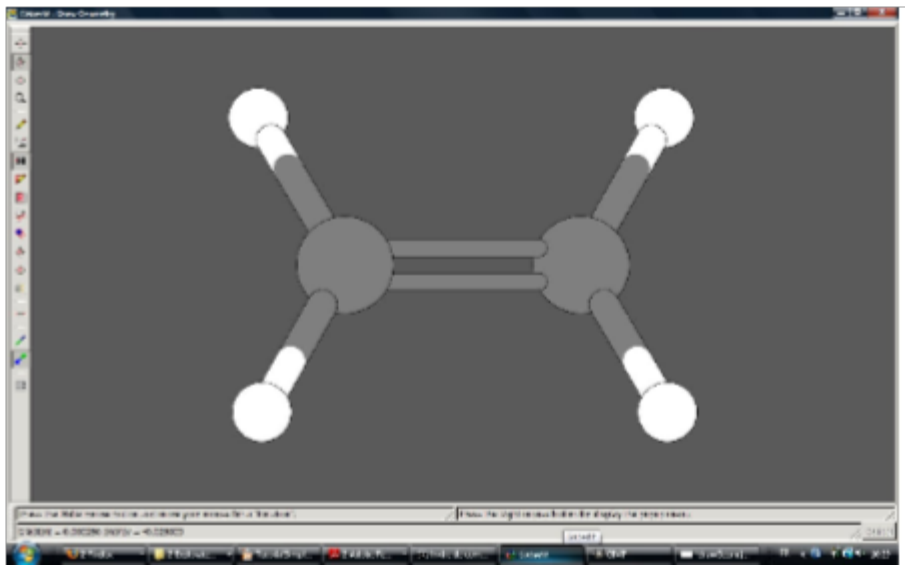
● Detailed Instructions

Building of the Molecule

Click on Draw/Display Geometry icon

On Drawing Area click, with left button of mouse and move your mouse (button always pressed). Release the button. Clic to the C-C bond.
On Drawing Area click, with RIGHT button of mouse and select « Molecular Machanics/Optimize. Click to OK button.
You have successfully built the desired structure.



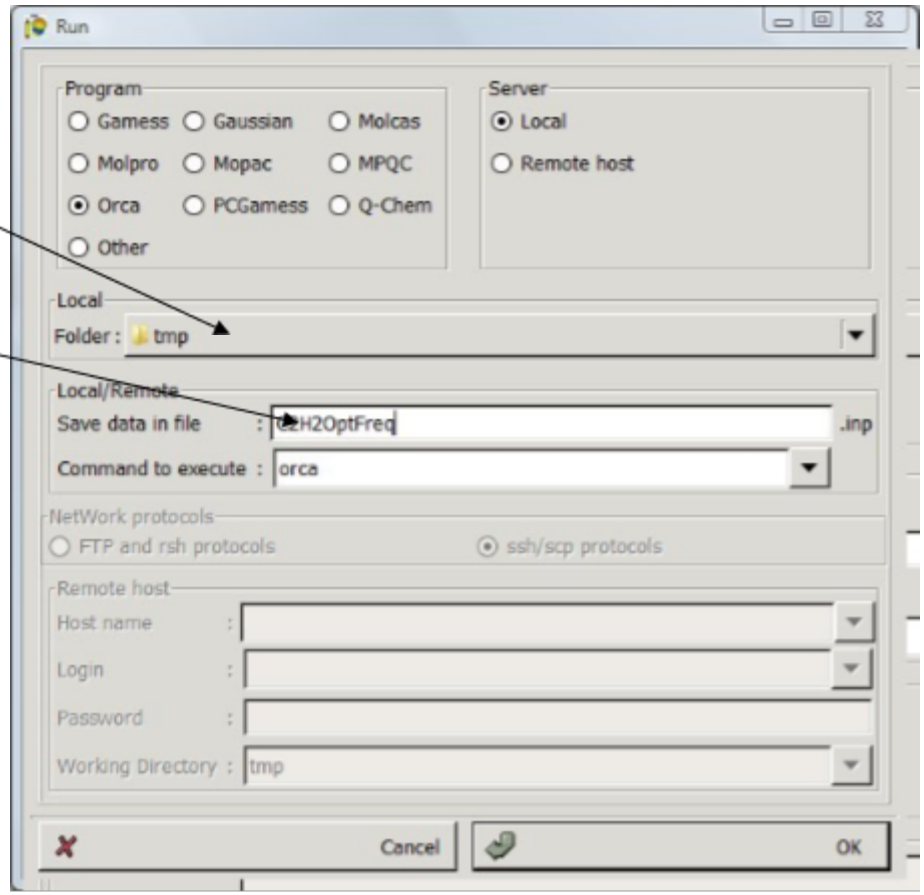


Optimizing the Molecule using HF/6-31+G* method

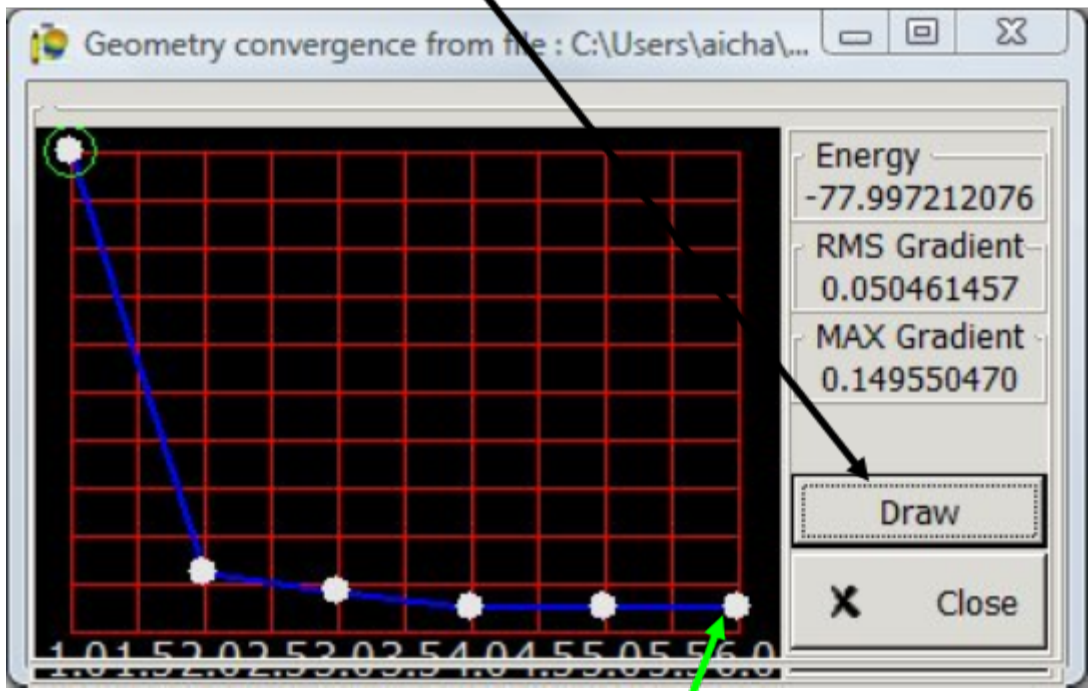
- Close Geometry Windows.
- Choose File/New Orca input (or Orca icon) from the Menu.
- Select **Equilibrium structure search + Frequencies**
- Select **Pople with one diffuse functions on non-hydrogen atom**
- Select **6-31+G***
- Click OK button.
- Click to Run icon (toolbar, top of window).

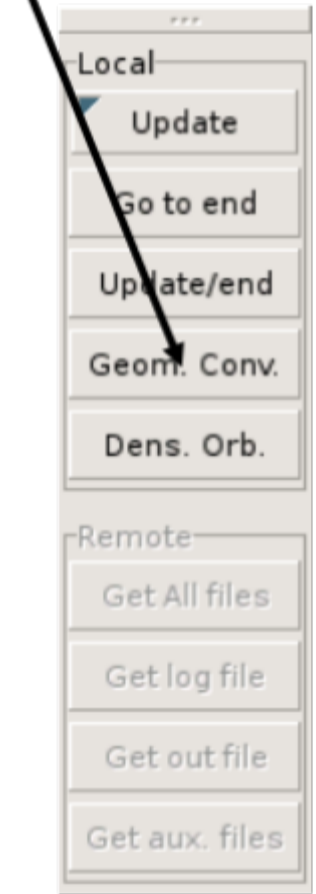
- Select your folder

- At save data file in text zone , type C2H4OptFreq



- Click to OK button.
- Orca is now started at background job.
- Select C2H4OptFreq.out notebook.
- Click to Update/End for reload the output file of Orca.
- When the job completes (and this may take several minutes, 7 minutes on my old computer, At the end of the output file you should obtain ****ORCA TERMINATED NORMALLY****) : Click to **Geom. Conv.** button
- Click to Draw button

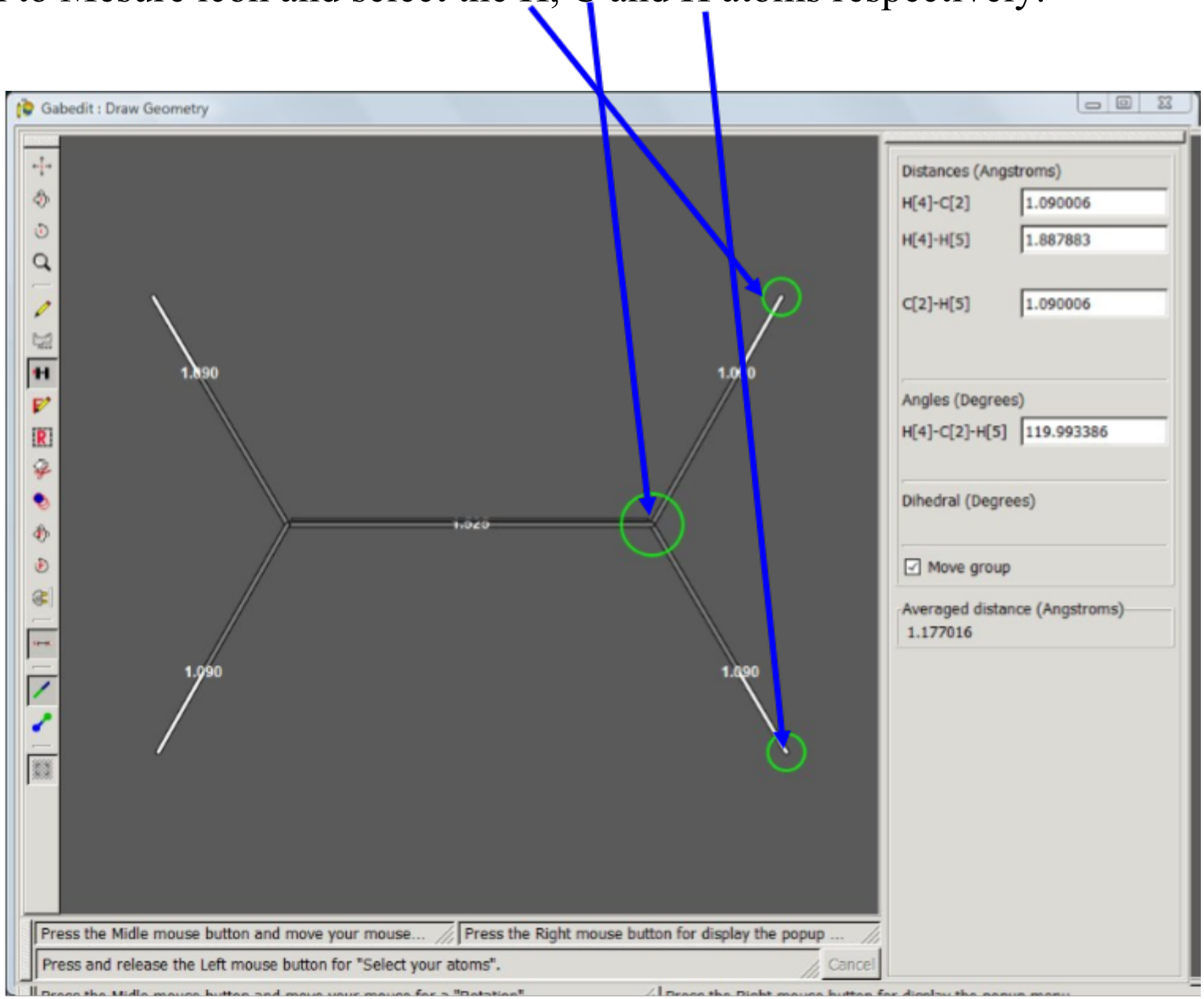




- Discover various optimized values for this structure by selection of various value. **Select the last point.**

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

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



Visualize the vibrational modes and draw the IR spectrum Ethylene

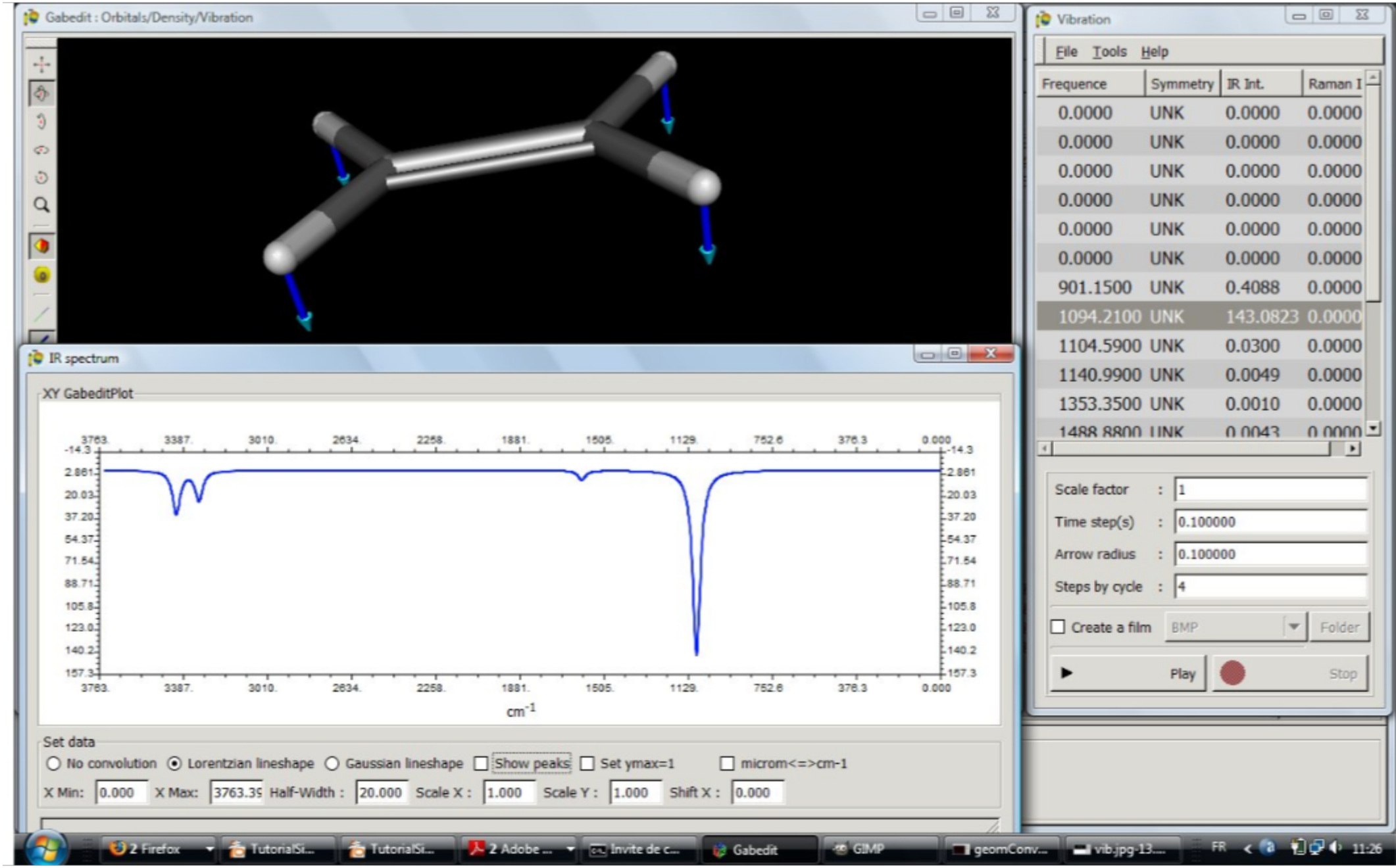
- Close Geometry Windows.
- Click to **"Dens. Orb."** icon

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/Orca and select C2H4OptFreq.out 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**.
You can change the Half-Width, value. You can use the middle button for do a zoom (or control + left button). You can use shif+left button for measuring the distance between 2 points on the curve. Double click to curve for change the color, line, ...


Gabedit : Orbitals/Density/Vibration
IR spectrum
XY GabeditPlot
3763.
3387.
3010.
2634.
2258.
1881.
1505.
1129.
752.6
376.3
0.000
-14.3
2.861
20.03
37.20
54.37
71.54
88.71
105.8
123.0
140.2
157.3
cm-1
Set data
No convolution
Lorentzian lineshape
Gaussian lineshape
Show peaks
Set ymax=1
microm<=>cm-1
X Min: 0.000
X Max: 3763.39
Half-Width : 20.000
Scale X : 1.000
Scale Y : 1.000
Shift X : 0.000
Vibration
File Tools Help
Frequence Symmetry IR Int. Raman I
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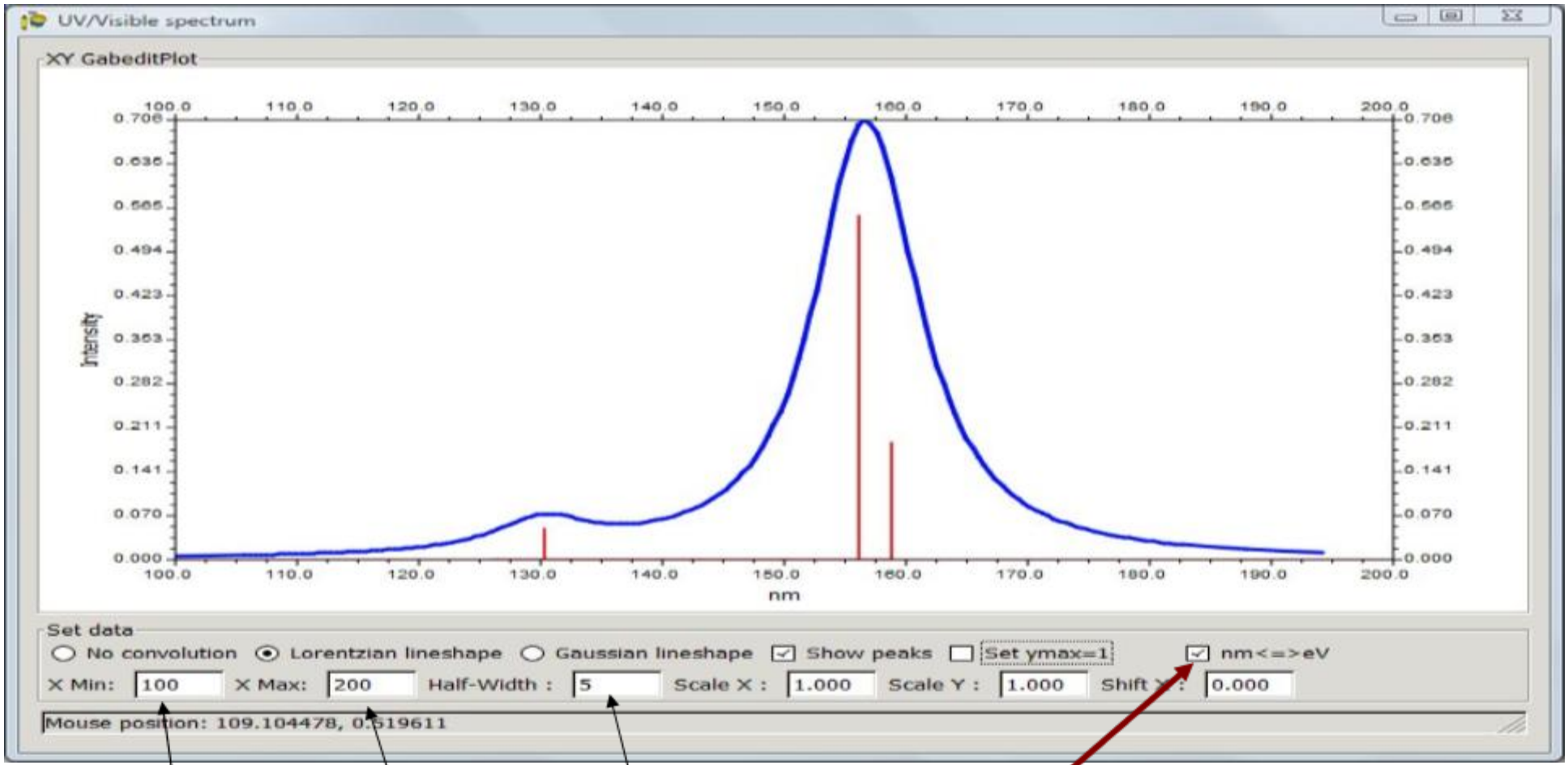
901.1500 UNK 0.4088 0.0000
1094.2100 UNK 143.0823 0.0000
1104.5900 UNK 0.0300 0.0000
1140.9900 UNK 0.0049 0.0000
1353.3500 UNK 0.0010 0.0000
Scale factor : 1
Time step(s) : 0.100000
Arrow radius : 0.100000
Steps by cycle : 4
Create a film
BMP
Folder
Play
Stop
2 Firefox
TutorialSi...
TutorialSi...
2 Adobe ...
Invite de c...
Gabedit
GIMP
geomConv...
vib.jpg-13....
FR
11:26

Computing of UV Spectrum by CIS method

- Close Geometry/Display window
- Choose File/New Orca input (or Orca icon) from the Menu.
- Select CIS method (For excited states method)
- Select Pople with one diffuse functions on non-hydrogen atom
- Select 6-31+G*
- Click OK button.
- Click to Run icon (toolbar, top of window).
- At save data file in text zone , type CIS
- Click to OK button.
- Orca is now started at background job.
- Select CIS.out notebook.
- Click to Update/End for reload the output file of Orca.
- When the job completes (and this may take several minutes, 2 minutes on my old computer, At the end of the output file you should obtain ****ORCA TERMINATED NORMALLY****).

Visualisation of the UV Spectrum

- From the menu, select **« Tools/UVSpectrum/Read energies and intensities form Orca output file »**
- Select CIS.out file



Click to « nm » button

Change Xmin (100); Xmax(200) ; Half-width(5)

Double click on the curve and save the data in CIS.txt

Visualisation of the orbitals implicated in transition of 156.2 nm (64020.3 cm^{-1})

- In CIS.out file, search the « CIS-EXCITED STATES » text
- We interest to state number 2
- This correpend to a transition from 7a to 10a (WARNNING in orca the numbering is started from 0 and not from 1)

We will visualize the orbitals number 8 and 11.

On Drawing Area of Geometry/Display window click with right button of mouse and select Orbitals/Read geometry and orbitals from a orca files.

Select the CIS.out file.

Select the orbital number 8 (already selected), click to OK button, click to OK button of the grid calculculation window, set isovalue to 0.1 and click to OK button.

Select Surfaces/delete All
Select Orbitals/Selection and select the orbital number 11, click to OK button, click to OK button of the grid calculculation window, set isovalue to 0.1 and click to OK button.

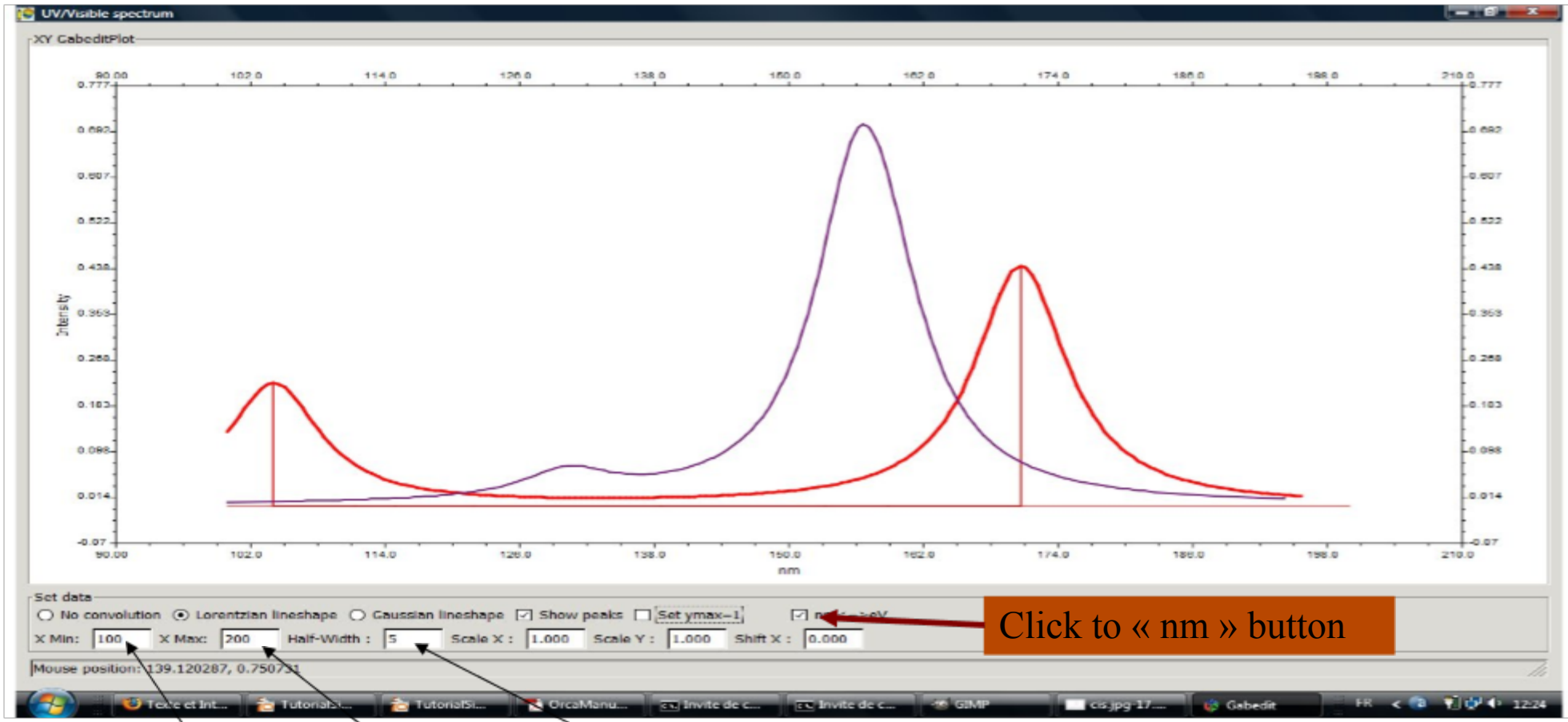
Computing of UV Spectrum by ZINDO/S and compare it to that of CIS method

Close Geometry/Display window

- Choose File/New Orca input (or Orca icon) from the Menu.
- **Select Semiemperical method (for Type of method)**
- Select CIS method (For excited states method)
- Click OK button.
- Click to Run icon (toolbar, top of window).
- At save data file in text zone , type ZINDO
- Click to OK button.
- Orca is now started at background job.
- Select ZINDO.out notebook.
- Click to Update/End for reload the output file of Orca.
- When the job completes (and this may take several seconds, 15 seconds on my old computer, At the end of the output file you should obtain ****ORCA TERMINATED NORMALLY****).

Visualisation of the UV Spectrums

- From the menu, select « Tools/UVSpectrum/Read energies and intensities form Orca output file ». Select ZINDO.out file



Change Xmin (100); Xmax(200) ; Half-width(5)

Add the CIS spectrum : right button : data/add data/read data from ASCII XY(2 columns) and select CIS. txt

Download the experimental spectrum from : http://webbook.nist.gov/cgi/cbook.cgi/74-85-1-UVVis.jdx?JCAMP=C74851&Index=0&Type=UVVis

and save it in UV.jdx file.. Add this to your spectrums (data/add data/read data from JDX file)