Tutorial : influence of environment on the uv-visible spectra of a small peptide : histidine amino-acid.

Prerequisite

- Gaussian
- Amber (sander, tleap)
- Amber 12 manual
- Any text editor (vi, emacs, gedit, geany or any you prefere)
- Visualisation programs : VMD, avogadro

1) Create a directory where you will put all your data. Go to this directory in a terminal
2) Creation of the small molecule histidine aminoacid using tleap

a) write done with an editor a script for tleap in the file tleap.in
$ vi tleap.in

```
source leaprc.ff14SB #Source leaprc file for ff14SB protein force field
source leaprc.gaff #Source leaprc file for gaff
source leaprc.tip3p #Source leaprc file for TIP3P water model
his=sequence {ACE HIS NME} #create the peptide and store in variable named his
desc his #check what you have created
savepdb his his-ini.pdb #save the initial structure in a pdb file named his-
ini.pdb
saveamberparm his his-ini.prmtop his-ini.inpcrd #Save AMBER topology and
coordinate files for the structure in vacuo
solvatebox his TIP3PBOX 8 #Solvate the molecule with a cubic water box
addions mol Cl- 0 #Add Cl- ions to neutralize the system
savepdb his his-solv.pdb #Save a pdb file of the coord of peptide + water
saveamberparm his his-solv.prmtop his-solv.inpcrd #Save AMBER topology and
coordinate files for the structure in a water box
quit #Quit tleap program
```

b) run tleap and check that in the output file tleap.log, there is no warning or problems.
$ tleap < tleap.in > tleap.log
you should now have created 6 files : `his-ini.pdb his-ini.prmtop his-ini.inpcrd his-solv.prmtop his-solv.inpcrd his-solv.pdb`
c) open with vmd the files his-solv.pdb and his-ini.pdb.
Check which protonation state of the histidine was chosen by tleap.
As you can see a structure is far from the ideal one (two Hydrogen atoms are too close).
We will first relax the structure before doing any calculations.

3) optimization of the structure using sander

a) create input file for sander program to perform a minimization (remove the comments in pink):

$ vi mini-ini.in

```
Minimize in vacuo
&cntrl
imin=1, maxcyc=200, (Perform minimization for 200 steps)
ntb=0, (Non-periodic simulation)
cut=20., (20 angstrom classical non-bond cut off)
&end
```

$ vi mini-solv.in

```
Minimize in Water
 &cntrl
  imin=1,
  ntx=1,
  irest=0,
  maxcyc=200,
  ntpr=10,
  ntwx=0,
  cut=8.0,
 /
```

b) run minimisation:

For structure in vacuo:

```
$ $AMBERHOME/bin/sander -O -i mini-ini.in -o his-iniMin.out -p his-
ini.prmtop -c his-ini.inpcrd -r his-iniMin.rst -inf his-iniMin.mdinfo &
```

sander uses a consistent syntax for each step of MD simulation. Here is a summary of the command line options of **sander**:

-O	Overwrite the output files if they already exist
-i 01_Min.in	Choose input file (default **mdin**)
-o 01_Min.out	Write output file (default **mdout**)
-p prmtop	Choose parameter and topology file **prmtop**
-c inpcrd	Choose coordinate file **inpcrd**
-r 01_Min.rst	Write output restart file with coordinates and velocities (default **restrt**)
-inf 01_Min.mdinfo	Write MD info file with simulation status (default **mdinfo**)
&	To make the calculation in background and be able to still use the terminal

Do the same for structure in water:

```
$ $AMBERHOME/bin/sander -O -i mini-solv.in -o his-solvMin.out -p his-
solv.prmtop -c his-solv.inpcrd -r his-solvMin.rst -inf his-solvMin.mdinfo &
```

check the .out files to see if the minimization is done (open with vi)

c) check that the obtained structures are indeed optimised (no more H atoms too close)

To do this, you need to creation of files .pdb using software ambpdb. Ambpdb need to have the correct topology file in name prmtop so the first command do a copy of the prmtopfile into prmtop and third command remove it after the use of ambpdb :

```
$ cp his-ini.prmtop prmtop
$ ambpdb <  his-iniMin.rst > his-iniMin.pdb
$ rm prmtop

$ cp his-solv.prmtop prmtop
$ ambpdb <  his-solvMin.rst > his-solvMin.pdb
$ rm prmtop
```

Open the .pdb files with vmd and check the structures.

d) If the structures do not seem to be optimized enough, rerun the minimization by increasing the number of cycles.

4) Calculation of the electronic transitions for the molecule in vacuo using Gaussian
With Avogadro software, open his-iniMin.pdb
Create a Gaussian input file in ground state of the structure, with the basis set 6-31G(d), functional B3LYP, and modify the file with an editor to have the heading for the calculation of the 3 first singlet states. Charge is equal to zero, spin should be singlet.
The file should look like this :
$vi his-iniMin-TDDFT.com

```
%chk=his-iniMin-TDDFT.chk
# td=(singlets,nstates=3) b3lyp/6-31g(d)

TDDFT in vacuo

0 1
 H            2.20900000   1.03600000   0.46300000
 C            2.12900000   2.10000000   0.23100000
 H            1.48800000   2.59300000   0.96300000
 H            1.71300000   2.22700000  -0.76900000
 C            3.50800000   2.71800000   0.28300000
 O            4.45500000   2.08100000   0.72700000
 N            3.61100000   3.96400000  -0.17600000
 H            2.77200000   4.44300000  -0.46800000
 C            4.85500000   4.74200000  -0.21200000
 H            5.43800000   4.49500000   0.67700000
 C            5.67800000   4.33500000  -1.45300000
 H            5.71400000   3.24500000  -1.51300000
 H            5.16600000   4.69400000  -2.35200000
 C            7.10500000   4.82900000  -1.46000000
 N            7.76300000   5.33600000  -2.58400000
 C            9.01500000   5.60400000  -2.18800000
 H            9.79900000   5.95200000  -2.85300000
 N            9.17400000   5.30400000  -0.88000000
 H           10.03300000   5.40100000  -0.35600000
 C            7.98500000   4.79200000  -0.41400000
 H            7.79600000   4.39200000   0.57400000
 C            4.56000000   6.25900000  -0.17600000
 O            3.40100000   6.66800000  -0.24300000
 N            5.60800000   7.09400000  -0.06000000
 H            6.52400000   6.67600000  -0.08400000
 C            5.53300000   8.55600000  -0.00100000
 H            4.49400000   8.88800000   0.01500000
 H            6.03300000   8.91600000   0.89800000
 H            6.02800000   8.98700000  -0.87300000
```

Check the transition energy (see in Gaussian output Excited States energies and oscillators section)
Remarks: It would be better to do before an optimization in vacuo using the same functional and basis set but it takes around one hour to perform it on one processor.

5) Calculation of the electronic transition for the molecule in implicit Water using Gaussian (QM/MM)

Take the obtained structure to perform a TD-DFT in Gaussian using the same basis set and functional for the 3 first singlet states but now with implicit water (PCM).

6) Calculation of the electronic transition for the molecule in explicit Water using Gaussian-ONIOM

Take the his-solvMin.pdb, file from the minimization in water.

a) First, we need to select only the water molecules that are at 6 Å from the peptide.

With VMD:

- Open his-solvMin.pdb
- To save pdb file with the selection of all the atoms of the peptide and the water where at least one atom is less than 6 Å from one atom of the peptide: First, check the selection "same resid as within 6 of resname ACE HIE NME" in the Graphical representation. Then, in VMD Main, right click on the molecule and save Coordinate with selected atoms "same resid as within 6 of resname ACE HIE NME"

Save in file his-solv6.pdb

b) Open his-solv6.pdb with Avogadro and create a Gaussian input file.

c) We will modify with an editor this input file to make a QM/MM input file. All the water molecules will be in the MM description and the peptide in the QM description. It is a 2-layer ONIOM calculation.

See http://gaussian.com/oniom/ for more information.

Modify the input to get this info:

$ vi his-QMMM-TDDFT-UFF.com

```
%chk=his-QMMM-TDDFT.chk
# td=(nstates=3,root=1) ONIOM(b3lyp/6-31g(d):UFF) geom=connectivity

QM/MM TD calculation

0 1 0 1 0 1
 H    0    11.57400000   11.09600000   13.96400000 H
 C    0    11.47300000   12.18600000   13.83500000 H
 H    0    10.73700000   12.53500000   14.55400000 H
 H    0    11.12000000   12.37900000   12.82200000 H
 C    0    12.78400000   12.85600000   14.10100000 H
 O    0    13.60600000   12.31800000   14.83300000 H
 N    0    12.98500000   14.02900000   13.51500000 H
 H    0    12.27700000   14.38600000   12.89300000 H
 C    0    14.22500000   14.81700000   13.55800000 H
 H    0    14.78000000   14.55000000   14.47700000 H
 C    0    15.10100000   14.43300000   12.35900000 H
 H    0    15.11100000   13.34600000   12.28500000 H
 H    0    14.64100000   14.82000000   11.45700000 H
 C    0    16.49800000   14.99900000   12.35800000 H
 N    0    17.24300000   15.30400000   11.20000000 H
 C    0    18.50300000   15.52300000   11.61900000 H
 H    0    19.31000000   15.90700000   10.98900000 H
 N    0    18.57400000   15.41900000   12.94400000 H
 H    0    19.40400000   15.52700000   13.50900000 H
 C    0    17.34000000   15.09800000   13.43000000 H
 H    0    17.15100000   14.74700000   14.43100000 H
```

```
 C    0    13.92800000    16.32700000    13.64000000 H
 O    0    12.75800000    16.71000000    13.75400000 H
 N    0    14.98100000    17.15400000    13.69600000 H
 H    0    15.91400000    16.76000000    13.57700000 H
 C    0    14.84900000    18.61200000    13.82000000 H
 H    0    13.80000000    18.95900000    13.87700000 H
 H    0    15.36600000    18.96700000    14.72000000 H
 H    0    15.30700000    19.10900000    12.96000000 H
 O    0    17.96200000    20.70200000    16.86200000 L
 H    0    16.98600000    20.73300000    16.67400000 L
 H    0    18.28900000    21.05400000    16.00400000 L
……
```

0 1 0 1 0 1 give the Charge and spin for entire molecule (real system), then the charge and spin for the high lever model (peptide) and the charge and spin for the low-model (waters)
You need to add the letter H at the end of each atom that is described in the high level model (peptide) and a L at the end of each atom that is described in the low-model (water).

The force field used is UFF
Check the transition energy (see in Gaussian output Excited States energies and oscillators section)

d) Let do the same with amber force field.
We need to modify the input file with the types of atoms :
$ vi his-QMMM-TDDFT-UFF.com

```
%chk=his-QMMM-TDDFT-amb.chk
# td=(nstates=3,root=1) ONIOM(b3lyp/6-31g(d):Amber) geom=connectivity

QM/MM TD calculation

0 1
 H-HC    0   11.57400000   11.09600000   13.96400000 H
 C-CT     0   11.47300000   12.18600000   13.83500000 H
 H-HC     0   10.73700000   12.53500000   14.55400000 H
 H-HC     0   11.12000000   12.37900000   12.82200000 H
 C-C-     0   12.78400000   12.85600000   14.10100000 H
 O-O-     0   13.60600000   12.31800000   14.83300000 H
 N-N-     0   12.98500000   14.02900000   13.51500000 H
 H-H-     0   12.27700000   14.38600000   12.89300000 H
 C-CT     0   14.22500000   14.81700000   13.55800000 H
 H-H1     0   14.78000000   14.55000000   14.47700000 H
 C-CT     0   15.10100000   14.43300000   12.35900000 H
 H-HC     0   15.11100000   13.34600000   12.28500000 H
 H-HC     0   14.64100000   14.82000000   11.45700000 H
 C-CC     0   16.49800000   14.99900000   12.35800000 H
 N-NB     0   17.24300000   15.30400000   11.20000000 H
 C-CR     0   18.50300000   15.52300000   11.61900000 H
 H-H5     0   19.31000000   15.90700000   10.98900000 H
 N-NA     0   18.57400000   15.41900000   12.94400000 H
 H-H-     0   19.40400000   15.52700000   13.50900000 H
 C-CW     0   17.34000000   15.09800000   13.43000000 H
 H-H4     0   17.15100000   14.74700000   14.43100000 H
 C-C-     0   13.92800000   16.32700000   13.64000000 H
 O-O-     0   12.75800000   16.71000000   13.75400000 H
 N-N-     0   14.98100000   17.15400000   13.69600000 H
 H-H-     0   15.91400000   16.76000000   13.57700000 H
 C-CT     0   14.84900000   18.61200000   13.82000000 H
 H-H1     0   13.80000000   18.95900000   13.87700000 H
 H-H1     0   15.36600000   18.96700000   14.72000000 H
 H-H1     0   15.30700000   19.10900000   12.96000000 H
 O-OW  0   17.96200000   20.70200000   16.86200000 L
```

```
 H-HW  0   16.98600000   20.73300000   16.67400000 L
 H-HW  0   18.28900000   21.05400000   16.00400000 L
 O-OW  0   19.92600000   19.21100000   17.96600000 L
 H-HW  0   20.21000000   19.96300000   18.53000000 L
 H-HW  0   19.10300000   19.61300000   17.58200000 L
 O-OW  0   17.88500000   23.13500000   18.31200000 L
 H-HW  0   17.88200000   23.86000000   17.64100000 L
 H-HW  0   17.80400000   22.36000000   17.71700000 L
 O-OW  0   23.59500000   16.55900000   16.56200000 L
 H-HW  0   22.87700000   16.50400000   17.22400000 L
 H-HW  0   23.90300000   15.62800000   16.54800000 L
 O-OW  0   16.58100000   18.66000000   20.07900000 L
 H-HW  0   16.12700000   18.01300000   20.67100000 L
 H-HW  0   16.79600000   18.09200000   19.32400000 L
 O-OW  0   15.60900000   23.30900000   14.61600000 L
 H-HW  0   16.57000000   23.37500000   14.74100000 L
 H-HW  0   15.42300000   24.09200000   14.07100000 L
 O-OW  0   19.23000000   14.87600000   19.17300000 L
 H-HW  0   19.26700000   14.80500000   20.15900000 L
 H-HW  0   18.28000000   14.64000000   19.04400000 L
 O-OW  0   20.67600000   19.71000000   15.25200000 L
 H-HW  0   21.62900000   19.91600000   15.34500000 L
 H-HW  0   20.47200000   19.40000000   16.15500000 L
 O-OW  0   18.58200000   22.47900000   14.67700000 L
 H-HW  0   19.37500000   22.04200000   14.27200000 L
 H-HW  0   18.93800000   23.39900000   14.73800000 L
 O-OW  0   20.59100000   21.55900000   13.10700000 L
 H-HW  0   20.64700000   20.63000000   13.39800000 L
 H-HW  0   20.47100000   21.44600000   12.14000000 L
 O-OW  0   22.96400000   17.38500000   14.03000000 L
 H-HW  0   22.73900000   16.48600000   13.74600000 L
 H-HW  0   23.17000000   17.23000000   14.98000000 L
 O-OW  0   15.43800000   21.18600000   16.24000000 L
 H-HW  0   14.64000000   21.34400000   16.78600000 L
 H-HW  0   15.37300000   21.94600000   15.61500000 L
 O-OW  0   21.36800000   16.93800000   18.41200000 L
 H-HW  0   20.66900000   16.27700000   18.60100000 L
 H-HW  0   20.79900000   17.71200000   18.17500000 L
 O-OW  0   16.89600000   18.73900000    6.33900000 L
 H-HW  0   16.64700000   17.83600000    6.61600000 L
 H-HW  0   16.17000000   19.25600000    6.76200000 L
 O-OW  0   20.04500000   16.54800000    8.03000000 L
 H-HW  0   20.02300000   17.26100000    7.33800000 L
 H-HW  0   19.16900000   16.14900000    7.87200000 L
 O-OW  0   19.61000000   18.51800000    6.26600000 L
 H-HW  0   19.86600000   19.46300000    6.17600000 L
 H-HW  0   18.63000000   18.61000000    6.23500000 L
 O-OW  0   18.30500000   19.41500000    9.61100000 L
 H-HW  0   17.65300000   20.14200000    9.76000000 L
 H-HW  0   17.72100000   18.71800000    9.27700000 L
 O-OW  0   24.33300000   18.93200000   12.39600000 L
 H-HW  0   23.73900000   18.40800000   13.00700000 L
 H-HW  0   24.89900000   19.35100000   13.09000000 L
 O-OW  0   17.16700000   23.82700000    8.70200000 L
 H-HW  0   16.68800000   24.33000000    9.39800000 L
 H-HW  0   17.04200000   22.91300000    9.05000000 L
 O-OW  0   16.33500000   25.03400000   11.13200000 L
 H-HW  0   16.83000000   24.29000000   11.55300000 L
 H-HW  0   15.64500000   25.17800000   11.81700000 L
 O-OW  0   17.79800000   22.94300000   12.04900000 L
 H-HW  0   17.93400000   22.65400000   12.98100000 L
 H-HW  0   18.73800000   23.05100000   11.77700000 L
 O-OW  0   19.94100000   21.48700000   10.40600000 L
```

```
 H-HW  0   19.47000000   20.74000000    9.98900000 L
 H-HW  0   20.44400000   21.83600000    9.64400000 L
 O-OW  0   20.84300000   18.38100000    9.95800000 L
 H-HW  0   20.70000000   17.63800000    9.33100000 L
 H-HW  0   19.93900000   18.77000000    9.95600000 L
 O-OW  0   23.46500000   17.42400000    7.26300000 L
 H-HW  0   23.10000000   17.51400000    6.34400000 L
 H-HW  0   22.70300000   17.01800000    7.70700000 L
 O-OW  0   22.96100000   20.10600000   10.35000000 L
 H-HW  0   23.40900000   19.69500000   11.12600000 L
 H-HW  0   22.18800000   19.49600000   10.26800000 L
 O-OW  0   16.58700000   21.47000000   10.05400000 L
 H-HW  0   15.70300000   21.22200000   10.43000000 L
 H-HW  0   16.97300000   21.91200000   10.85000000 L
 O-OW  0   17.07100000   15.60600000    4.54500000 L
 H-HW  0   17.89500000   15.23400000    4.14100000 L
 H-HW  0   17.40800000   15.85300000    5.42200000 L
 O-OW  0   16.94800000   15.94500000    7.66300000 L
 H-HW  0   16.95500000   15.78700000    8.62800000 L
 H-HW  0   16.21100000   15.33200000    7.41000000 L
 O-OW  0   24.73700000   16.68900000   10.88900000 L
 H-HW  0   24.53700000   17.53600000   11.35400000 L
 H-HW  0   25.62000000   16.91900000   10.51500000 L
 O-OW  0   16.06500000    8.42700000   15.89000000 L
 H-HW  0   16.39000000    8.92700000   15.11500000 L
 H-HW  0   16.10800000    9.13700000   16.57700000 L
 O-OW  0   16.56600000    9.53500000   20.23100000 L
 H-HW  0   16.47400000    9.77900000   19.27900000 L
 H-HW  0   17.51300000    9.32500000   20.27000000 L
 O-OW  0   21.27000000   13.36500000   18.15700000 L
 H-HW  0   21.06000000   12.46300000   18.46200000 L
 H-HW  0   20.52200000   13.86800000   18.55000000 L
 O-OW  0   22.31000000   11.37500000   15.27300000 L
 H-HW  0   22.08300000   12.16900000   14.73900000 L
 H-HW  0   21.40600000   11.05400000   15.48600000 L
 O-OW  0   16.22300000   10.44500000   17.68200000 L
 H-HW  0   15.32300000   10.84900000   17.64200000 L
 H-HW  0   16.76400000   11.21400000   17.39600000 L
 O-OW  0   21.90700000   13.50800000   13.64100000 L
 H-HW  0   22.72500000   14.00100000   13.36000000 L
 H-HW  0   21.80100000   12.94900000   12.82800000 L
 O-OW  0   18.33500000    9.30900000   13.92200000 L
 H-HW  0   18.87500000    9.86800000   14.52900000 L
 H-HW  0   18.84900000    8.47000000   13.97200000 L
 O-OW  0   16.70600000   13.77700000   19.08800000 L
 H-HW  0   16.48200000   13.28300000   19.91100000 L
 H-HW  0   15.79200000   13.93900000   18.75000000 L
 O-OW  0   17.95800000   12.54400000   16.97400000 L
 H-HW  0   18.50800000   13.22400000   16.53300000 L
 H-HW  0   17.60800000   13.06700000   17.73000000 L
 O-OW  0   20.15800000   14.19300000   15.66100000 L
 H-HW  0   20.77700000   13.98400000   14.92600000 L
 H-HW  0   20.73500000   14.00900000   16.42900000 L
 O-OW  0   19.69600000   10.67700000   15.82700000 L
 H-HW  0   19.10700000   11.29000000   16.31400000 L
 H-HW  0   19.77600000    9.94900000   16.48100000 L
 O-OW  0   21.90000000   11.96500000   11.40400000 L
 H-HW  0   21.82300000   12.51400000   10.58900000 L
 H-HW  0   21.55500000   11.11000000   11.06200000 L
 O-OW  0   17.63900000    8.08500000    9.51100000 L
 H-HW  0   17.12500000    7.52200000   10.13400000 L
 H-HW  0   17.89600000    8.81500000   10.12200000 L
 O-OW  0   21.74200000   13.49000000    9.12000000 L
```

```
 H-HW  0   21.09900000   14.11000000    8.73900000 L
 H-HW  0   21.89200000   12.89200000    8.34800000 L
 O-OW  0   24.36600000   14.42800000    9.35100000 L
 H-HW  0   24.33600000   15.28200000    9.83000000 L
 H-HW  0   23.42500000   14.16600000    9.38500000 L
 O-OW  0   15.99600000   13.10200000    4.98500000 L
 H-HW  0   15.66400000   13.27800000    5.89100000 L
 H-HW  0   16.34700000   13.99200000    4.75800000 L
 O-OW  0   18.47800000    9.94800000   11.29500000 L
 H-HW  0   18.37900000    9.73100000   12.25400000 L
 H-HW  0   18.10400000   10.84400000   11.27800000 L
 O-OW  0   24.06400000   14.76300000   12.69200000 L
 H-HW  0   24.89900000   14.26900000   12.67300000 L
 H-HW  0   24.26100000   15.47500000   12.04100000 L
 O-OW  0    9.81600000   21.51300000   15.35600000 L
 H-HW  0   10.58700000   22.08200000   15.11900000 L
 H-HW  0   10.16100000   20.64000000   15.08200000 L
 O-OW  0   11.78600000   23.22500000   14.53800000 L
 H-HW  0   11.78900000   23.27000000   13.56600000 L
 H-HW  0   12.71300000   23.40900000   14.75000000 L
 O-OW  0   11.82800000   19.51300000   17.08000000 L
 H-HW  0   11.44300000   19.21000000   16.23200000 L
 H-HW  0   11.37600000   18.91900000   17.71100000 L
 O-OW  0    9.38000000   16.47000000   15.24100000 L
 H-HW  0    9.74800000   15.97800000   15.99000000 L
 H-HW  0    8.62000000   16.92300000   15.68400000 L
 O-OW  0   10.81300000   18.73900000   14.66000000 L
 H-HW  0   11.53800000   18.25600000   14.20800000 L
 H-HW  0   10.16500000   18.00300000   14.75600000 L
 O-OW  0   13.75400000   24.12900000   18.20000000 L
 H-HW  0   13.54700000   23.16400000   18.09800000 L
 H-HW  0   12.83300000   24.47500000   18.27300000 L
 O-OW  0   13.33500000   21.49300000   17.97600000 L
 H-HW  0   13.65300000   20.95400000   18.74100000 L
 H-HW  0   12.71800000   20.82000000   17.57600000 L
 O-OW  0   14.25300000   20.17200000   20.17500000 L
 H-HW  0   14.16500000   19.73200000   21.05200000 L
 H-HW  0   15.14200000   19.82500000   19.92000000 L
 O-OW  0   15.06100000   20.35000000    7.55400000 L
 H-HW  0   14.43100000   21.06200000    7.26700000 L
 H-HW  0   15.40300000   20.75900000    8.37300000 L
 O-OW  0   14.05600000   20.83100000   10.60200000 L
 H-HW  0   13.66400000   21.68600000   10.28400000 L
 H-HW  0   13.25800000   20.26800000   10.55500000 L
 O-OW  0   11.41100000   20.29700000    9.43400000 L
 H-HW  0   10.55900000   20.22300000    9.91700000 L
 H-HW  0   11.14300000   20.89800000    8.70600000 L
 O-OW  0   11.90600000   14.94400000   10.68800000 L
 H-HW  0   12.48500000   14.19900000   10.40700000 L
 H-HW  0   11.92000000   15.46500000    9.84500000 L
 O-OW  0   12.96200000   18.58400000    7.98000000 L
 H-HW  0   12.40300000   19.18400000    8.52500000 L
 H-HW  0   13.74000000   19.16000000    7.83500000 L
 O-OW  0   11.04700000   23.30200000   11.47000000 L
 H-HW  0   11.74800000   23.02500000   10.83900000 L
 H-HW  0   10.71900000   24.10600000   11.00600000 L
 O-OW  0    8.99200000   19.91900000   10.86300000 L
 H-HW  0    8.41100000   19.23700000   10.46100000 L
 H-HW  0    9.30000000   19.43700000   11.65200000 L
 O-OW  0   13.05200000   23.04200000    9.50100000 L
 H-HW  0   13.11400000   22.81700000    8.54700000 L
 H-HW  0   13.21000000   24.02100000    9.44300000 L
 O-OW  0   12.22200000   16.03200000    8.16500000 L
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 H-HW  0   12.65900000   16.90100000    7.99400000 L
 H-HW  0   12.21700000   15.66900000    7.25000000 L
 O-OW  0    8.25300000   17.22700000   10.42000000 L
 H-HW  0    8.87300000   17.22600000    9.65600000 L
 H-HW  0    8.78000000   16.68700000   11.06000000 L
 O-OW  0    9.82100000   17.52900000    8.23200000 L
 H-HW  0    9.57000000   16.70000000    7.73400000 L
 H-HW  0   10.78900000   17.36100000    8.29600000 L
 O-OW  0    9.64800000   15.89400000   12.28600000 L
 H-HW  0    9.78300000   16.01500000   13.24000000 L
 H-HW  0   10.53900000   15.64100000   11.98500000 L
 O-OW  0    8.03900000    8.13500000   18.13300000 L
 H-HW  0    7.61000000    8.48800000   17.31600000 L
 H-HW  0    7.88100000    8.89600000   18.73400000 L
 O-OW  0   11.68400000    9.62000000   18.17600000 L
 H-HW  0   11.53600000    8.67200000   18.41700000 L
 H-HW  0   11.22800000   10.05300000   18.92000000 L
 O-OW  0    9.22900000    6.25100000   15.20800000 L
 H-HW  0    9.69500000    5.42300000   15.39700000 L
 H-HW  0    9.96100000    6.90200000   15.34300000 L
 O-OW  0    7.20000000   10.63300000   19.28200000 L
 H-HW  0    7.95700000   11.19500000   19.00300000 L
 H-HW  0    6.84900000   11.21400000   20.00600000 L
 O-OW  0    9.11400000   12.88200000   19.62500000 L
 H-HW  0    9.71600000   12.26300000   20.10200000 L
 H-HW  0    9.45100000   13.73700000   19.96300000 L
 O-OW  0    6.46300000    9.20100000   16.12000000 L
 H-HW  0    6.32300000   10.06700000   15.68200000 L
 H-HW  0    5.63800000    9.12600000   16.63600000 L
 O-OW  0   13.67700000   11.33600000   17.36100000 L
 H-HW  0   12.95600000   10.70900000   17.60600000 L
 H-HW  0   13.49900000   11.43500000   16.40100000 L
 O-OW  0   11.32900000    7.88500000   15.70700000 L
 H-HW  0   11.29100000    8.52800000   16.43700000 L
 H-HW  0   12.20800000    7.48000000   15.86800000 L
 O-OW  0    6.02500000   11.57000000   14.63900000 L
 H-HW  0    6.38400000   11.17900000   13.81600000 L
 H-HW  0    5.13400000   11.83800000   14.32700000 L
 O-OW  0    7.23400000    7.55000000   13.97700000 L
 H-HW  0    6.89100000    8.07600000   14.73500000 L
 H-HW  0    7.95400000    7.05300000   14.44600000 L
 O-OW  0    6.02300000   13.82000000   16.34300000 L
 H-HW  0    6.88000000   14.11700000   16.00000000 L
 H-HW  0    5.93600000   12.95400000   15.88300000 L
 O-OW  0   13.84200000    6.81500000   15.97600000 L
 H-HW  0   14.64600000    7.36900000   16.11300000 L
 H-HW  0   13.88500000    6.26300000   16.79000000 L
 O-OW  0   14.49000000    7.05700000   13.30100000 L
H-HW  0   13.97700000    7.77000000   12.88800000 L
 H-HW  0   14.15400000    7.09900000   14.22400000 L
 O-OW  0   12.37400000   14.07800000   20.09500000 L
 H-HW  0   13.05600000   13.84600000   19.43100000 L
 H-HW  0   12.49900000   13.34000000   20.73300000 L
 O-OW  0   14.17800000   13.86000000   18.05400000 L
 H-HW  0   14.00100000   12.92000000   17.79900000 L
 H-HW  0   13.66300000   14.32600000   17.37900000 L
 O-OW  0   11.21600000   12.72900000    7.66200000 L
 H-HW  0   10.71900000   13.44900000    7.23900000 L
 H-HW  0   10.49200000   12.16600000    8.00300000 L
 O-OW  0   13.94000000   10.09300000    9.41500000 L
 H-HW  0   14.68300000    9.95100000    8.77600000 L
 H-HW  0   13.62100000    9.17700000    9.49900000 L
 O-OW  0    7.72400000   13.37500000    8.29200000 L
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 H-HW  0     8.05400000   13.06500000    9.14800000 L
 H-HW  0     6.91200000   13.86600000    8.58300000 L
 O-OW  0     7.24000000   10.04600000    9.87500000 L
 H-HW  0     7.09800000    9.07100000    9.88800000 L
 H-HW  0     6.50800000   10.32500000   10.47200000 L
 O-OW  0     9.70100000   10.80700000    9.01900000 L
 H-HW  0     9.97700000   10.77700000    9.95200000 L
 H-HW  0     8.75100000   10.54000000    9.12000000 L
 O-OW  0     5.47000000   10.60500000   11.91100000 L
 H-HW  0     5.05100000    9.88200000   12.44900000 L
 H-HW  0     4.65400000   11.10400000   11.67300000 L
 O-OW  0     8.71400000    9.26000000   12.26400000 L
 H-HW  0     7.99500000    9.58000000   11.69800000 L
 H-HW  0     8.22700000    8.66700000   12.87400000 L
 O-OW  0     9.79300000    6.85300000   10.25000000 L
 H-HW  0    10.25900000    7.61700000   10.63000000 L
 H-HW  0     8.86000000    7.10300000   10.43600000 L
 O-OW  0    13.36100000   12.82400000    9.35300000 L
 H-HW  0    12.59800000   12.74200000    8.73500000 L
 H-HW  0    13.58400000   11.86800000    9.46300000 L
 O-OW  0    11.39000000    9.01200000    7.74400000 L
 H-HW  0    10.82300000    9.68900000    8.18200000 L
 H-HW  0    11.86500000    9.61100000    7.10400000 L
 O-OW  0    14.82600000   14.16500000    7.29200000 L
 H-HW  0    13.99300000   14.39600000    6.83400000 L
 H-HW  0    14.46500000   13.72600000    8.09600000 L
 O-OW  0     5.37200000   14.69300000   12.55700000 L
 H-HW  0     6.27100000   14.32100000   12.57200000 L
 H-HW  0     5.53500000   15.50500000   12.01300000 L
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Check the transition energy (see in Gaussian output Excited States energies and oscillators section)