Computational Chemistry 2, CHEM-E4225, Exercise 1 23.4.2021

To run Orca you need to load it: module load orca

to run it (in Wihuri) jsub -np 4 orca H2O.inp

There are a lot of example file in /home/kari/CC2-2021-example

To see what is in this dir type ls -l /home/kari/CC2-2021-example (ls is the list command)

you can copy the example files to your own directory: cp /home/kari/CC2-2021-example/h2o.inp . (there is a dot at the end it is your working directory)

1) Compare the Mulliken and Lowdin charges of the N2C3 molecule in the lecture notes (Chapter 4). Do a PBE calculation and large basis (TZ or QZ, like cc-pVQZ) of the molecule. The coordinates are in the CC2-2021-example dir. (you can also look the n2c3-mol.charge.txt file for Bader charges and PBE0, MP2 values) . Does the Mulliken and Lowdin charges agree with each other and to the values in the lectures?

2) Find how to computer the molecular polarization. Compute polarization of some molecules, like water, methanol, methyl-phenol.

3) Do a vibrational calculation for a water and methanol molecules. Note that you need to optimize the molecule first. What can you say of the IR intensities. (additional: use orca_mapspc tool to make the IR plot, note that the upper limit need to be increased to 4500 cm-1. You can use gnuplot to plot the spectra. inside gnuplot plot 'h2o-PBE-vib.oout.ir.dat' w l)

4) Use the orca_pltvib tool to visualize some frequency modes. Use the ase-gui to visualize the modes.

5) Use the polarization to compute the Raman intensities. NOTE that you need to do frequencies as numerical freq (numfreq keyword).

6) Do calculation of water dimer with PBE. Use ma-def2-TZVP basis. You may want to use the van der Waals correction (D3zero). What is the binding energy. (for this you need the water monomer energy). Do the frequency calculations for water molecule and dimer. Compare the energy and Free energy. What is the temperature in these calculations.

Extra: (old) Find out how to make molecules with ChemDraw software. You can use directly the Chem3D module or draw the molecule with ChemDraw and copy it to Chem3D. Make 2-Me-phenol, 3-Me-phenol, and 4-Me-phenol structures. Learn to transfer the xyz coordinates to wihuri. The xyz format in

Chem3D is stupid because it is not standard. One can save the file in Gaussian or Games format. They are almost correct.

Extra: do the benzene vibration calculation compare that the lectures. (Chapter 4)

ase-gui can be started with ‘module load ase’

The instructions of Wihuri are included.

In the first time make your own directory in /home/kari/CC2-2021-results
mkdir /home/kari/CC2-2021-results/ossi (ossi should be your own name)
At end of exercise copy the results to your result dir: cp *out /home/kari/CC2-2021-results/ossi

Orca input library: https://sites.google.com/site/orcainputlibrary/home