Computational Chemistry 2, CHEM-E4225, Exercise 3 30.9.2021

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

2) Do the benzene vibration calculation compare that the lectures. (Chapter 4)

3) Use the orca_pltvib tool to visualize some frequency modes. Use the ase gui of vmd to visualize the modes.

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

5) 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.

ase gui can be started with 'module load python/3.8-gpaw'

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