Computational Chemistry 1, CHEM-E4110, Quantum chemistry Exercise 2 11.1.2019

1) Find out the ethane and ethene torsional scan input and do the scan calculations. What are the torsional potentials.

2) Find from the input library a transition state calculation of $CH_3Cl + F^- \rightarrow Cl^- + CH_3F$ and do it.

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.)

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

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

ag can be started with 'module load ase' and 'module load gpaw-setups'

The instructions of Wihuri are included. Also example files of the exercises are included.

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