Computational Chemistry 1, CHEM-E4110, Quantum chemistry Exercise 1 8.1.2019

1) Find the ORCA manual and find out the basis sets

2) 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.

3) Do a HF geometry optimization calculation for H_2O and n-me-phenol molecules. Use TZVP basis sets. Compute the energy differences of the n-me-phenol molecules.

4) What are the dipole moments and some of the bond lengths of the computed molecules. VMD (in windows) and ag (in wihuri) are convenient tools to look the molecules. The read the .xyz file of the molecule.

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

ag can be started with 'module load ase'

The instructions of Wihuri are included. Also example files of the exercises are in the dir /home/kari/CC-example.

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