Computational Chemistry 2, CHEM-E4225, Exercise 1 16.9.2021

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

to run it (in Wihuri) jsub -np 4 orca H2O.inp (H2O.inp can be any .inp file)

There are a lot of example files 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 the ORCA (quantum chemistry program) manual and find out the methods like HF BLYP and 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 PBE (or 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 ase gui (in wihuri) are convenient tools to look the molecules. The read the .xyz file of the molecule.

5) Do a HF, MP2, CCSD(T), CASSCF(8,6) and CASSCF(8,12) calculations for water. What is the correlation energy in these cases? In CASSCF you need to subtract the HF energy form the total energy. Optimize the molecules geometry with PBE and use the same geometry in all calculations. Use TZVPP basis. In case of CCSD(T) try also QZVPP basis. (The grep command is useful: grep FINAL h2o-MP2.oout the grep fill print all lines that have text FINAL in file h2o-MP2.oout, you can also type: grep FINAL h2o*.oout)

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

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 to this dir: cp *out /home/kari/CC2-2021-results/ossi

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