Computational Chemistry 2, CHEM-E4225, Exercise 1 26.10.2023

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

see available modules: module avail

to run it (in mylly2**)** **jsub orca H2O.inp** or jsub -np 4 orca xx.inp (H2O.inp can be any .inp file)

There are a lot of example files in /home/kari/CC2-2023-examples

To see what is in this dir type ls -l /home/kari/CC2-2023-examples (ls is the list command)

you can copy the example files to your own directory: cp /home/kari/CC2-2023-examples/h2o.inp . (there is a dot at the end. It is your working directory.)

1) Find the ORCA 4.x (quantum chemistry program) manual and find out the methods like HF, BLYP and the basis sets. The manual of 5.0 requires registration. Version 4.x is good enough.

2) Do a PBE (or HF) geometry optimization calculation for H_2O and n-me-phenol molecules. Use cc-pVTZ basis sets. Compute the energy differences of the n-me-phenol molecules. How many basis functions are used in the computations. How many SCF iterations were done at the first iteration. How long the computations take. Note orca used au in energy (see below). (The grep command is useful: grep FINAL *phenol-PBE.out the grep will print all lines that have text FINAL in file that ends phenol-PBE.out)

3) What are the dipole moments and some of the bond lengths of the computed molecules. ase gui (in mylly2) is a convenient tool for looking the molecules. It reads the .xyz file of a molecule. The *_traj.xyz will contain the optimization geometries.

4) 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 from the total energy. Optimize the molecules geometry with PBE and use the same geometry in all calculations. Use cc-pVTZ basis. In case of CCSD(T) try also cc-pVQZ basis. (The grep command is useful: grep FINAL h2o-MP2.out the grep will print all lines that have text FINAL in file h2o-MP2.out, you can also type: grep FINAL h2o*.out)

5) Extra: 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 mylly2. 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.

ase gui can be started with 'module load python'

The instructions of mylly2 are included.

1 au = 27.211 eV = 2625 kJ/mol = 627.5 kcal/mol

See also constants.dvi (yorku.ca)

In the first time make your own directory in /home/kari/CC2-2023-results
mkdir /home/kari/CC2-2023-results/ossi (ossi should be your own name)
It is convenient to make an own directory for each exercise: mkdir exer1
and then go to this dir: cd exer1 (you can move between dirs. cd ../exer2 (.. means one dir above in the tree)

At end of exercise copy the results to your result to this dir: cp *.out /home/kari/CC2-2023-results/ossi

In Orca input library there are several input examples:
https://sites.google.com/site/orcainputlibrary/home