Computational Chemistry 2, CHEM-E4225, Exercise 2 2.10.2023

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

to run it (in mylly2) jsub -np 4 -mem 3G orca big-xxx.inp

There are a lot of example file 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) Try the extrapolation method with MP2 for a big molecule (coordinates big-test.xyz and other big starting files). Do an extrapolation with DZ and TZ basis (for example cc-pV* basis, check that the input files have the parallel mode on, use 12 cores and 3G of memory. This will take more than ½ hour). Compare the FINAL energies of big*CCSD*DZ-p.out. Do also a PBE calculation with DZ basis. Compare the computer times.

2) Compare the Mulliken, Lowdin ChelpG charges of the N2C3 molecule in the lecture notes (Chapter 4). Do a PBE calculation and large basis (TZ or QZ, like cc-pVQZ) of the molecule. The coordinates are in the CC2-2023-example dir. The CHELPG charges can be computed with orca_chelpg tool by giving it the wavefunction (n2c3…gbw file) (you can also look the n2c3-mol.charge.txt file for Bader charges and PBE0, MP2 values, Warning in this file the atom order is different). Does the Mulliken, Lowdin, ChelpG charges agree with each other and to the values in the lectures?

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

4) 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. inside gnuplot plot 'h2o-PBE-vib.oout.ir.dat' w l)

5) Use the orca_pltvib tool to visualize some frequency modes. Use the ase gui to visualize the modes.

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

ase gui can be started with ‘module load python’

The instructions of mylly2 are included.

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

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