Lab3

Objectives

- Single point energy calculations
- Geometry optimization
- Frequencies and normal mode calculations
- Basis set effect

H2O single point energy

1. Calculate single point energy of H_2O dimer at HF/6-31* for several distances between two molecules. Generate plots for
    a. Total energy

as functions of the distance. Use HF method. Write down your observations.

Geometry optimization

Gaussian logfile:

Item	Value	Threshold	Converged?
Maximum Force	0.000006	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.000111	0.001800	YES
RMS Displacement	0.000052	0.001200	YES

H2O geometry optimization

1. Optimize the geometry of the H_2O molecule while varying basis sets, including 3-21, 6-31, 6-31*, 6-311, 6-311*, cc-pVDZ, and cc-pVTZ. Generate plots for
   a. Total energy
   b. r(HO) distance
   c. θ(HOH) angle
   d. Dipole moment

as functions of the basis sets. Use HF method. Write down your observations.

Experimental values:

r(OH) = 0.9578 Å; θ(HOH)= 104.48° , $\boldsymbol{\mu}$=1.85D

H2O dimer frequency calculation

1. Optimize the geometry of the H_2O dimer at HF/6-31* and do frequency calculation. Report,
   a. Binding energy
   b. Interaction energy
   c. r(H - - -O) distance
   d. θ(H - - - O-H) angle
   e. Total number of frequencies reported in Gaussian log file
   f. Zero-point energy

Basis set superposition error (BSSE)

Gaussian input file for water dimer:

```
%chk=water.chk
%nprocshared=2
# hf/3-21g counterpoise=2

Title Card Required

0 1 0 1 0 1
 O(Fragment=1)     -1.97619047   -1.11904760    0.00000000
 H(Fragment=1)     -1.01619047   -1.11904760    0.00000000
 H(Fragment=1)     -2.29664505   -0.21411177    0.00000000
 O(Fragment=2)      0.80952381   -0.38095238    0.00000000
 H(Fragment=2)      1.76952381   -0.38095238    0.00000000
 H(Fragment=2)      0.48906922    0.52398346    0.00000000
```

Basis set superposition error (BSSE)

$ grep A.U. water.log

```
SCF Done:  E(RHF) =  -151.183376551     A.U. after   10 cycles
SCF Done:  E(RHF) =  -75.5871648459     A.U. after    9 cycles
SCF Done:  E(RHF) =  -75.5908152208     A.U. after    9 cycles
SCF Done:  E(RHF) =  -75.5858099772     A.U. after   10 cycles
SCF Done:  E(RHF) =  -75.5858099773     A.U. after   10 cycles
```

```
grep -A 4 'Counterpoise ' water.log
Counterpoise corrected energy =    -151.177016439265
                  BSSE energy =       0.006360112084
             sum of fragments =    -151.171619954583
          complexation energy =      -7.38 kcal/mole (raw)
          complexation energy =      -3.39 kcal/mole (corrected)
```

Hands-on

1. Compute the BSSE for the water dimer
2. Determine the BSSE for the water dimer for several distances between the water molecules
3. Determine BSSE for the water dimer as a function of basis set size?

(Use HF method in all cases)

References

1. https://avogadro.cc/
2. https://gaussian.com/gaussian16/
3.