Experiment 10: Computational Chemistry: Geometry optimization using Avogadro software

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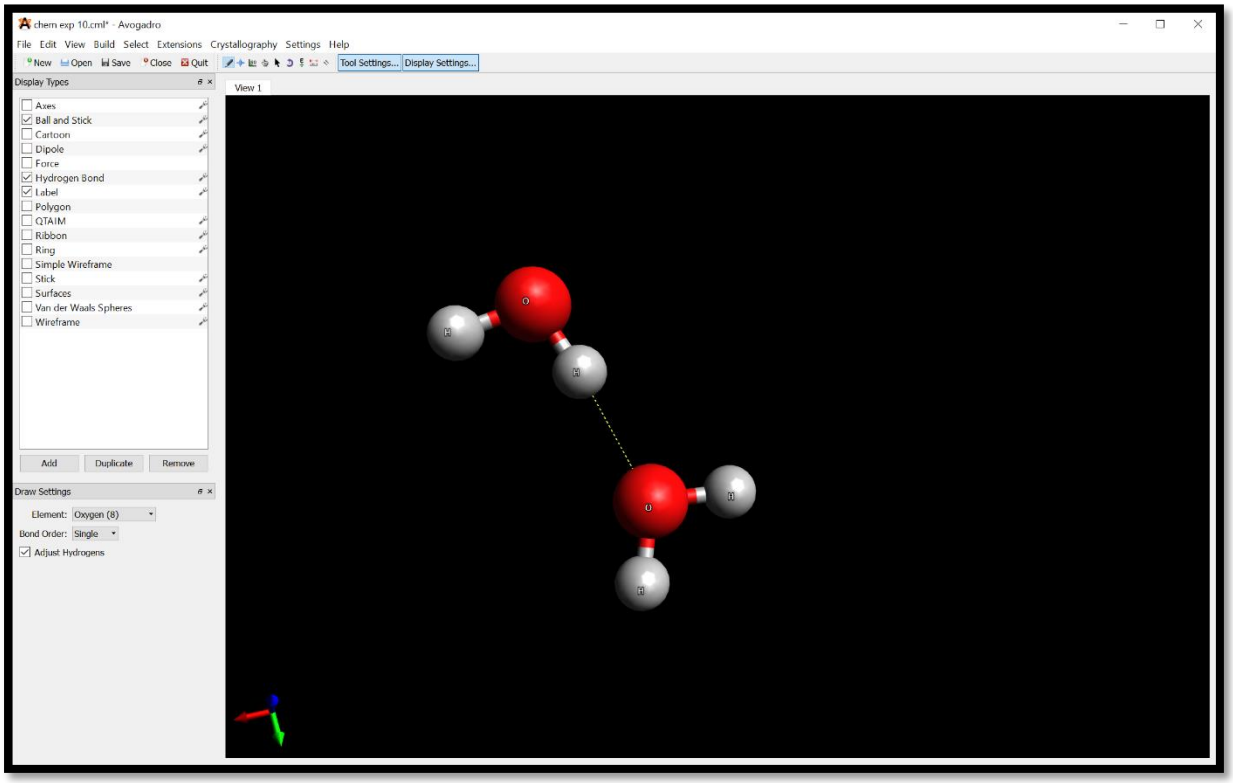
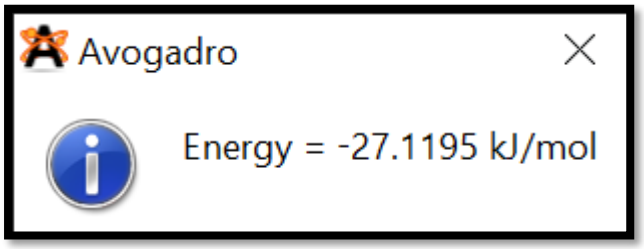
Slot: L11-L12

Date: 21/12/21

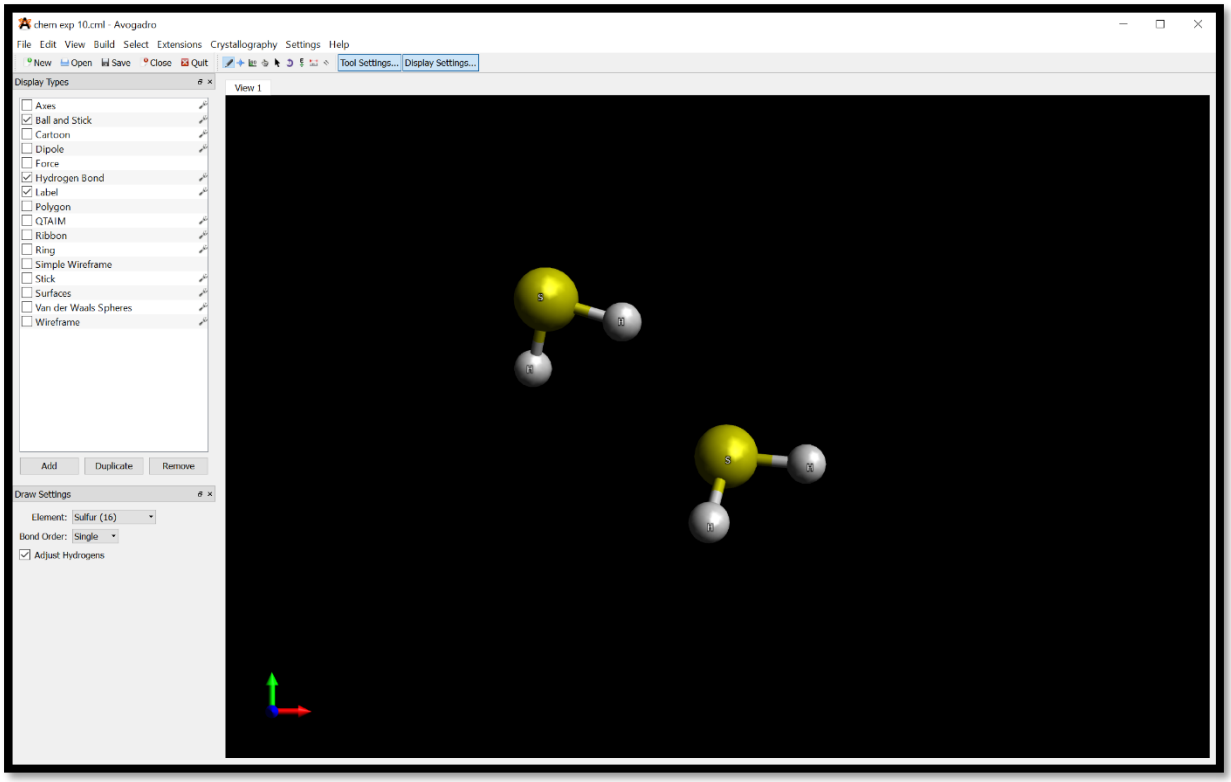
1) Comparison and modelling of **water (H_2O) dimer** and **H_2S dimer** to investigate the influence of ***intermolecular*** **hydrogen bonding**.

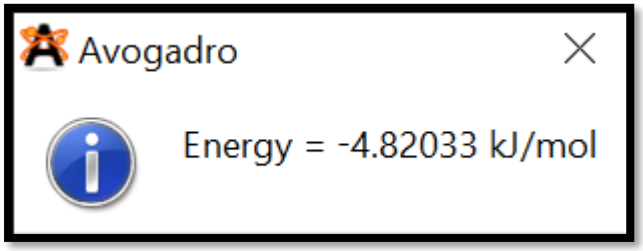
a) H_2O



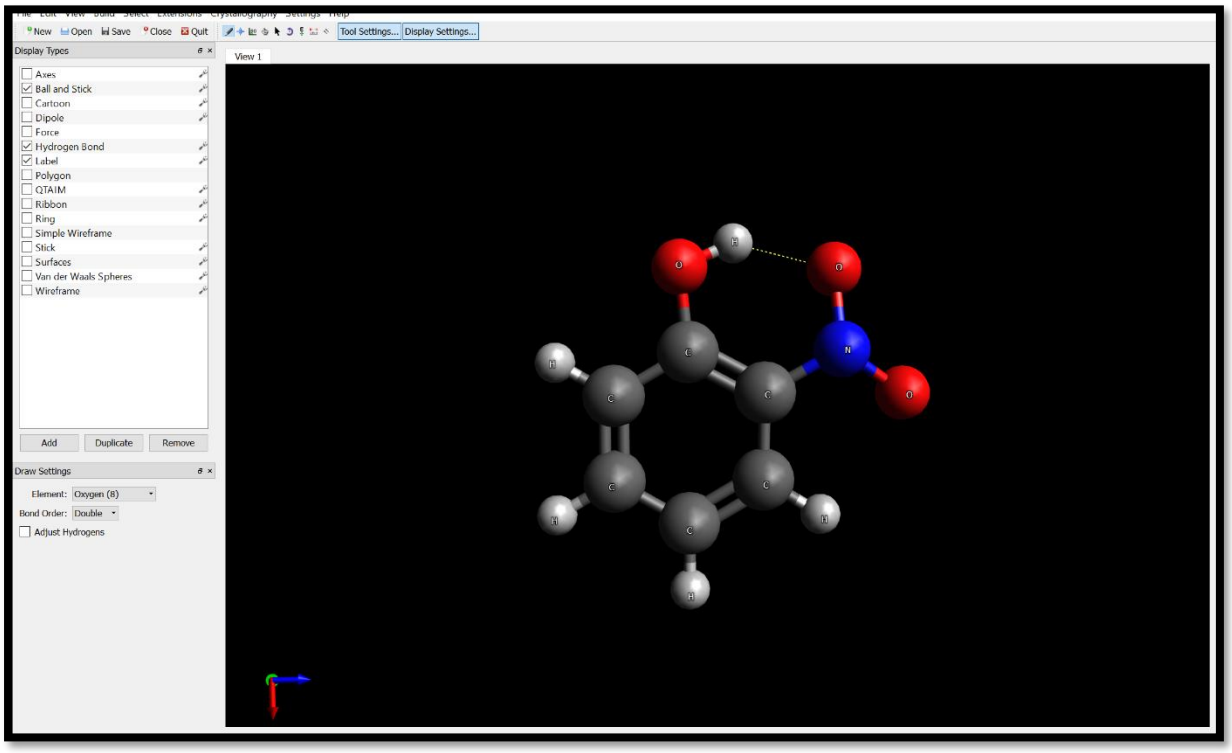


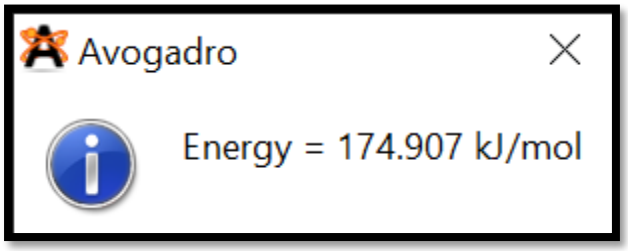
b) $\underline{H_2S}$





2) Modelling of **2-nitrophenol** to study the influence of ***intramolecular*** **hydrogen bonding**.





Results:

1. Visualize the geometry of H_2O and H_2S dimers.
2. The energy of **H_2O dimer** = **-27.1195 kJ/mol**

   H_2S dimer = **-4.82033 kJ/mol**
3. Visualize the geometry of 2-nitrophenol.
4. The energy of **2-nitrophenol** = 1**74.907 kJ/mol**