10月9日上机实习安排

使用Gaussian软件完成：

1. $(H_2O)_3$团簇结构的优化，并进一步计算该团簇中氢键的平均键能
2. S_{N2}反应机理研究：F^- (g) + CH_3Cl (g) → CH_3F (g) + Cl^- (g)，以及主要反应物、产物的IR、UV-vis、NMR光谱

PPT展示：2名同学

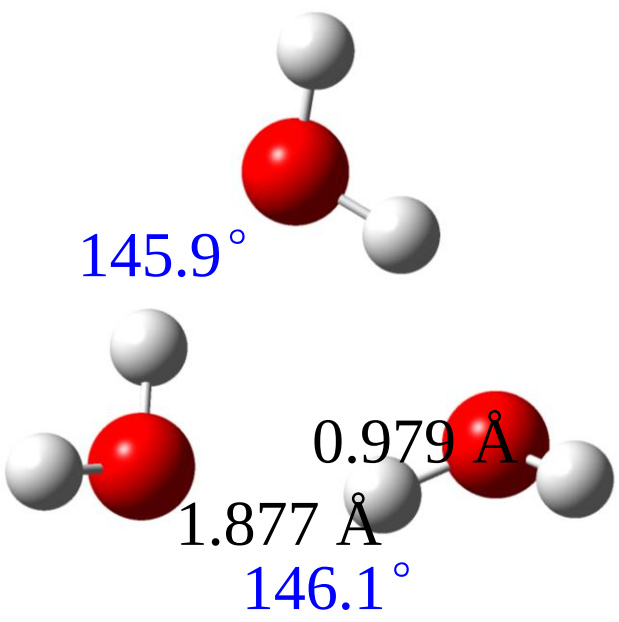
李振兴(+10)：NBO分析，给出H_2O孤对电子的自然键轨道

钱思源 (+10) ：NMR原理

上机操作：作业逐项完成，下课前10 min告之完成情况

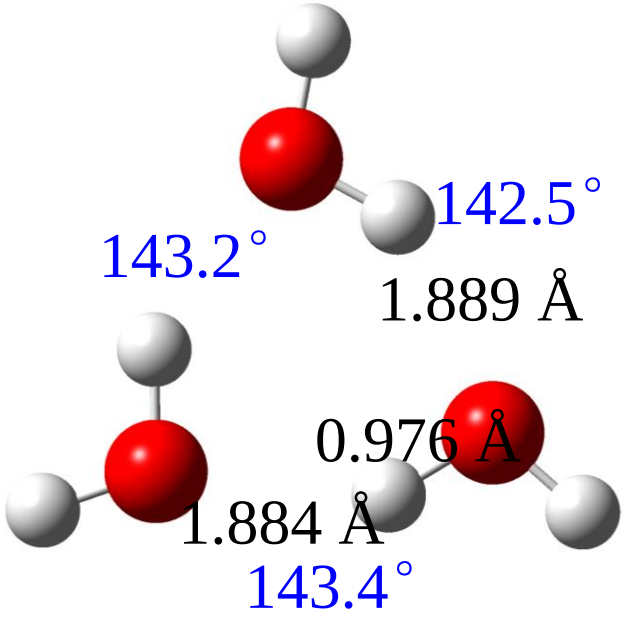
Geometry Optimization of $(H_2O)_3$ Cluster

➢Computational level: M06-2X/6-31+G(d)



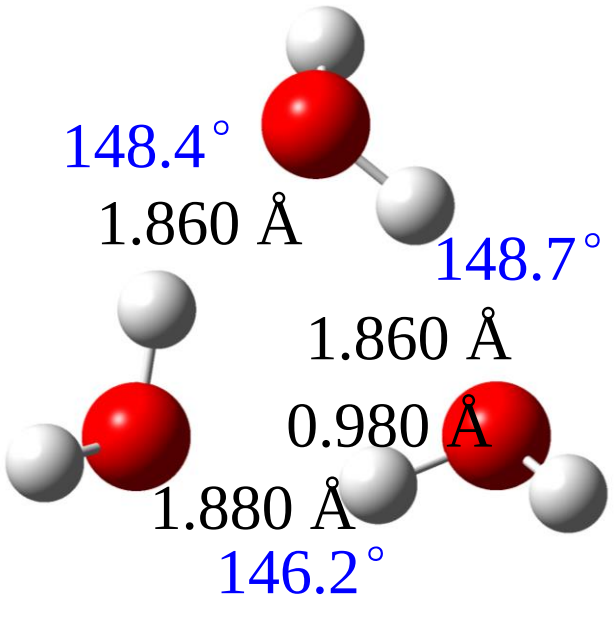
Isomer I

-229.18487148 a.u.



Isomer II

-229.18436347 a.u.

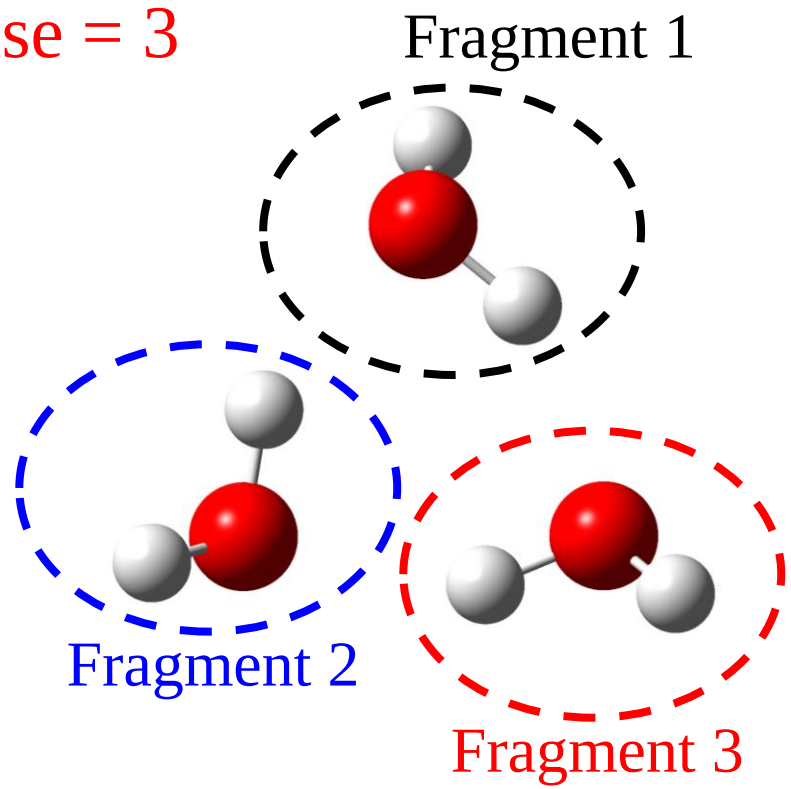


Isomer III

-229.18657639 a.u.

Geometry Optimization of $(H_2O)_3$ Cluster

- Computational level: M06-2X/6-31+G(d)
- Counterpoise = 3

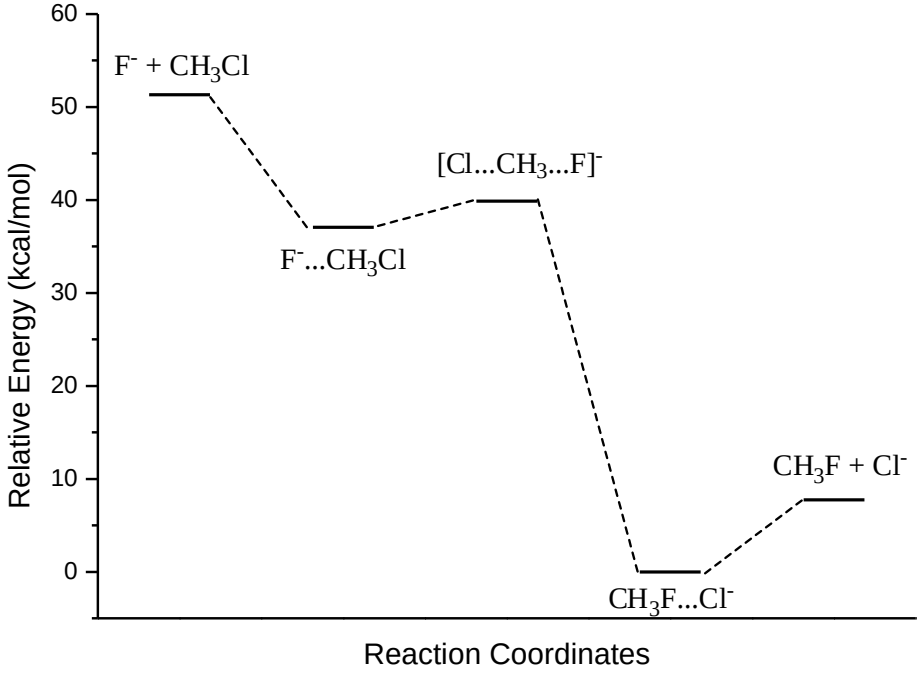


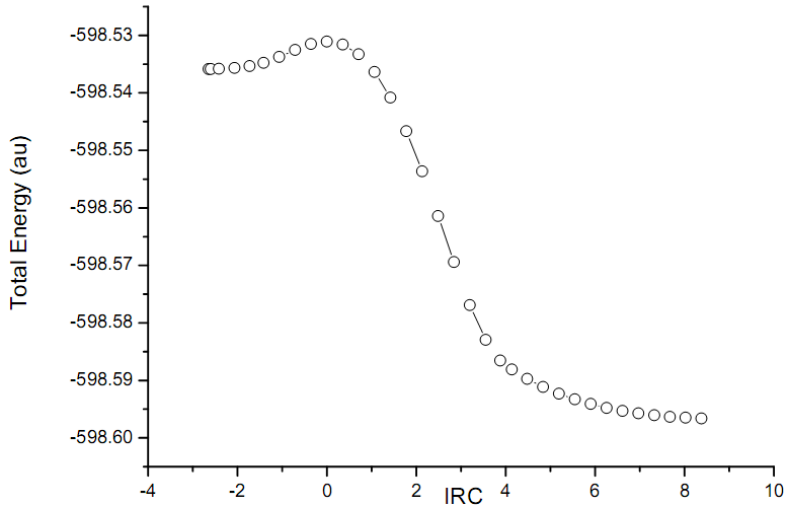
Isomer III

$$E_I(\text{corrected}) = [E_{123} - (E_1 + E_2 + E_3) - E_{BSSE}]/3$$

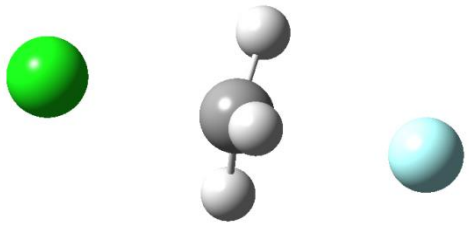
S_{N2}-Reaction Mechanism:
$F^- (g) + CH_3Cl (g) \rightarrow CH_3F (g) + Cl^- (g)$

- Computational level: CAM-B3LYP/6-31+G(d)





The structure of the TS:



r(C-Cl)=2.134

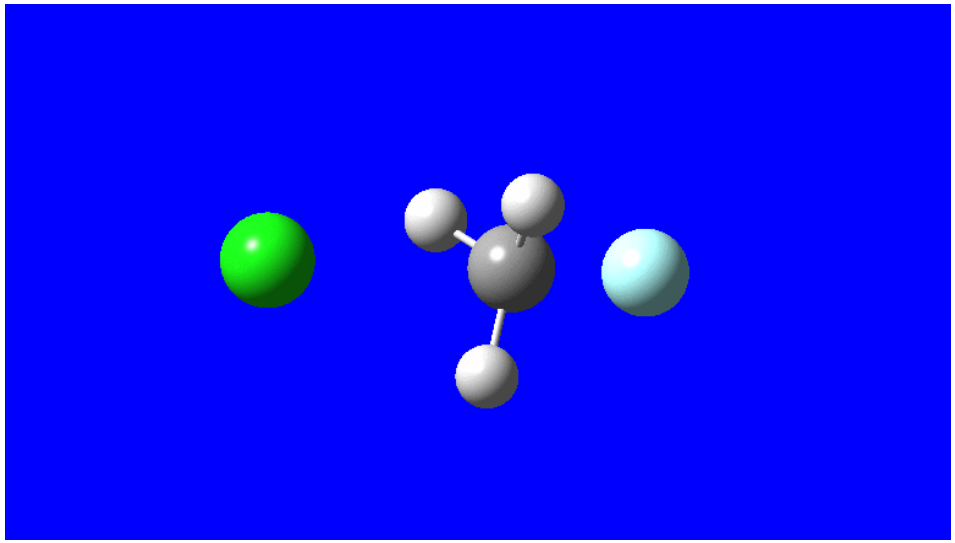
r(C-F)=2.125

∠H-C-H=118.4°

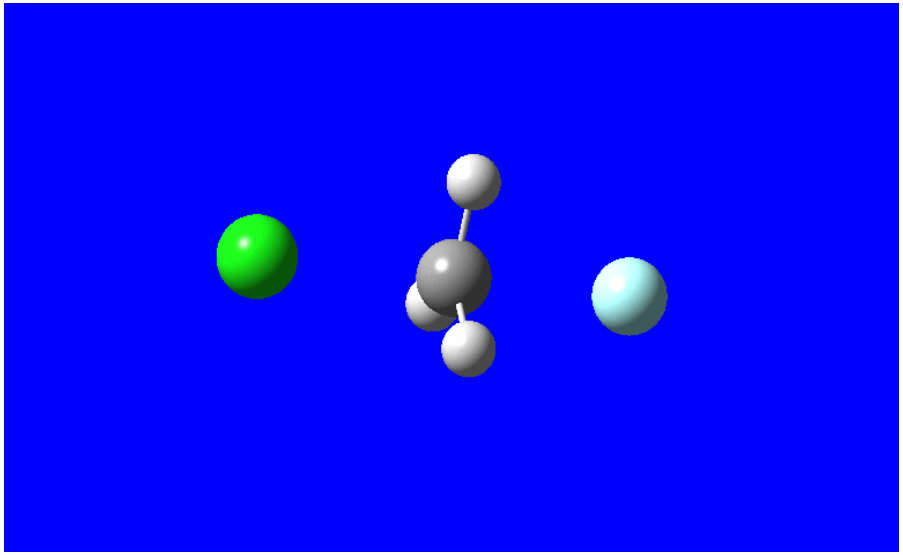
S_{N2}-Reaction Mechanism:

$$F^- (g) + CH_3Cl (g) \rightarrow CH_3F (g) + Cl^- (g)$$

- Computational level: CAM-B3LYP/6-31+G(d)



Animation of IRC



Animation of TS

E_a = ? kcal/mol^{-1} (298.15 K & 1 atom)

Properties of Reactant CH_3Cl (g) & Product CH_3F (g)

- Computational level: CAM-B3LYP/6-31+G(d)
- IR: freq
- NMR: nmr test
- UV-vis: TD=(50-50,nstates=50)