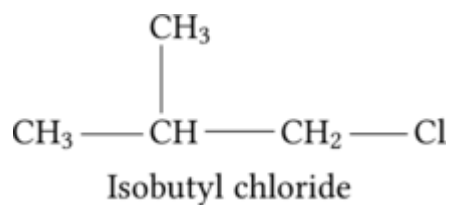


Spartan 初階検定

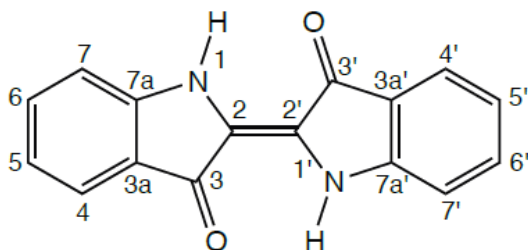
(2017/9/1)

1 hartree = 627.5095 kcal/mol

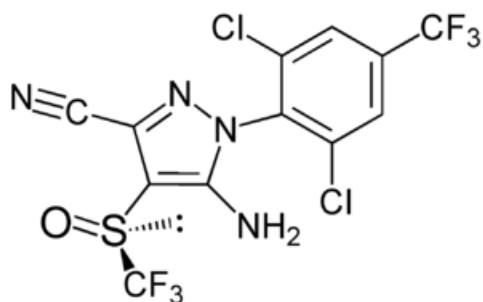
1. Isobutyl Chloride (10%)



2. Indigo (10%)



3. Fipronil (10%)



4. L-Alanine and D-Alanine (15%)

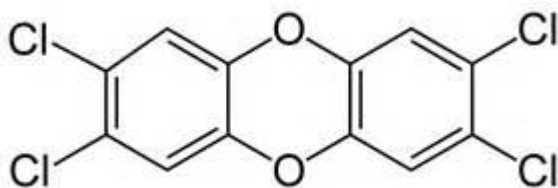


Mirror

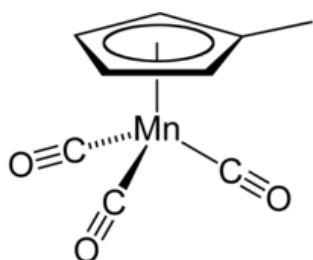
L-Alanine

D-Alanine

5. Plot a TCDD electrostatic map (PM3) (15%)



6. Build the following (MeCp)Mn(CO)₃ structure and estimate the Mn–C, C–O bond lengths and C–Mn–C bond angle at MMFF level? (15%)

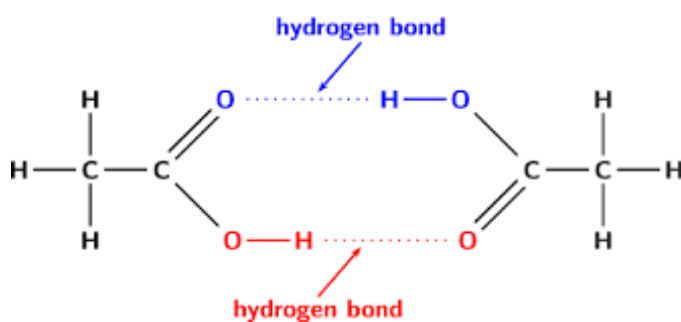


Mn–C = Å

C–O = Å

C–Mn–C = degrees

7. Build acetic acid dimers, and estimate the O...H distance at MMFF level (15%)



O...H–O = Å

8. Please calculate the structures of *trans* and *cis*-1,2 dichloroethene at B3LYP/6-31+G* level (20%)

(A) show the calculated structures

(B) measure the C=C and C-Cl distances and H-C-Cl angle

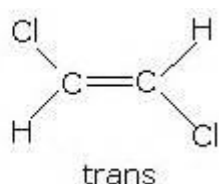
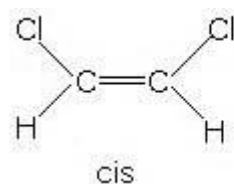
(C) find the relative energies of the two isomers (in kcal/mol)

C=C = Å

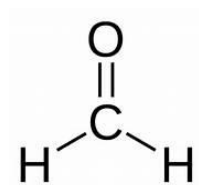
C-Cl = Å

H-C-Cl = degrees

Relative energies: *cis* = 0.0, *trans* = kcal/mol



9. Calculate the molecular structure and vibrational frequencies of HCHO at MP2/6-31+G* level. Compare the IR spectra with experimental data. (20%)



C=O = Å

C-H = Å

H-C-H = degrees

Frequencies (cm⁻¹) =