計算生物（二）第四周作業
0317033 謝明修

1. Complete the energy profiles about the C-C bond rotation of 1,2-dichloroethane in Example 2, using rigid and relaxed PES scan, respectively.

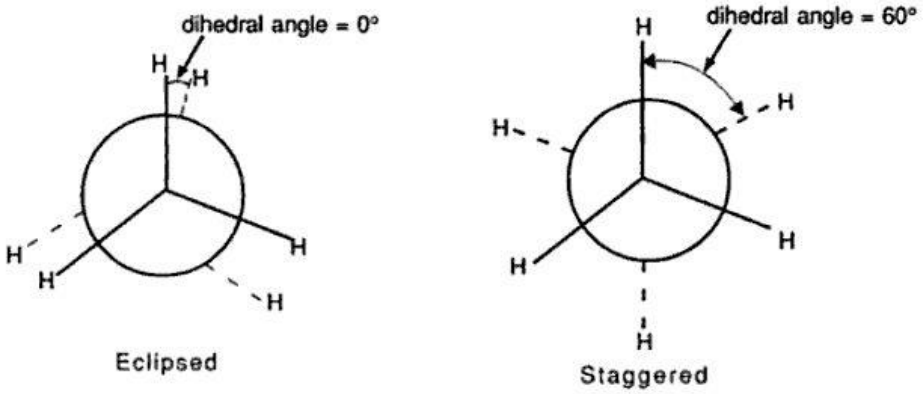

Fig. 93–14. The eclipsed and staggered conformations of ethane.

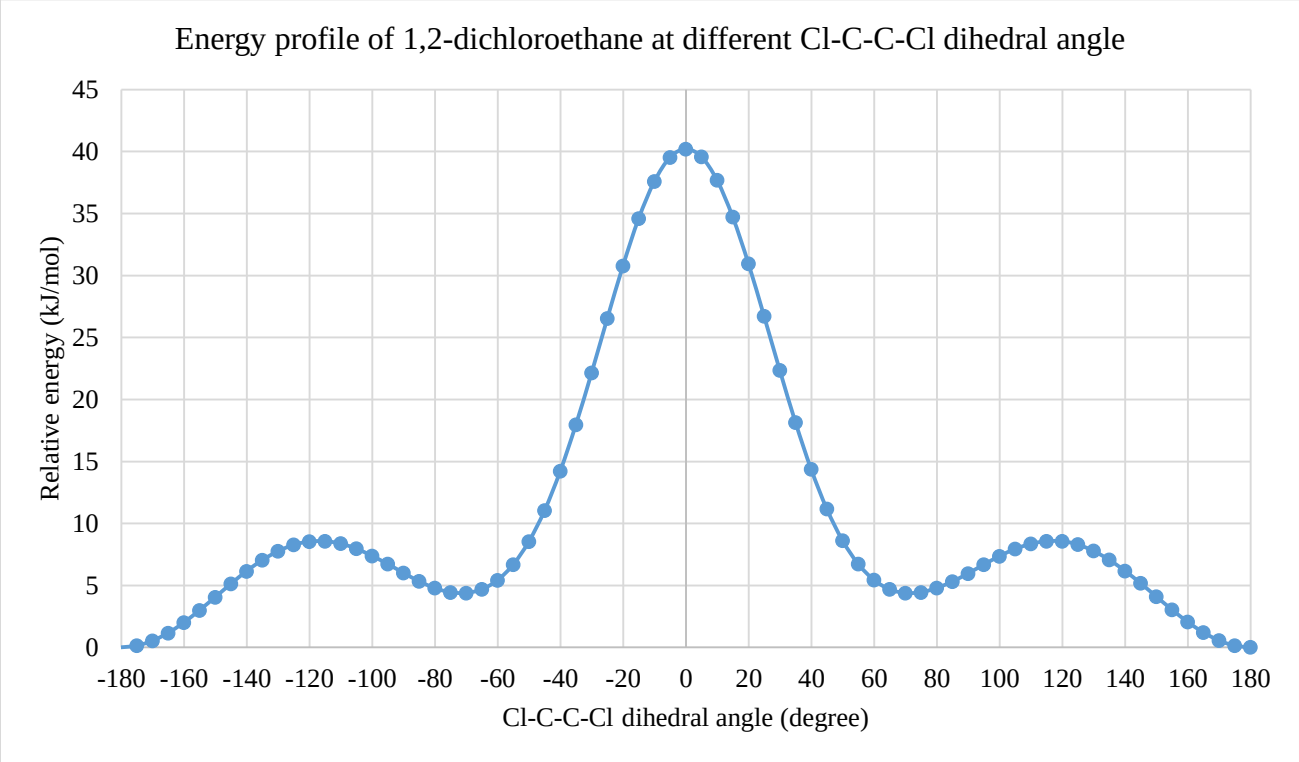

Figure1. The energy profile of 1,2-dichloroethane at different Cl—C—C—Cl dihedral angle. Using the rigid potential energy surface scan at AM1 level, and the fixed geometry is optimized at the same level.

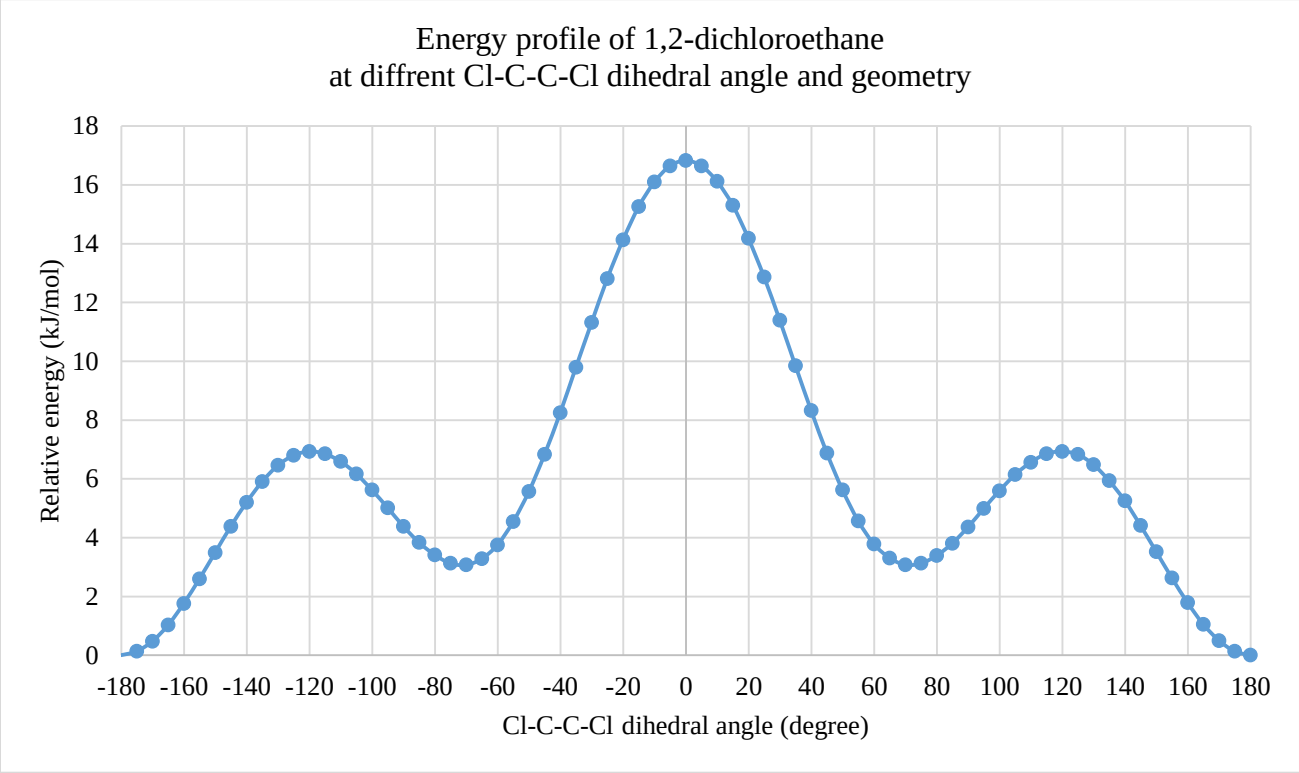

Figure2. The energy profile of 1,2-dichloroethane at different Cl—C—C—Cl dihedral angle and geometry. Using the relaxed potential energy surface scan at AM1 level, at which the geometries are optimized at each dihedral angle. Note that the relative energy is lower compared with the rigid potential energy surface scan.

2.Calculate the reaction energy and activation energy of the reaction and plot the energy profile:

$HCO^+ \longrightarrow [TS]^+ \longrightarrow COH^+$

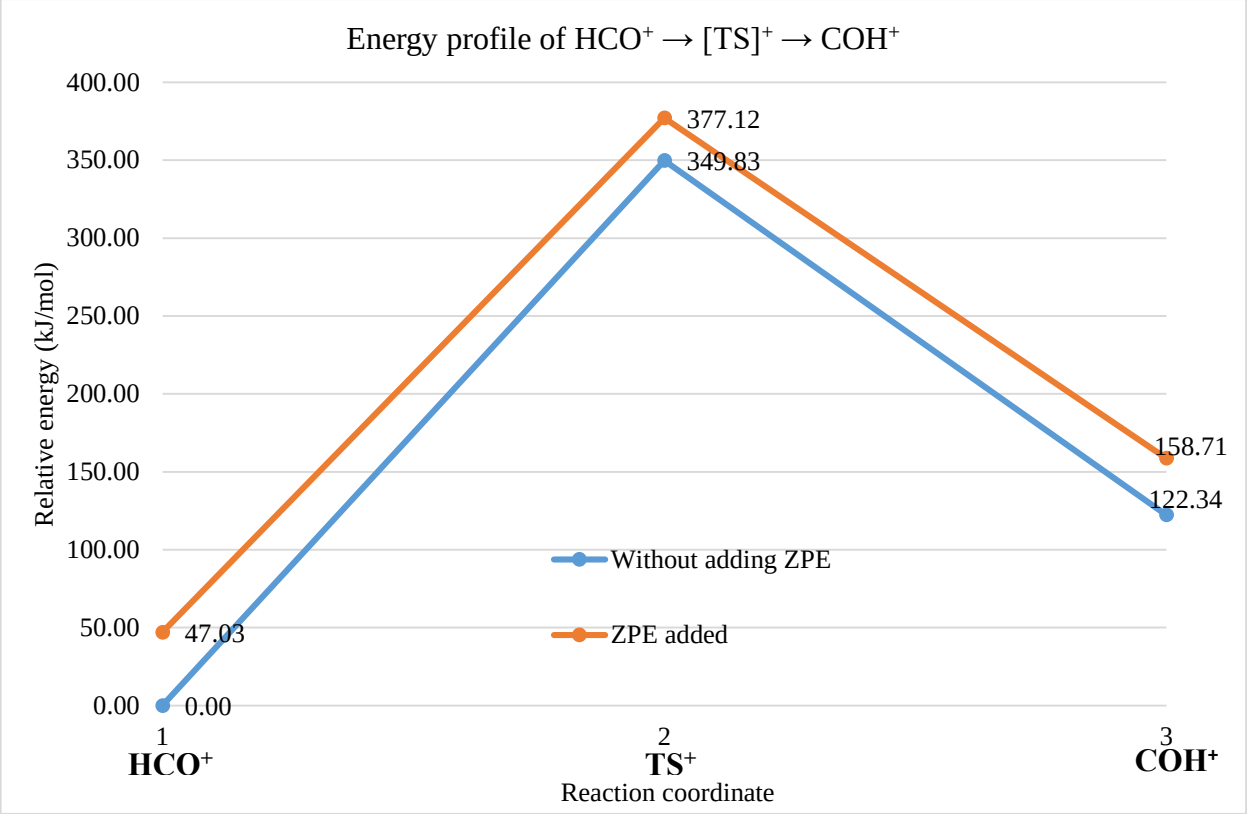

Figure3. The energy profile of the reaction at the level of HF/6-31G(d,p).

	HF/631G(d,p)
HCO^+ (cation singlet)	
Energy (hartree)	-112.9680897
Zero Point Energy (hartree)	0.0179138
COH^+ (cation singlet)	
Energy (hartree)	-112.9214923
Zero Point Energy (hartree)	0.0138502
$[Transition\ state]^+$ (cation singlet)	
C—O bondlength (angstrom)	1.12
O—H bondlength (angstrom)	1.44
C—H bondlength (angstrom)	1.27
Energy (hartree)	-112.834848
Zero Point Energy (hartree)	0.0103964
ΔE_{rxn} (kJ/mol)	122.34
ΔE_{rxn} + ZPE (kJ/mol)	111.67
ΔE_a (kJ/mol)	349.83
ΔE_a + ZPE (kJ/mol)	330.09

Table1. The calculated result at the level of HF/6-31G(d,p)

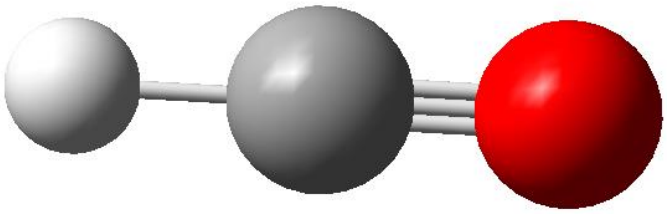

Figure4. The optimized geometry of HCO^{+}.

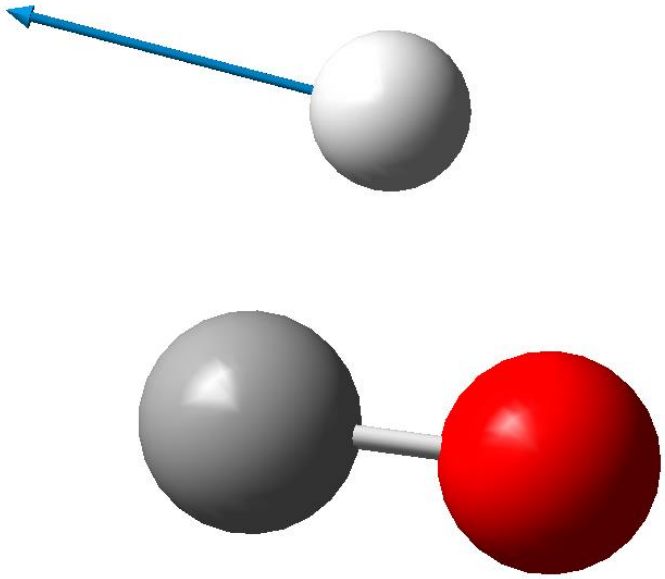

Figure5. The optimized geometry of transition state^{+}.

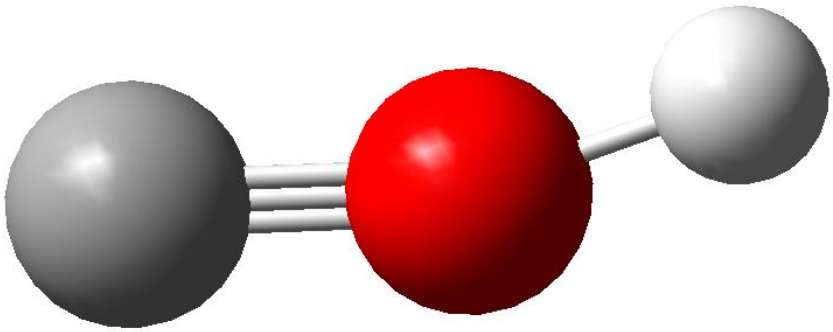

Figure6. The optimized geometry of COH^{+}.