計算生物（二）第五周作業
0317033 謝明修

1.Calculate the reaction energy and activation energy of the reaction and plot the energy profile at MP2/cc-pvTZ level

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

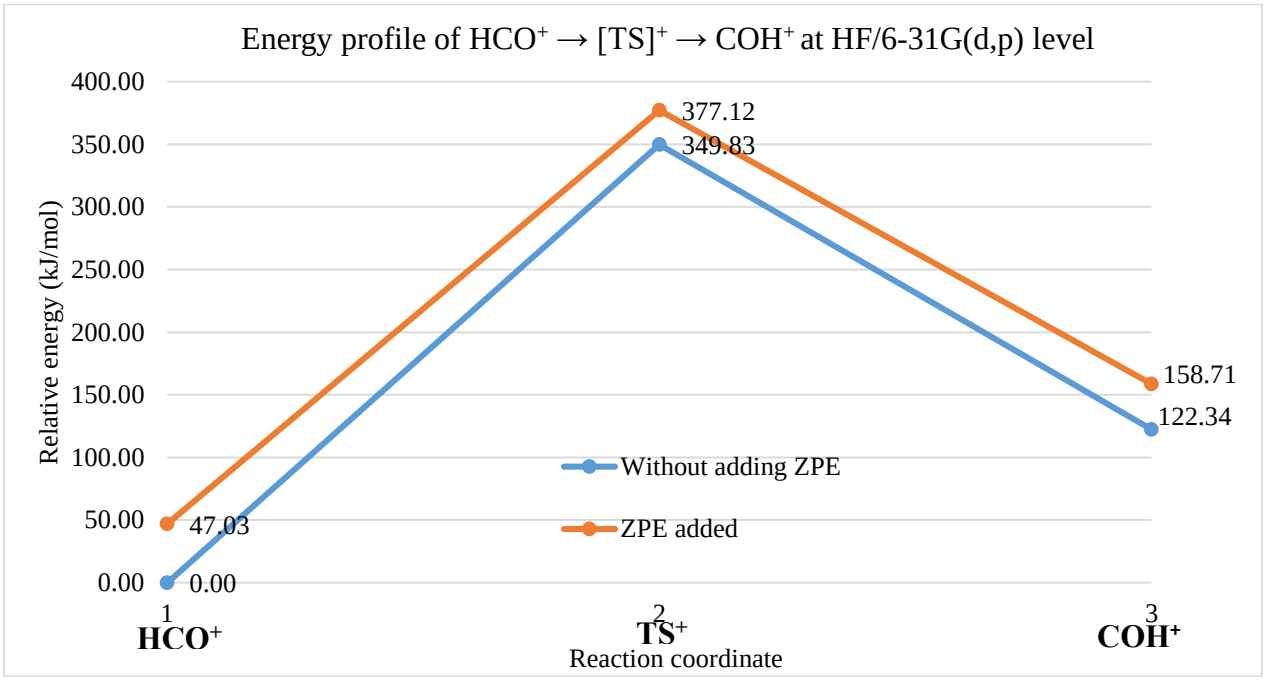

Figure1. The energy profile of the reaction at the level of HF/6-31G(d,p).

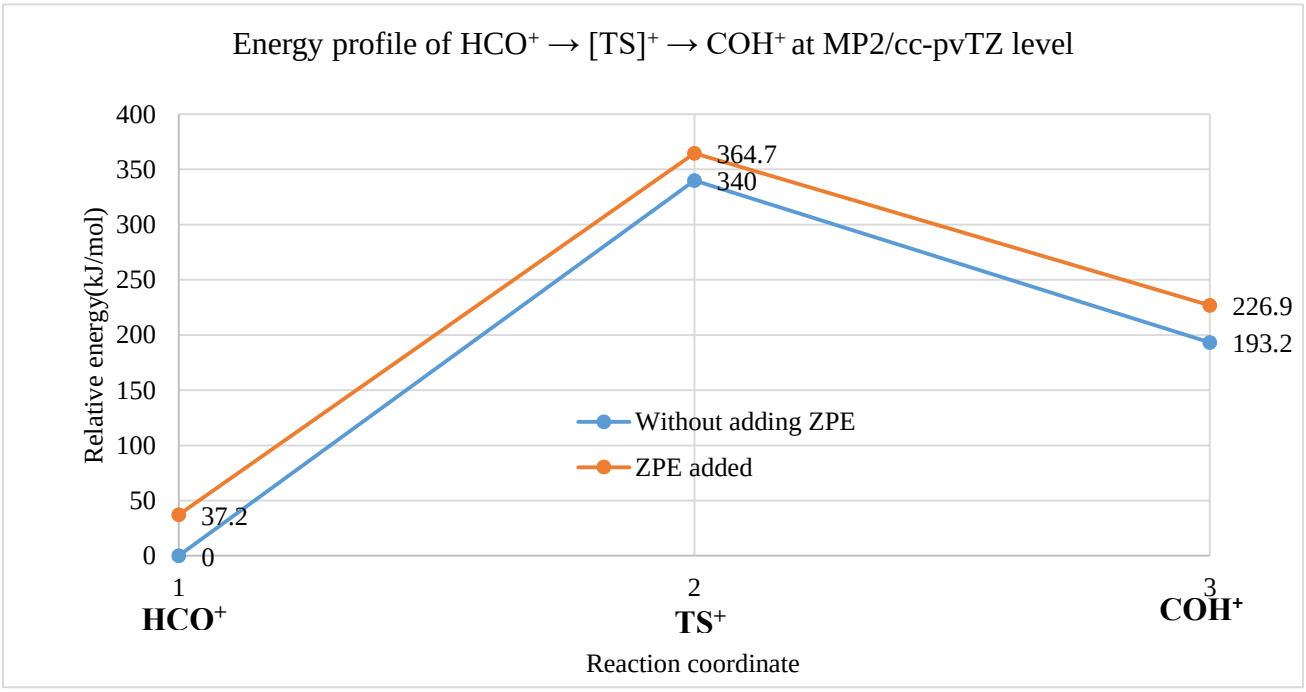

Figure2. The energy profile of the reaction at the level of MP2/cc-pvTZ.

	HF/6-31G(d,p)	MP2/cc-pvTZ
HCO^+ (cation singlet)		
Energy (hartree)	-112.9680897	-113.3750829
Zero Point Energy (hartree)	0.0179138	0.0141715
COH^+ (cation singlet)		
Energy (hartree)	-112.9214923	-113.3014971
Zero Point Energy (hartree)	0.0138502	0.0128344
[Transition state]$^+$ (cation singlet)		
C—O bondlength (angstrom)	1.12	1.16
O—H bondlength (angstrom)	1.44	1.36
C—H bondlength (angstrom)	1.27	1.31
Energy (hartree)	-112.834848	-113.2455668
Zero Point Energy (hartree)	0.0103964	0.0093913
ΔE_{rxn} (kJ/mol)	122.34	193.20
ΔE_{rxn} + ZPE (kJ/mol)	111.67	189.69
ΔE_a (kJ/mol)	349.83	340.04
ΔE_a + ZPE (kJ/mol)	330.09	327.49

Table1. The calculated result at the level of HF/6-31G(d,p) and MP2/cc-pvTZ.

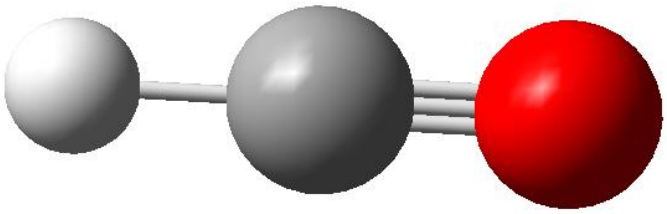

Figure4. The optimized geometry of HCO^{+}.

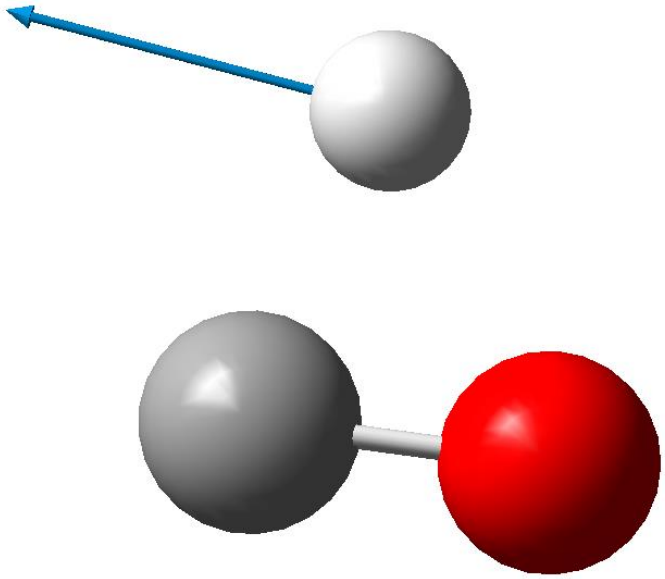

Figure5. The optimized geometry of transition state^{+}.

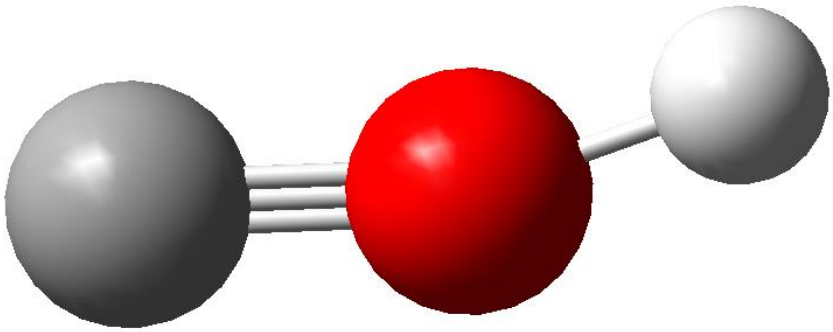

Figure6. The optimized geometry of COH^{+}.

2. Calculate the energy of the following S_N2 reaction, IRC result included.

$$CH3Br+OH^- \rightarrow CH3OH + Br^-$$

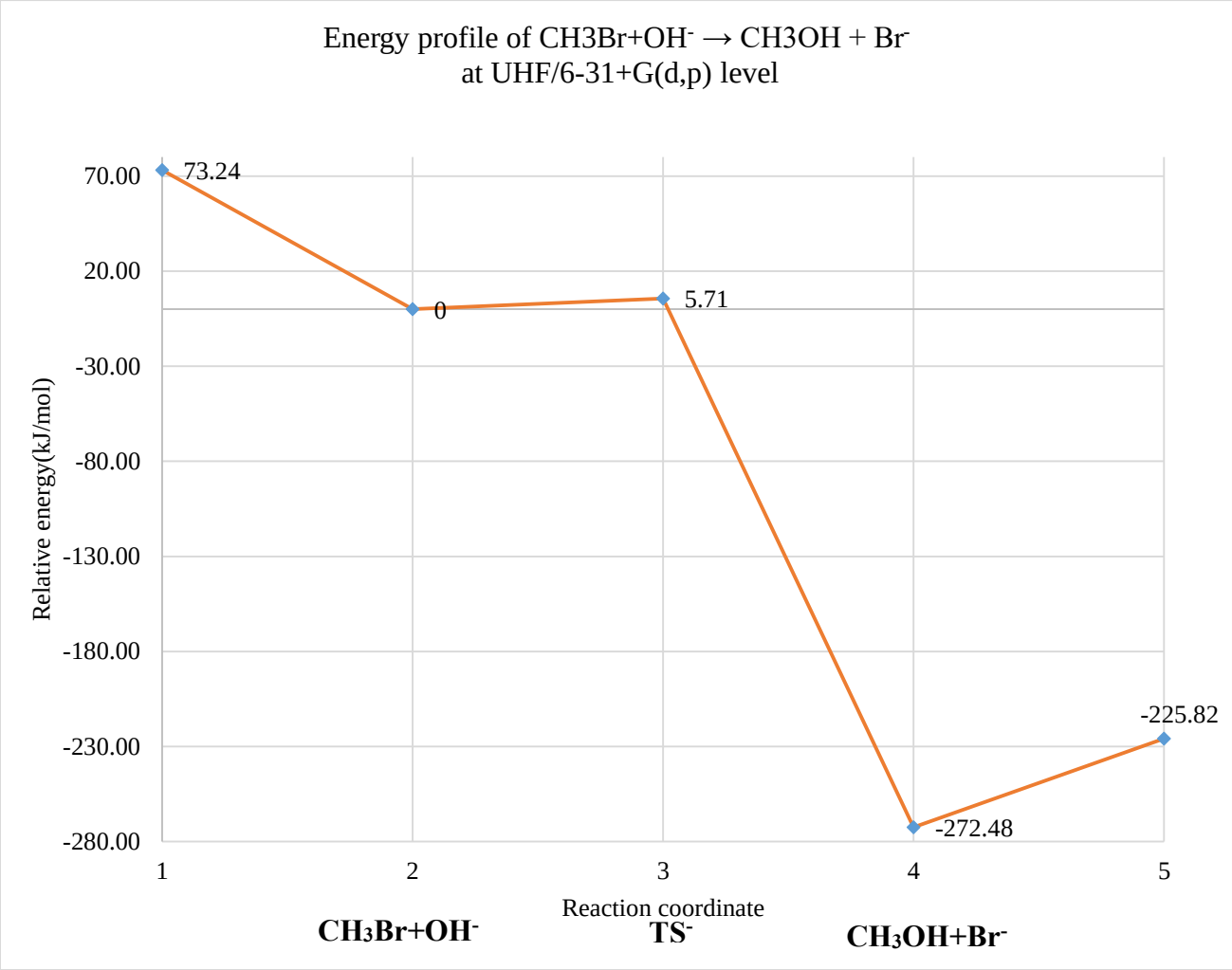

Figure6. The energy profile of the reaction at the level of UHF/6-31+G(d,p).

	UHF/6-31+G(d,p)
$CH_3Br + OH^-$ (anion singlet)	
Energy (hartree)	-2684.8824
Zero Point Energy (hartree)	0.0179138
$CH_3OH + Br^-$ (anion singlet)	
Energy (hartree)	-112.9214923
Zero Point Energy (hartree)	0.0138502
$[Transition\ state]^-$ (anion singlet)	
Energy (hartree)	-112.834848
Zero Point Energy (hartree)	0.0103964
$CH_3Br + OH^-$ (anion singlet) IRC result	
Energy (hartree)	-2684.8824
$CH_3OH + Br^-$ (anion singlet) IRC result	
Energy (hartree)	-2684.9814
$CH_3Br + OH^-$ (anion singlet) IRC result further optimized	
Energy (hartree)	-2684.9326526
Zero Point Energy (hartree)	0.0500044
$CH_3OH + Br^-$ (anion singlet) IRC result further optimized	
Energy (hartree)	-2685.042737
Zero Point Energy (hartree)	0.056308
ΔE_{rxn} (kJ/mol)	-272.48
ΔE_a (kJ/mol)	5.71

Table2. The calculated result of the S_N2 reaction at the level of UHF/6-31+G(d,p).