計算生物（二）第六周作業

0317033 謝明修

1. Calculate the energy of the following S_N2 reaction at MP2/aug-cc-pVTZ level. This involves the reoptimization of each geometry.

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

2. Perform single-point energy calculations at the level of CCSD(T)/aug-cc-pVTZ using the geometries optimized at MP2/aug-cc-pVTZ.

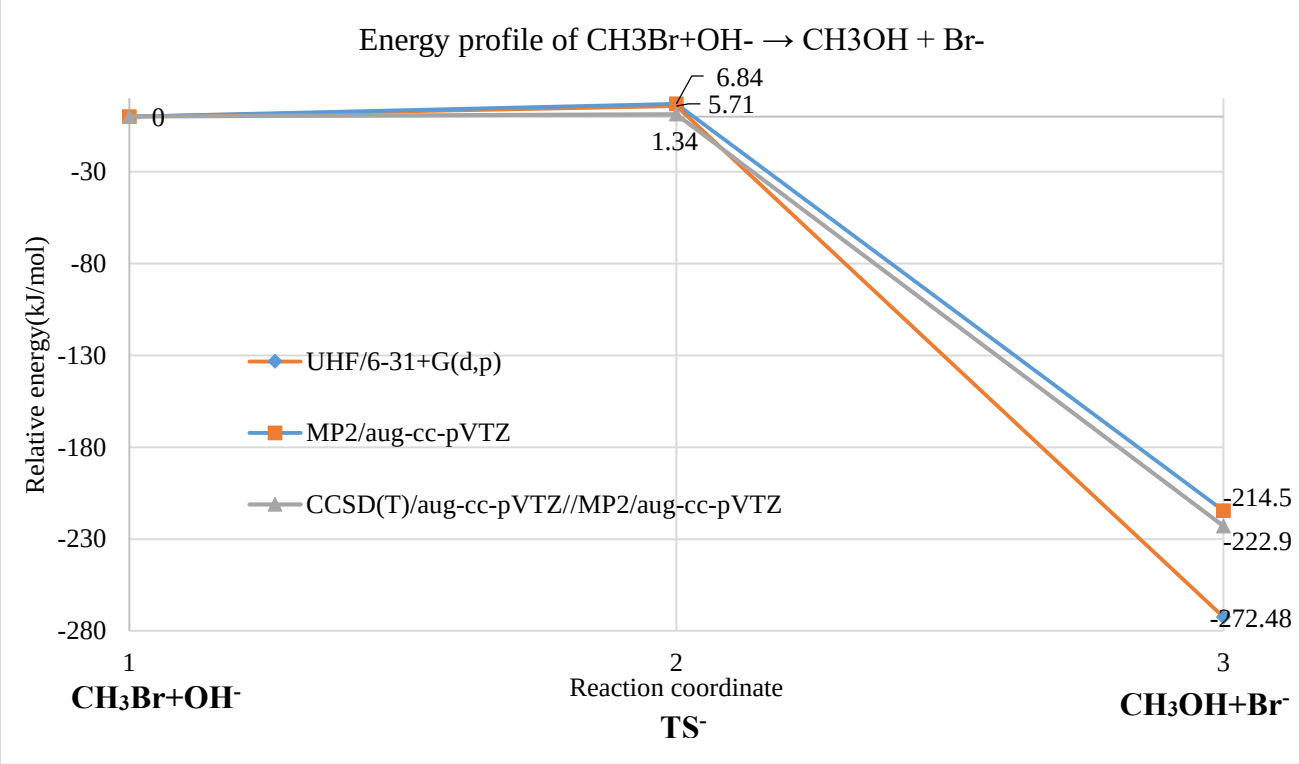

Figure1. The energy profile of the reaction at the level of UHF/6-31+G(d,p).

	UHF/6-31+G(d,p)	MP2/aug-cc-pVTZ	CCSD(T)/aug-cc-pVTZ// MP2/aug-cc-pVTZ
$CH_3Br + OH^-$ (anion singlet)			
Energy (hartree)	-2684.9326526	-2688.242384	-2688.290256
Zero Point Energy (hartree)	0.0500044	0.0473039	0.0473039
$CH_3OH + Br^-$ (anion singlet)			
Energy (hartree)	-2685.0427381	-2688.3294022	-2688.3804757
Zero Point Energy (hartree)	0.056308	0.052626	0.052626
$[TS]^-$ (anion singlet)			
Energy (hartree)	-2684.9307278	-2688.2399965	-2688.2899619
Zero Point Energy (hartree)	0.0502526	0.0475211	0.0475211
ΔE_{rxn} (kJ/mol)	-272.48	-214.5	-222.9
ΔE_a (kJ/mol)	5.71	6.84	1.34

Table1. The calculated result of the S_N2 reaction.