ICC Report I

TS Investigation Exercise

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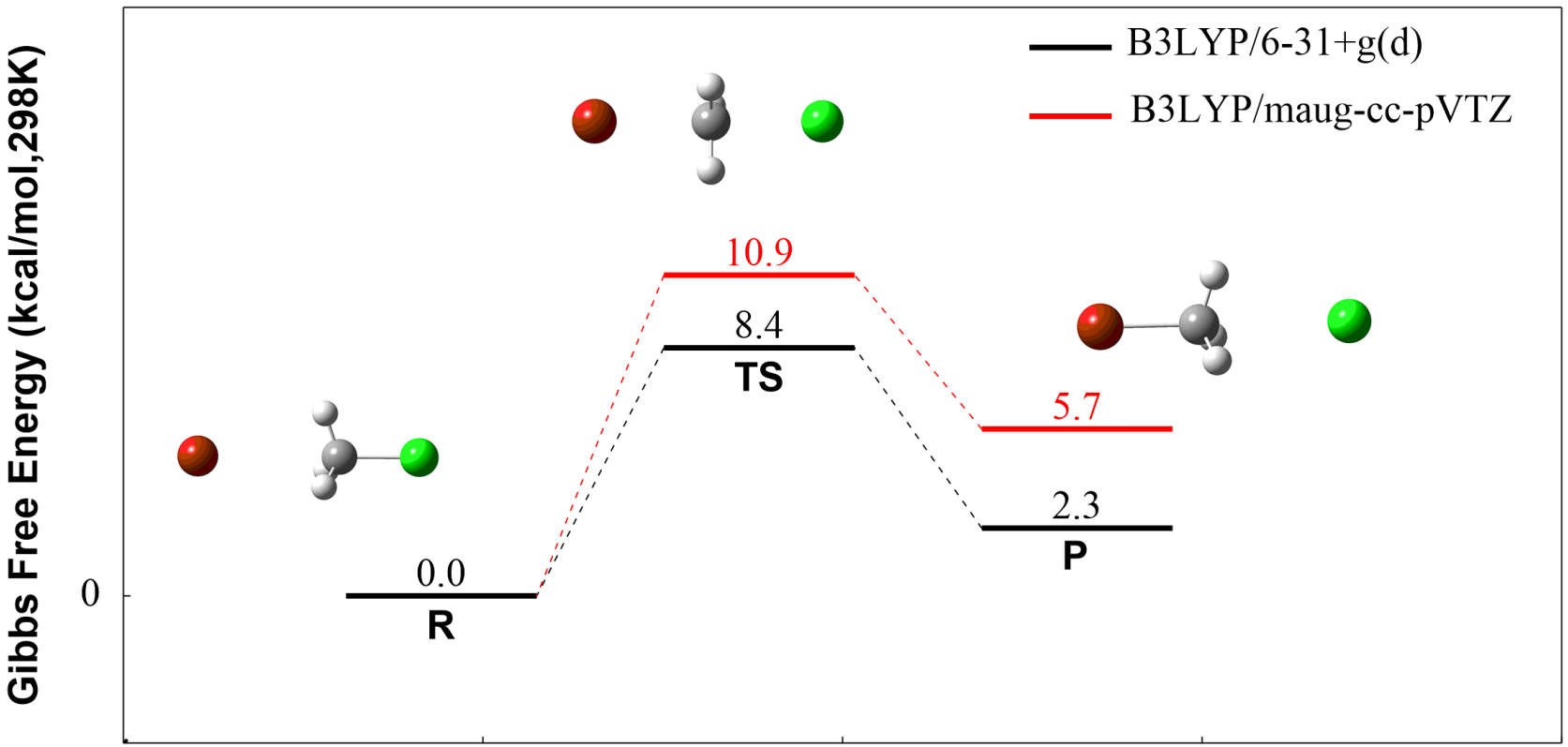
Contents

S_N2 of Chloromethane

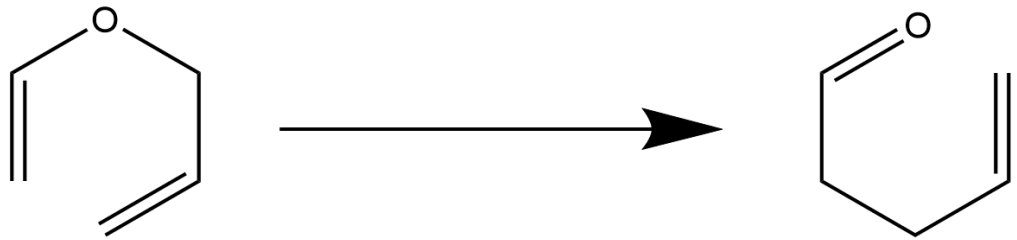
$$\mathrm{CH_3Cl} + \mathrm{Br^-} \longrightarrow \mathrm{CH_3Br} + \mathrm{Cl^-} \tag{1}$$



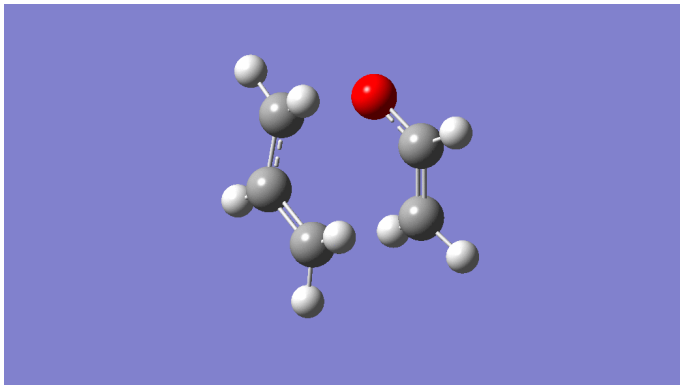
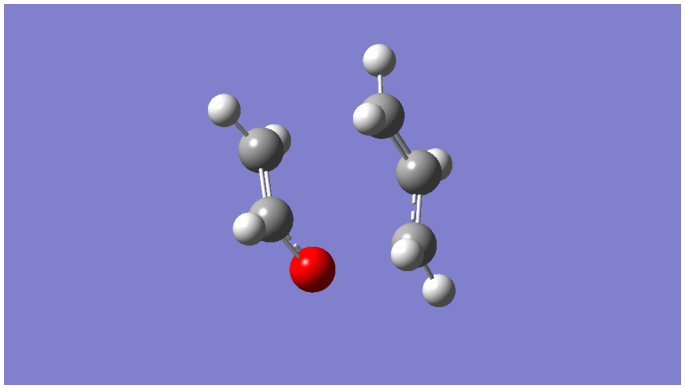
	C−Cl (R)	C−Cl (TS)	C−Br (TS)	C−Br (P)
B3LYP/6-31+g(d)	1.856	2.370	2.482	2.021
B3LYP/maug-cc-pVTZ	1.845	2.415	2.453	2.023

Table: Bond length (Å) in configurations above

Claisen Rearrangement

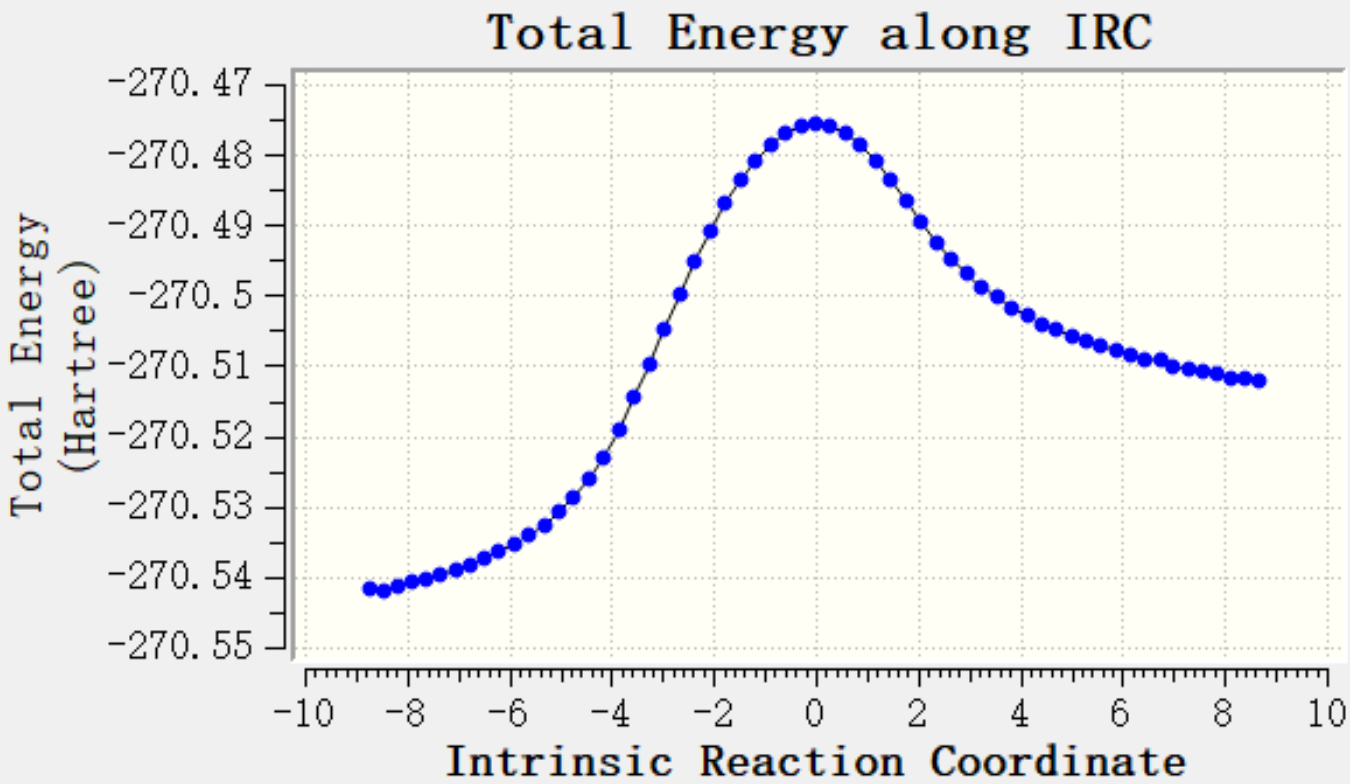


Transition State I – Chair A

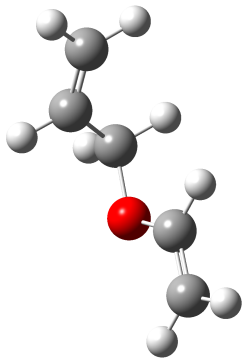



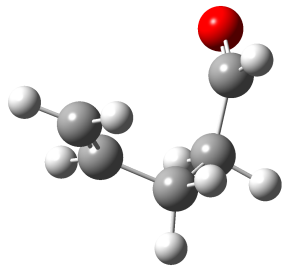
All the results in this case are calculated with B3LYP/6-31+g(d)

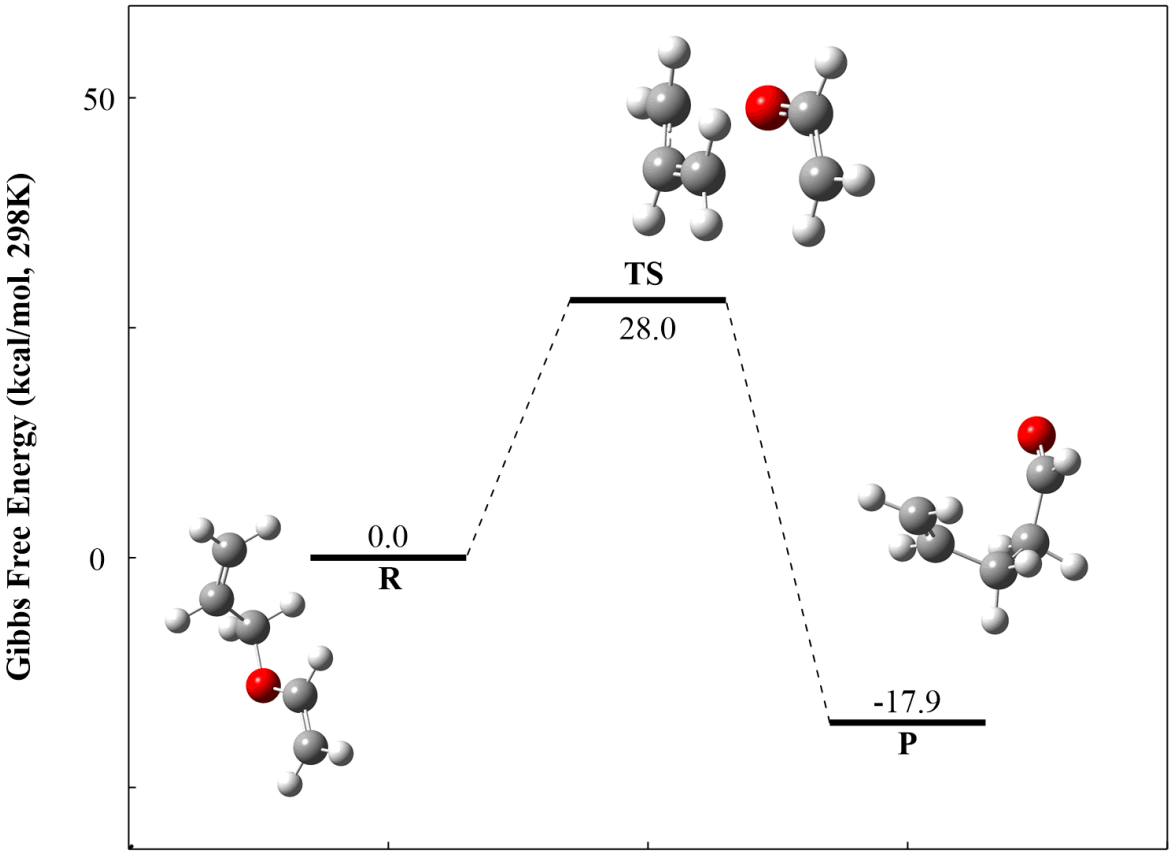
Chair A


Total Energy along IRC
Total Energy (Hartree)
-270.47
-270.48
-270.49
-270.5
-270.51
-270.52
-270.53
-270.54
-270.55
-10
-8
-6
-4
-2
0
2
4
6
8
10
Intrinsic Reaction Coordinate

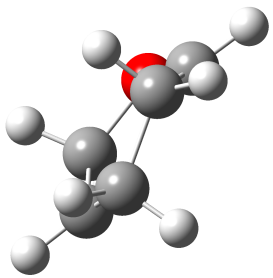
Extract the first and last structure from IRC and do optimization, we get the reactant and product

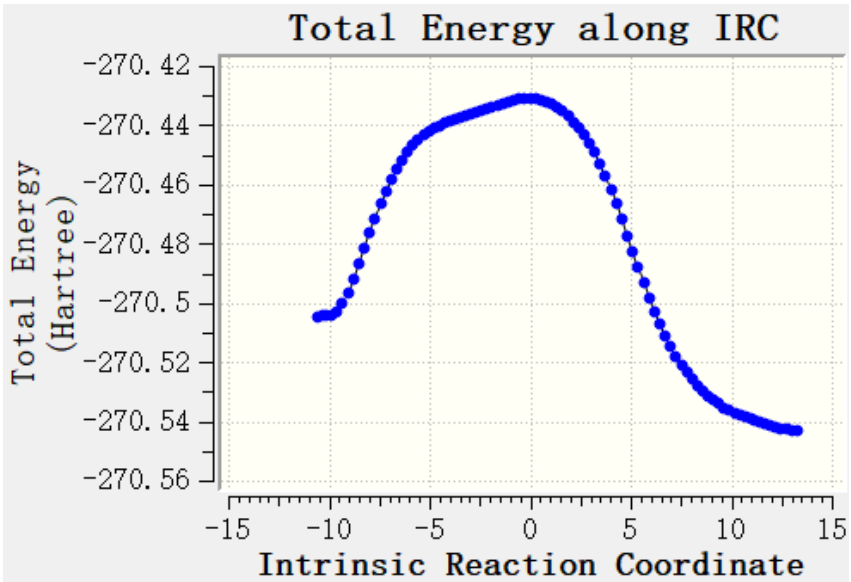





Gibbs Free Energy (kcal/mol, 298K)
50
0
TS
28.0
0.0
R
-17.9
P

Transition State II – Chair B



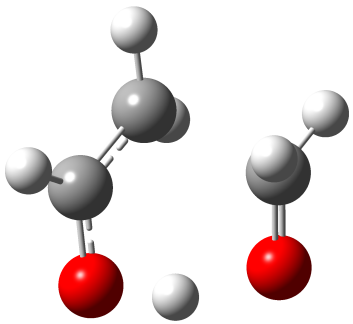


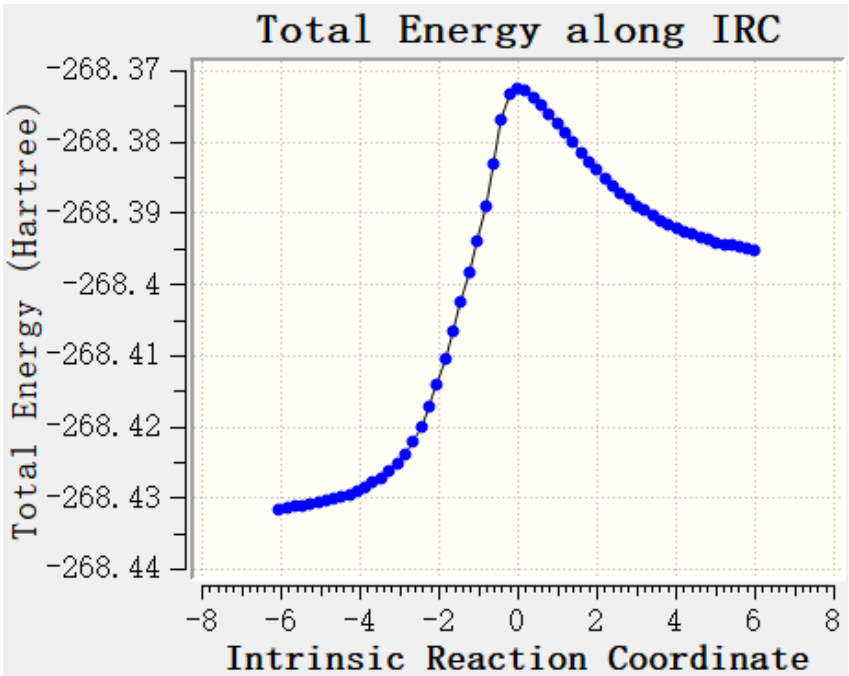
Others

1. Boat
2. ...

Aldol Reaction

$$CH_2{=}CH{-}OH + O{=}CH_2 \longrightarrow CHO{-}CH_2{-}CH_2{-}OH \qquad (2)$$





All calculated with B3LYP/6-311+g(d)