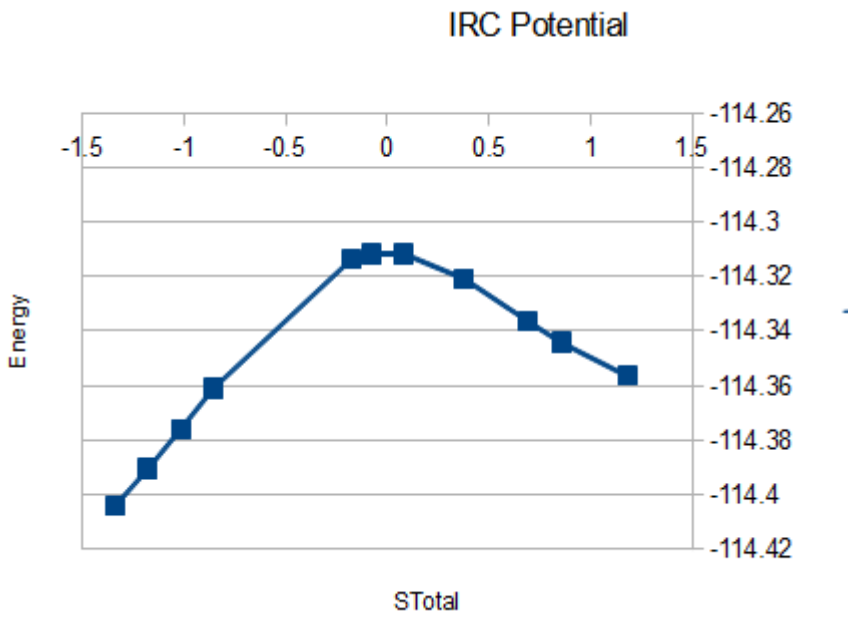
Tanuj Gupta **Assignment 5**

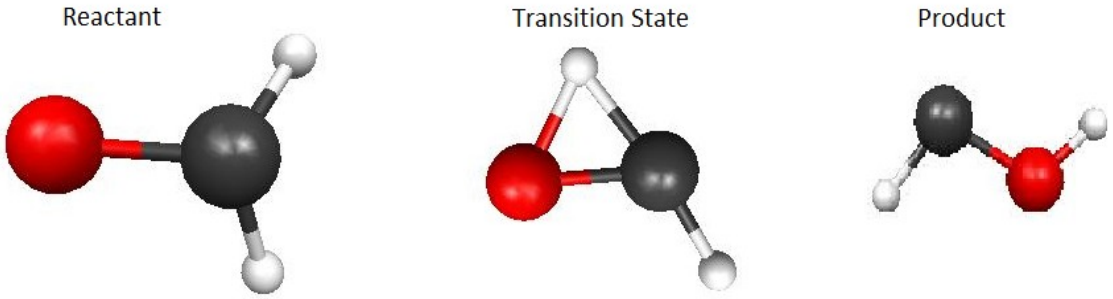
Property	Reactant(HF/cc-pvdz)	Reactant(DFT/cc-pvdz)	Product(HF/cc-pvdz)	Product(DFT/cc-pvdz)	Transition(HF/cc-pvdz)	Transition(DFT/cc-pvdz)
BondLength(CO)	1.182	1.204	1.297	1.318	1.271	1.294
BondLength(CH)	1.102	1.121	0.988	0.975	1.114	1.187
Energy	-113.877	-114.448	-113.8	-114.365	-114.297	-114.311
Max. Frequency	3183.44	2914.17	8356.12	3656.09	---	----

IRC Potential

Stotal (Ang)	Energy (Hartree)
1.34086	-114.3605280879
1.179047	-114.3564417104
1.017598	-114.3509733892
0.855104	-114.3442152071
0.695177	-114.3365746777
0.528540	-114.3281413022
0.378618	-114.3208941007
0.178623	-114.3135511782
0.07862	-114.3116080243
0	-114.3111212908
-0.07862	-114.3116310606
-0.17862	-114.3137575277
-0.378621	-114.3227124156
-0.528613	-114.3328684601
-0.695277	-114.3465264074
-0.855268	-114.3609603380
-1.017759	-114.3760193994
-1.179282	-114.3906083516
-1.341164	-114.4042088954



IRC Potential surface constructed from the IRC calculations



Activation Energy = -114.3116080243+114.4042088954
= 0.0926008711 Hartrees
= 243.1236055932 Kcal/mol

In this assignment, we have optimized the geometry of HCHO in the product , transition and reactant state using the Hartree-Fock and DFT methods in order to locate the geometry of transition state.
DFT is higher level of theory and gives more accurate result compared to Hartree-Fock method and hence is more time consuming. Once we have optimized our geometry, we have found the saddle point of reaction which is basically the transition state. At saddle point energy is at a stationary point i.e. energy increases if the migrating hydrogen is moved in any direction except in only one possible direction. We have done IRC calculations to see that it is actually the transition state and plotted energy as a function of migration of hydrogen along the length of the C=O bond. It is clear from the plot that transition state is indeed the stationary point and its energy decreases in moving along the reactant and product path and is consistent with the typical transition energy curves.