

Table S3.

	R_R	R_{TS}	R_P	E_{TS-R}	E_{P-R}
MP2/6-31G(d)	-1.83	-0.12	1.56	22.47	-3.13
MP2/cc-pVDZ	-1.83	-0.12	1.38	19.89	-5.53
B3LYP/6-31G(d)	-1.83	0.13	1.38	25.14	3.57
B3LYP/cc-pVDZ	-1.83	0.13	1.38	23.76	2.35

The reaction coordinates in Å for the reactant, transition state and product are R_R , R_{TS} and R_P , respectively. The barrier height of the transition state E_{TS-R} and the overall reaction energy E_{P-R} are in kcal/mol.