Table S5.

	R_R	R_{TS}	R_P	E_{TS-R}	E_{P-R}
MP2/6-31G(d)	-1.83	-0.09	1.39	23.53	-3.08
MP2/cc-pVDZ	-1.83	-0.09	1.39	20.67	-5.29
B3LYP/6-31G(d)	-1.83	-0.09	1.39	26.11	3.28
B3LYP/cc-pVDZ	-1.83	-0.09	1.39	24.65	2.13

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 $E_{\mathrm{TS-R}}$ and the overall reaction energy $E_{\mathrm{P-R}}$ are in kcal/mol.