Table S2.

	R_R	R_{TS}	R_P	E_{TS-R}	E_{P-R}
MP2/6-31G(d)	-1.83	0.13	1.56	22.34	-3.17
MP2/cc-pVDZ	-1.83	-0.36	1.38	20.06	-5.52
B3LYP/6-31G(d)	-1.83	0.13	1.38	25.29	3.55
B3LYP/cc-pVDZ	-1.83	0.13	1.38	23.91	2.32

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.