

Supplementary Table S1. T1 Diagnostic value of all transition states.

Species	T1/cc-pVDZ	Species	T1/cc-pVDZ
TSa	0.00937886	TSb''''	0.01615893
TSb	0.00923366	TSc''''	0.01631231
TSc	0.00932056	TSd''''	0.01633832
TSd	0.00932826	TS1	0.01033944
TSa'	0.01326566	TS2	0.01170139
TSb'	0.01341476	TS3	0.01065141
TSc'	0.01352642	TS4	0.02186546
TSd'	0.01339797	TS5	0.01069461
TSa''	0.02052348	TS6	0.01207125
TSb''	0.02089072	TS7	0.02177074
TSc''	0.02119248	TS8	0.02069242
TSd''	0.02099783	TS9	0.01070617
TSa'''	0.02024957	TS10	0.02175401
TSb'''	0.03472506	TS11	0.02042362
TSc'''	0.04070773	TS12	0.02150316
TSd'''	0.03801255	TS13	0.02166020
TSa''''	0.01577936		

T₁ diagnostic values calculated at the CCSD(T)/cc-pVDZ level.