

Supplementary Table S5. Kinetic parameters predicted for the essential isomerization and decomposition reactions of n-heptane radicals at $P = 0.01$ atm.

Reactions	A	n	E
int1→int4	1.18E+11	-1.47	1.68E+04
int1→Pa1	1.01E+15	-1.01	2.45E+04
int2→int3	1.92E+10	-0.8	2.63E+04
int2→Pb1	6.43E+14	-0.98	2.60E+04
int2→Pb2	2.58E+12	-0.69	3.28E+04
int3→int1	1.83E+10	-0.88	2.55E+04
int3→int4	2.66E+13	-1	2.22E+04
int3→Pc1	1.63E+15	-0.99	2.39E+04
int4→int1	2.84E+10	-1.33	1.93E+04
int4→Pd1	1.06E+15	-1.13	2.70E+04