

Supplementary Table S8. Kinetic parameters predicted for the essential isomerization and decomposition of n-heptane radicals at $P = 100$ atm.

Reactions	A	n	E
int1→int4	2.78E+12	-1.67	1.97E+04
int1→Pa1	1.26E+17	-1.27	2.91E+04
int2→int3	6.48E+12	-0.9	3.27E+04
int2→Pb1	4.43E+16	-1.89	3.14E+04
int2→Pb2	3.69E+14	-0.81	4.04E+04
int3→int1	4.26E+12	-0.93	3.19E+04
int3→int4	1.99E+15	-1.16	2.63E+04
int3→Pc1	1.45E+17	-1.11	2.85E+04
int4→int1	9.64E+11	-1.56	2.25E+04
int4→Pd1	6.06E+15	-1.07	3.20E+04