

Supplementary Table S3 Reaction kinetic parameters for the H-abstraction of n-heptane in the temperature range of 300–2,000 K. The rate constants are fitted in the form $K = AT^n \exp(-E/RT)$, units of rate constants for bimolecular reaction are $\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$ and E is cal/mol.

Reactions	A	n	E
n-C ₇ H ₁₆ +H→int1+H ₂	4.30E-01	4.42	4.26E+00
n-C ₇ H ₁₆ +H→int2+H ₂	3.00E+00	4.07	3.95E+00
n-C ₇ H ₁₆ +H→int3+H ₂	2.51E+00	4.09	1.10E+00
n-C ₇ H ₁₆ +H→int4+H ₂	4.60E-01	4.24	3.51E+00
n-C ₇ H ₁₆ +HO ₂ →int1+H ₂ O ₂	2.08E+00	4.32	1.83E+04
n-C ₇ H ₁₆ +HO ₂ →int2+H ₂ O ₂	2.35E+00	4.16	1.12E+04
n-C ₇ H ₁₆ +HO ₂ →int3+H ₂ O ₂	5.24E+04	3.21	2.05E+04
n-C ₇ H ₁₆ +HO ₂ →int4+H ₂ O ₂	3.44E+00	4.38	2.03E+04
n-C ₇ H ₁₆ +NO ₂ →int1+cis-HONO	3.02E+04	3.58	3.46E+04
n-C ₇ H ₁₆ +NO ₂ →int2+cis-HONO	7.20E-01	4.58	2.19E+04
n-C ₇ H ₁₆ +NO ₂ →int3+cis-HONO	1.44E+04	3.45	2.66E+04
n-C ₇ H ₁₆ +NO ₂ →int4+cis-HONO	7.80E-01	4.15	1.28E+04
n-C ₇ H ₁₆ +NO ₂ →int1+trans-HONO	8.67E+04	3.77	4.62E+04
n-C ₇ H ₁₆ +NO ₂ →int2+trans-HONO	2.65E+00	4.89	4.01E+04
n-C ₇ H ₁₆ +NO ₂ →int3+trans-HONO	1.65E+04	3.7	4.13E+04
n-C ₇ H ₁₆ +NO ₂ →int4+trans-HONO	2.43E+00	4.11	2.39E+04
n-C ₇ H ₁₆ +NO ₂ →int1+HNO ₂	3.22E+00	3.97	2.21E+04
n-C ₇ H ₁₆ +NO ₂ →int2+HNO ₂	2.49E+00	4.08	1.32E+04
n-C ₇ H ₁₆ +NO ₂ →int3+HNO ₂	1.20E+05	3.21	2.92E+04
n-C ₇ H ₁₆ +NO ₂ →int4+HNO ₂	2.83E+00	4.43	2.32E+04