

**Supplementary Table S4** Reaction kinetic parameters for the isomerization and decomposition reactions of n-heptane radicals in the temperature range of 300–2,000 K at HPL.

| Reactions | A        | n     | E        |
|-----------|----------|-------|----------|
| int1→int2 | 1.08E+13 | -0.32 | 3.96E+04 |
| int1→int3 | 2.62E+12 | -0.73 | 3.86E+04 |
| int1→int4 | 5.07E+11 | -1.39 | 2.06E+04 |
| int1→Pa1  | 1.27E+16 | -0.81 | 3.20E+04 |
| int2→int1 | 3.94E+12 | -0.12 | 4.33E+04 |
| int2→int3 | 1.40E+12 | -0.19 | 4.10E+04 |
| int2→int4 | 2.10E+11 | -0.65 | 3.97E+04 |
| int2→Pb1  | 1.48E+15 | -0.68 | 3.22E+04 |
| int2→Pb2  | 7.86E+12 | -0.18 | 4.25E+04 |
| int3→int1 | 1.14E+12 | -0.6  | 4.23E+04 |
| int3→int2 | 1.52E+12 | -0.24 | 4.10E+04 |
| int3→int4 | 9.54E+11 | -0.27 | 4.05E+04 |
| int3→Pc1  | 1.31E+15 | -0.76 | 3.21E+04 |
| int3→Pc2  | 1.57E+13 | -0.31 | 4.16E+04 |
| int3→Pc3  | 8.85E+16 | -0.64 | 3.51E+04 |
| int4→int1 | 3.11E+11 | -1.3  | 2.44E+04 |
| int4→int2 | 1.84E+11 | -0.68 | 3.96E+04 |
| int4→int3 | 1.03E+12 | -0.29 | 4.05E+04 |
| int4→Pd1  | 6.21E+14 | -0.77 | 3.18E+04 |