

A Shock Tube Study of C4 - C6 Straight Chain Alkenes + OH Reactions

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Alkenes are known to be good octane boosters and they are major components of commercial fuels. Detailed theoretical calculations and direct kinetic measurements of elementary reactions of alkenes with combustion radicals are scarce for C4 alkenes and they are practically absent for C5 and larger alkenes. In this work, the overall rate coefficients for the reaction of OH radical with 1-butene (kI), 1-pentene (kII), cis/trans 2-pentene (kIII and kIV), 1-hexene (kV) and cis/trans 2-hexene (kVI and kVII) were measured behind reflected shock waves over the temperature range of 833 – 1377 K and pressures near 1.5 atm. The reaction progress was followed by measuring mole fraction of OH radicals near 306.7 nm using UV laser absorption technique.

It is found that the rate coefficients of OH + trans-2-alkenes are larger than those of OH + cis-2-alkenes, followed by OH + 1-alkenes. Also, comparison with available rate measurements at low temperature allowed us to stipulate that C4-C6 alkenes + OH reactions proceed mainly through H-abstraction for $T > 700$ K and via addition to the double bond at $T < 350$ K. In the intermediate temperature range ($700 \text{ K} > T > 350 \text{ K}$), both H-abstraction and additions channels contribute to the overall rate coefficients.

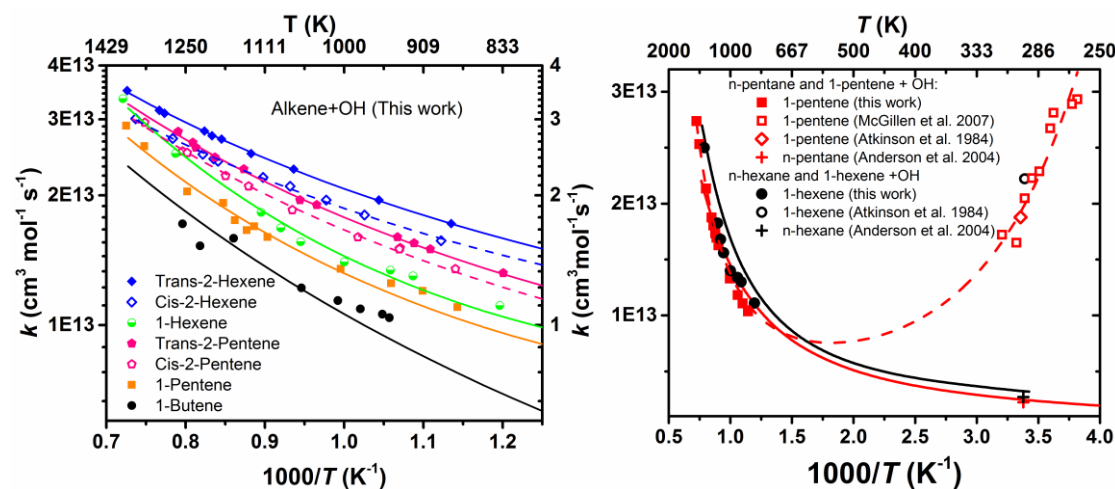


Figure: Left: Rate coefficients of the reaction of C4, C5 and C6 alkenes with OH radicals. Right: Comparison between C5/C6 alkenes + OH and alkanes + OH reactions.

References

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