

Chemical Kinetics of Hydrogen Atom Abstraction from Allylic Sites by O₂

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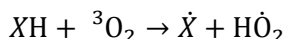
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Abstract

Alkenes are important intermediates formed by the combustion of larger fuel molecules including alkanes and alcohols. Moreover, liquefied petroleum gas (LPG) produced during oil refining contains significant amount of olefins, particularly propene and butenes, with gasoline fuel containing butenes, pentenes and hexenes in various amounts. Furans including 2,5-dimethylfuran (25DMF), and 2-methylfuran (2MF) as possible alternative biofuels have received much attention in recent years. Alkyl aromatic hydrocarbons comprise a significant fraction of the molecular components found in petroleum-derived gasoline, diesel, and gas turbine fuels. Their chemical reactivity is markedly different from other chemical functional classes.

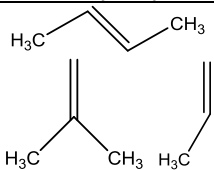
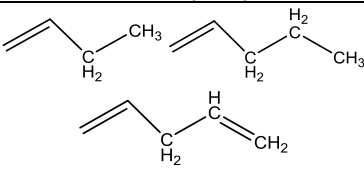
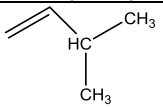
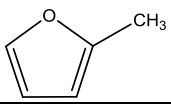
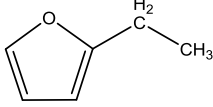
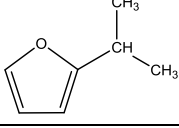
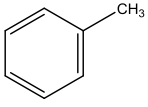
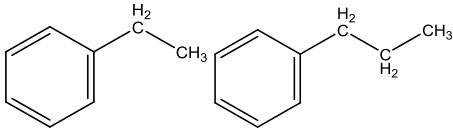
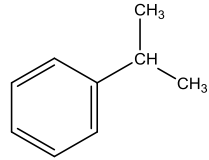
Chemical kinetic models of propene¹, isobutene², 1-and 2-butene³, 25DMF⁴, 2MF⁵ and toluene⁶ have been developed in our group. H-atom abstraction from allylic site by molecular oxygen is found to be very important in determining the reactivity of those fuels at low to intermediate temperatures, but with similar type of H-atom abstraction, we found the rate constants can vary by one order of magnitude. To our knowledge there are no previous systematic studies on these compounds.

In this work we explore the chemical kinetic consequences of structural variants of allylic H-atom sites from which O₂ abstracts a hydrogen atom:



where X is allyl, 2-furyl or phenyl. Rate constants were calculated in the temperature range of 500 to 2000 K. All of the species investigated in this work are listed in Table 1. Rate constants roles for abstracting different allylic hydrogen type will be provided in this work.

Table 1. Species investigated in this work for H-atom abstraction by ³O₂.

	Primary allylic	Secondary allylic	Tertiary allylic
alkenes			
Furans			
Alkyl Aromatics			

References

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