

# Ring-Opening Reactions of $\dot{R}$ and $\dot{Q}OOH$ Radicals in Cyclic Hydrocarbons: Cyclohexene and Tetrahydropyran

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Reaction mechanisms in low-temperature oxidation of hydrocarbons and biofuels remain of central importance to the development of numerical chemical kinetics models, which serve as input to simulation tools in the design of next-generation combustion systems. The degree to which such models are useful hinges on insight obtained from rigorous experimental measurements. Of particular utility are speciation data in the region where  $R\cdot + O_2$  reactions dominate ( $< 1000$  K) and, in specific, the identification of isomers formed via reactions of  $R\cdot$  and  $\cdot QOOH$  radicals and/or species connected to subsequent ketohydroperoxide formation pathways.

Molecular structure plays a central role in reactions mechanisms unfolding below 1000 K. Accordingly, the seminar presents results from a concerted set of studies on cyclohexane, cyclohexene, and tetrahydropyran – six-membered cyclic molecules with different bonding motifs. The results were obtained using multiplexed photoionization mass spectrometry (MPIMS) applied to molecular beams and confirm that ring-opening reactions are facilitated in both cyclohexene and tetrahydropyran, which ultimately impacts the degree of chain-branching expected during combustion.

Date: Fri, March 9, 2018

Time: 12:30-1:30 pm

Location: 208 Clark Hall

Students, pizza will be provided during this special lunch time seminar!