

# SEMINAR

## Comprehensive laboratory studies of hydrocarbon oxidation mechanisms

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### Abstract:

The phenomenon of air pollution is underpinned by a rich chemistry that is largely determined by the interplay between anthropogenic and biogenic emissions into the atmosphere. Central to this chemistry are the oxidation reactions of hydrocarbons, which play a pivotal role in determining the capacity of a hydrocarbon to pollute the air. However, quantitative and complete measurements of the mechanisms by which oxidation occurs are very uncommon, especially as a function of temperature.

A comprehensive study of one such mechanism, that of *i*-butanol with the OH radical, will be presented. In this example, multiple branching and sequential oxidation reactions lead to different end products that are determined by the initial site of OH attack. These branching ratios are found to exhibit temperature dependence, and therefore, under real-world conditions would lead to an end product distribution that changes according to both the time and location of *i*-butanol emission. Accordingly, a parameterization of this temperature dependence is developed, whereby product branching ratios can be estimated accurately throughout the atmospheric temperature range.

Although this is a satisfying result, it is acknowledged that in this case these data are hard-won. In fact, *i*-butanol provides a concise summary of the kinds of challenges associated with studying atmospheric chemistry in a chamber environment, notably: secondary chemistry, convergent (non-unique) product formation, reservoir species and side chemistry. Accordingly, the latter part of this seminar will explore the potential of chemistries besides “atmospheric chemistry” to study oxidation reactions and how these types of experiments might complement conventional chamber experiments.

**Tuesday, 16 August**  
**2:45 pm**  
**FL-1022, Large Auditorium**

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