Physical Chemistry Seminar

Tuesday, January 26, 2010 | **11:00 a.m.** | **Room 1315 Chemistry Building**

Laboratory Studies of Hydrocarbon Oxidation Mechanisms Under Atmospheric Conditions

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The Earth's lower atmosphere contains an array of hydrocarbon compounds of all shapes, sizes and functionalities, including saturated and unsaturated species, as well as those containing oxygen and halogens. Emissions from natural (mostly vegetative) sources provide the major source on a global scale, but emissions from human activity are clearly of importance in and near populated areas. These hydrocarbon species can be thought of as the 'fuel' that drives much of the chemistry of the troposphere. Their oxidation is initiated by photolysis or by reaction with atmospheric oxidants, such as OH, O_3 and NO_3. This oxidative chemistry, through the production of so-called "secondary pollutants" such as ozone, organic acids, organic nitrates and secondary organic aerosols, impacts air quality and human health, the oxidative capacity of the atmosphere and the Earth's climate system.

Understanding the intricacies of the atmospheric behavior of the wide variety of organic species present in the atmosphere can, at first glance, appear a daunting task. However, the atmospheric oxidation of essentially all hydrocarbons follows a familiar pattern, involving the successive formation and reaction of an alkyl radical, an alkyl peroxy radical, and finally an alkoxy species. While this general pattern is indeed well established, it is also the case that, for each individual hydrocarbon, differences in the structure and energetics of the radicals involved impacts the rates and branching to the relevant processes, and hence determines the eventual environmental impact of that species.

In this presentation, an overview of the basic atmospheric hydrocarbon oxidation process will first be presented. Data from our laboratory will then be used to examine the chemistry of alkyl peroxy and alkoxy radicals in more detail.

Topics to be covered include:

1) Competition between radical chain propagation and chain termination in reactions of organic peroxy radicals with HO_2 and with NO; and

2) Competition between unimolecular reactions of alkoxy radicals and their reaction with O_2, and the effects of chemical activation on this competition.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:15 p.m. in Room 8305f