Youngstown State University Chemistry Seminar Program - Fall 2005

Friday November 18th (3:15)

8th Fall Seminar

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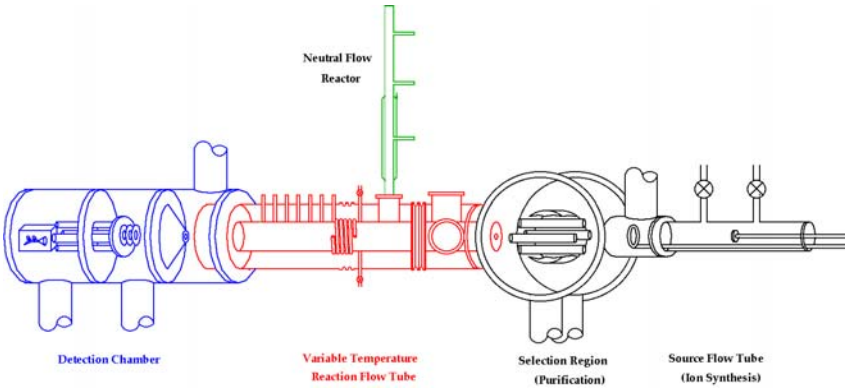
Department of Chemistry

"Reactive Oxygen Species in Chemistry: Experiment and Theory"

Abstract

Reactive Oxygen Species (ROS) are important in chemistry in a variety of areas, from toxicological damage in biological systems to atmospheric, combustion and geomedia chemistry for how we pollute (and clean) our environment and efficiently (or inefficiently) use fuel resources. Within this family of ROS species, hydroxyl radical is a key player. For understanding hydroxyl radical in atmospheric and combustion chemistry, we utilize a chemical ionization mass spectrometric apparatus. Our apparatus is similar to that used for determining the rate of ozone depletion by stratospheric Cl radicals. We have successfully explored the reactions of hydroxyl (OH) radical with volatile organic compounds (VOCs) for tropospheric oxidation reactions of relevance to ozone (smog) generation. For applications in biological, atmospheric and environmental chemistry, we are developing methods for generating OH radicals (and other ROS) in the condensed phase in order to probe H-atom abstraction and addition pathways in polycyclic aromatic hydrocarbons, many of which are environmental pollutants. These studies utilize laser flash photolysis (with UV and IR detection) as well as time-resolved EPR spectroscopy. Fundamental computational studies of the oxidative pathways of ROS species with aromatic hydrocarbons provide complete analysis of the potential energy surfaces, including transition states. From these studies, we have noted an unusual solvation effect for HO reactions in water vs organic solvent, and theory has been used to rationalize this effect and to predict its importance for other electron-rich substrates.



Variable temp. flowing afterglow - selected ion flow tube - neutral flow reactor.