

NCA&T: Atmospheric Chemistry Group (Bililign group)

Interdisciplinary group involving faculty and students from physics, chemistry, chemical engineering and Energy and Environmental systems



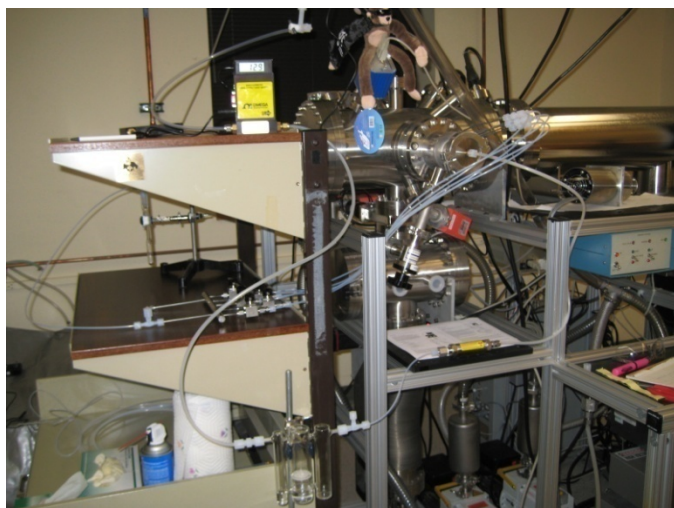
Proton Transfer Mass Spectrometry in Negative Ion

Negative Ion Proton Transfer Mass Spectrometry (NI-PTRMS) is a new method with a potential to provide on-line measurement of organic acids with better time resolution than existing methods. The method involves selective ionization of acidic species via transfer of protons to a carboxylate ion. The implementation of the method requires a clean and intense source of ions and accurate measurements of acidity of carboxylic acids in the gas phase.

This project focuses on two aspects that lead toward the development of NI-PTRMS: (1) the development of a clean dependable source of acetate ions under different conditions of pressure,

temperature and water vapor concentration and (2) determination of gas phase acidity of carboxylic acids of potential atmospheric interest. (3) Estimates of free energy of hydration of carboxylic ions; (4) Determination of the effective gas phase acidity of hydrated carboxylic acids

This project addresses critical problems in air quality and climate change, because organic acids (carboxylic acids) are key to the chemistry of volatile organic compounds (VOCs). VOCs are in turn are related to the formation of ozone and organic aerosols which have a significant impact on regional air quality.



Vibrational O-H overtone Spectroscopy of Carboxylic Acids Using CRDS

The vibrational O-H overtone absorption cross section of carboxylic acids is a necessary quantity to calculate the photochemical reaction rate (J) for reactions initiated by the excitation of the O-H overtone. These reactions have been shown to include unimolecular reactions such as decarboxylation and photodissociation. An experimental setup consisting of a Cavity Ring-Down Spectroscopy (CRDS) instrument and a Ultra-Violet Absorption Spectroscopy (UV-Abs) instrument was built, calibrated,

tested and used to measure the fourth O-H overtone absorption cross sections of acetic acid and peracetic acid.

Future work includes applying the technique to measure O-H overtone absorption cross sections of carboxylic acids.

