

A MODULAR DESIGN FOR REACTION TRAPS IN CRYOGENIC ION TRAP MASS SPECTROMETERS

GINA ROESCH, ETIENNE GARAND, *Department of Chemistry, University of Wisconsin–Madison, Madison, WI, USA.*

Innovations in cryogenic ion traps greatly enhance our ability to control ion-neutral chemistry and spectroscopically probe ionic species in real time. Currently, our lab studies microsolvated species and reaction intermediates using a home-built dual cryogenic ion mass spectrometer. The dual trap design allows for controlled ion manipulation and subsequent tagging in preparation for infrared action spectroscopy. The first trap, a liquid nitrogen cooled octupole “reaction trap”, is used for the condensation of solvent molecules to the analyte or to perform temperature-controlled ion-neutral reaction chemistry to access unstable intermediates. The second “tagging” trap is held at 10K to cluster weakly perturbative tags such as D₂, which can serve as messengers for the subsequent action spectroscopy step.

Currently, the “reaction trap” is the sole location for ion manipulation which limits us to one chemical reaction or the addition of a single type of solvent molecules. To overcome these limitations, we have developed a mass selective, multi-reaction trap setup via a modular housing design. The modular design also reduces the cost and increases the adaptability. In addition, the ion traps utilize digital ion technology (DIT) to facilitate mass-selection, improve the signal-to-noise and increase the mass range for the study of larger clusters.

Preliminary results suggest that a prototype of a dual reaction trapping system can form clusters with two different solvents. For example, water clusters were made in the first trap, mass-selected and methanol was added to the cluster in the second trap. Thus, the multi-reaction trap design provides solvent position selectivity which is of great advantage for simulating more complex environments. Future plans for the multi-reaction trap CIVS instrument include characterizing a water network around an ion by inserting a D₂O as a spectroscopic molecular probe.