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

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

Innovations in ion traps have made it possible to control ion chemistry in real time. Currently, our lab studies micro-solvated species and reaction intermediates using a home-built dual cryogenic ion mass spectrometer. CIVS, Cryogenic Ion Vibrational Spectroscopy, produces high-resolution IR spectra using action spectroscopy. The dual trap design allows for ion manipulation and tagging. The first trap, a liquid nitrogen cooled octopole reaction trap, is used for the adding solvent molecules to the analyte or performing reaction chemistry to form unstable intermediates. The second trap, a liquid helium cooled main trap, is held at 10K to promote the adherence of a non-perturbative tag such as D_2.

At the current moment, the octopole reaction trap is the sole location for ion manipulation. Thus, we are limited to one chemical reaction or the addition of one solvent molecule. Both intermediate formation and solvation are restricted by the time the ions spend in the reaction trap and the gas pressure. To overcome these limitations, we have developed a mass selective, multi-reaction trap setup via a modular housing design. In addition to addressing the limited number of ion manipulation that can occur, the modular design reduces the cost and increases the adaptability.

Preliminary results suggest that a prototype of a dual reaction trapping system can form clusters with different solvents. For example, water clusters were made in the first trap and methanol was clustered in the second trap. Thus, the multi-reaction trap design provides solvent position selectivity for ion manipulation, which is of great advantage for simulating more complex environments. For example, future plans for the multi-reaction trap CIVS instrument include characterizing bulk water using the red-shifted IR peaks of D_2O as a molecular probe.