DEVELOPMENT OF A CRYOGENIC, MASS SELECTIVE, MULTI-REACTION TRAP ION SPECTROMETER

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Development of cryogenic ion traps have greatly enhanced the ability to control ion-neutral chemistry and spectroscopically probe the resulting reaction products. Currently, our lab uses a dual cryogenic ion trap instrument for controlled ion manipulation and subsequent tagging in preparation for infrared action spectroscopy studies. This allows, for example, the study of microsolvated ionic species and catalytic reaction intermediates. The first ion trap is a liquid nitrogen cooled "reaction trap". It is the sole location for ion manipulation and thus limits us to a single chemical reaction or the addition of a single type of solvent molecule. To overcome this limitation, we have developed a cryogenic, mass selective, sequential multi-reaction trap setup with a modular housing design. Mass selectivity is achieved via frequency and duty cycle manipulations of the RF square wave trapping potential. In addition, the modular design reduces the cost and allows for easier adaptability and expansion.

We show that such digital linear quadrupole can efficiently form clusters at low temperature and subsequently mass-select a single species within a series of different cluster sizes before ion transfer. Additionally, we show that manipulation of the square wave duty cycle during the clustering process can be used to enhance the formation of a specific cluster size. This single species enhancement and selection is expected to decrease the amount of time required for spectroscopic characterization. Careful ion transfer into a second reaction trap can be done to cluster a different species and simulate more complex ion environments. Future plans for the multi-reaction trap instrument include characterizing water networks around small peptides by inserting a D_2O as a position sensitive spectroscopic molecular probe.