

TANDEM CRYOGENIC MASS-SELECTIVE DIGITAL ION TRAPS TO PRODUCE MOLECULAR CLUSTERS WITH COMPLEX ENVIRONMENTS

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Cryogenic Ion Vibrational Spectroscopy (CIVS) is a tandem mass spectrometry and infrared spectroscopy technique used to gather structural information about ionic species. When coupled with a “reaction trap”, the technique is especially powerful because ion manipulations can be performed prior to spectroscopic investigation. Species which are difficult to obtain directly in the solution phase (i.e. solvated species, catalytic intermediates, etc.) can be accessed in the gas phase via ion-molecule reactions. Despite the robustness of the technique, there are still limitations in the complexity of the clusters that are achievable because only one synthetic step can be performed. Additionally, the inability to perform mass selection creates heavily cluttered spectra which can hinder the subsequent spectroscopic characterization step.

Here, we present a next-generation prototype instrument with a pair of cryogenic mass-selective digital ion traps. The advantages of the new design include a smaller footprint, less expensive circuitry and modular ion trap design to create a larger number of ion manipulation and mass filtering steps. The digital ion traps run on square wave RF potentials whose frequency and duty cycle can be manipulated to create high- and low-mass pass filters, respectively. Together, frequency and duty cycle filtering allow for mass selection within each cryogenic ion trap. These RF manipulations are compatible with the high pressure and low temperature necessary for solvent clustering. We show preliminary studies highlighting the performance in creating microsolvated clusters followed by in-situ mass selection of a specific cluster size. We also show that the preferential formation of a particular cluster size can be achieved with duty cycle manipulation during the clustering process. Finally, we show that a mass-selected cluster can be transferred to a second ion trap and undergo a second clustering step, resulting in a multi-solvent cluster. Future plans for the multi-reaction trap instrument include characterizing water networks around small peptides by inserting a D₂O as a position sensitive spectroscopic molecular probe.