Infrared Spectroscopy of Mass/Charge Selected Cations and Anions in Helium Droplets

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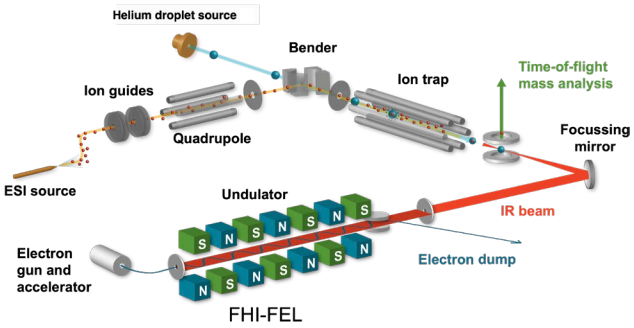
Helium droplets can pick up mass/charge selected ions from an ion trap and the doped droplets can be investigated using optical spectroscopy. We use that technique to investigate cations and anions ranging in size from ions containing only a few atoms up to mass/charge selected protein ions containing several thousand atoms. The figure below shows a schematic of the experimental setup. Ions are generated using a nano electrospray source. After mass/charge selection using a quadrupole, ions are injected and stored in an ion trap. Helium nanodroplets, generated by a cooled pulsed valve, are then allowed to traverse the trap. The droplets travel at a beam velocity of ≈500 m/s and even relatively small droplets containing only a few hundred helium atoms have a kinetic energy that is higher than the longitudinal trapping potential of the ion trap.



When a droplet picks up an ion via mechanical impact, the ion will be cooled to the equilibrium temperature of the droplet (0.4 K), and the ion doped droplet can exit the trap. Doped droplets are irradiated using tunable IR light from the FHI free electron laser. After resonant absorption of multiple photons, droplets evaporate and the bare ion is detected in a time of flight mass spectrometer. Plotting the IR yield as a function of IR frequency gives an IR spectrum. The droplet evaporation process involves the absorption of many IR photons. Results from kinetic modeling of the absorption/evaporation process will be presented.

During the presentation, several systems will be discussed. Among them is the proton-bound dimer of dihydrogen phosphate and formate for which high resolution IR spectra were recently measured. The results show that, contrary to the initial expectation that the stronger phosphoric acid would donate a proton to formate, both experiment and theory show that all exchangeable protons are located in the phosphate moiety. Some H-bending modes of the non-deuterated complex are found to be sensitive to the helium environment. In the case of the partially deuterated complexes, the experiments indicate that internal dynamics leads to isomeric interconversion upon IR excitation.

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