Coupling mass spectrometry with ion mobility spectrometry, helium droplet isolation and infrared spectroscopy

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Abstract:

Mass-spectrometry can be coupled to infrared-spectroscopy to obtain additional information on ion structure and dynamics. In the frequently used IR multiple photon dissociation (IRMPD) approach, ions are m/z selected, irradiated by intense and tunable IR light and fragmentation is monitored as a function of IR wavelength. IRMPD spectroscopy has been proven to be a powerful, robust and fast method, however, two complications that can arise in IRMPD spectroscopy. First, different isomers or conformers may be present and the resulting spectra represent the sum of the spectra of the individual components. Second, intrinsic in the IRMPD process are line shifts and spectral broadening.

The address the question of different isomers and conformers, we constructed a setup, in which ion mobility methods are used to obtain m/z selected ions of defined shape, which are then further investigated by IR spectroscopy. The approach has been applied to a variety of biomolecules, ranging from amino acids to proteins as well as clusters, ranging from inorganic clusters to peptide aggregates.

To avoid line shifts and broadening, IR spectroscopy on cold ions can be performed. To do so, m/z selected ions are captured in liquid helium droplets prior to IR spectroscopic investigation. The conditions inside a helium droplet are isothermal at 0.38 K and the interaction between the helium matrix and the molecules are weak so that only small perturbations on the ion are expected. IR spectra for m/z small molecules as well as proteins containing more than 100 amino acids have been measured. The spectra of the smaller species show very narrow lines. For the larger species, band envelopes are obtained and for the case of highly charged proteins, a transition from helical to extended structures is observed.