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The site of protonation and proton delocalization in gaseous molecules elucidated by IR spectroscopy

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In electrospray ionization mass spectrometry (ESI-MS), molecules are usually ionized by protonation. The site of protonation is not necessarily the site of highest proton affinity, especially in cases where site-specific proton affinities in gas and solution phase deviate significantly. We use infrared ion spectroscopy employing the FELIX free-electron laser to determine the protonation site in the gas phase of the mass spectrometer. In addition to ion spectroscopy, various groups have employed ion mobility to differentiate between different protomers. We will relay recent experiments combining ion spectroscopy and ion mobility (as implemented on our modified Bruker SolariX FTMS platform) that indicate that post-mobility scrambling of the proton may occur.

For systems with two (nearly) equally nucleophilic sites in close proximity, the ionizing proton may become shared between the two nucleophiles. We discuss the spectroscopic signatures of such delocalized protons in infrared multiple-photon dissociation (IRMPD) spectra. Quantum-chemical modelling provides a basis for understanding these spectra, where static versus dynamic approaches reveal interesting insights into the vibrations involving the delocalized proton.

Keywords

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