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Gas-phase fragmentation chemistry of protonated ions: Models, structures, energetics and dynamics

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Fundamentally, chemical structure determines the properties and potential functions of any given molecule. Consequently, to effectively and consistently identify chemicals with tandem mass spectrometry the gas-phase structures occupied by our analyte ions will have direct influence on which fragmentation pathways are populated, and thus, on the resulting mass spectrum. Ideally, we desire the ability to decipher both the elemental composition (CcHhNnOoSsPp) and structural information on unknown compounds. To accomplish this successfully, an understanding of the gas-phase fragmentation chemistries likely to be in play is of substantial benefit. Consequently we need a reasonable means of modelling the processes occurring within the mass spectrometer or a spectral database of all possible compounds under the particular experimental conditions employed. The latter, optimal approach is impractical for many compound types as it requires reference spectra generated from prior confident identification of each possible synthesized/isolated analyte. Thus, we require a robust model for our particular compound class that is flexible and accurate enough to deal with how and why different analyte ions form particular conformations, and what affect this has on their gas-phase fragmentation chemistry and resultant mass spectra. The author will discuss recent density functional theory and experimental findings and their implications for structural identification of protonated systems with MS/MS.

Biography

Benjamin J Bythell received his MChem degree from the University of Bath, UK, in 2002 and PhD from Oregon State University in 2007. He held Postdoctoral fellowships at the German Cancer Research Center in Heidelberg (2008-2010) and at the National High Magnetic Field Laboratory at Florida State University (2010-2013). He joined the University of Missouri-St. Louis faculty in 2013. He works at the interface between analytical, computational and biophysical chemistry where he strives to understand the structure, reactivity and gas-phase behavior of biologically- and industrially-important chemicals.

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