INFRARED ION SPECTROSCOPY AT FELIX: APPLICATIONS IN PEPTIDE DISSOCIATION AND ANALYTICAL CHEMISTRY

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Infrared free electron lasers such as those in Paris, Berlin and Nijmegen have been at the forefront of the development of infrared ion spectroscopy. In this contribution, I will give an overview of new developments in IR spectroscopy of stored ions at the FELIX Laboratory. In particular, I will focus on recent developments made possible by the coupling of a new commercial ion trap mass spectrometer to the FELIX beamline.

The possibility to record IR spectra of mass-selected molecular ions and their reaction products has in recent years shed new light on our understanding of collision induced dissociation (CID) reactions of protonated peptides in mass spectrometry (MS). We now show that it is possible to record IR spectra for the products of electron transfer dissociation (ETD) reactions

$$[M + nH]^{n+} + A^- \rightarrow [M + nH]^{(n-1)+} + A \rightarrow \text{dissociation of analyte}$$

These reactions are now widely used in novel MS-based protein sequencing strategies, but involve complex radical chemistry. The spectroscopic results allow stringent verification of computationally predicted product structures and hence reaction mechanisms and H-atom migration.

The sensitivity and high dynamic range of a commercial mass spectrometer also allows us to apply infrared ion spectroscopy to analytes in complex "real-life" mixtures. The ability to record IR spectra with the sensitivity of mass-spectrometric detection is unrivalled in analytical sciences and is particularly useful in the identification of small (biological) molecules, such as in metabolomics. We report preliminary results of a pilot study on the spectroscopic identification of small metabolites in urine and plasma samples.