DEVELOPMENT OF A HYBRID LASER-MASS SPECTROMETER WITH TWO INSTRUMENT ARMS: IRMPD AND HENDI COLD ION SPECTROSCOPIC EXPERIMENTS

MATTHIAS HEGER, JOSEPH CHERAMY, FAN XIE, ZHIHAO CHEN, HAOLU WANG, WOLFGANG JÄGER, YUNJIE XU, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada*.

In this talk, we present a new hybrid laser-mass spectrometer with two instrument arms: one for infrared multiphoton dissociation (IRMPD) and the other for helium nanodroplet isolation (HENDI) cold ion spectroscopic experiments. The spectrometer features an electrospray source for ion production, using either traditional atmospheric nanospray or a novel Subambient Pressure Ionization with Nanoelectrospray (SPIN) design.[1] Ionic species of interest are isolated in a quadrupole mass filter and stored in a Paul trap for OPO IR laser irradiation. The ion trap is coupled to a TOF tube for fast wide-range mass spectrometry at high resolution. The second arm contains in addition an ion deflector and a linear quadruple ion trap which is currently being integrated into an existing HENDI spectrometer. This will enable higher resolution investigations of mass-selected ionic species in an ultra-cold environment.

IRMPD spectroscopy has emerged as a powerful asset in the spectroscopist's toolbox to investigate the isomerization and aggregation behavior of small molecules.[2] For example, this technique has been coupled with mass spectrometry to elucidate the structures of some amino acid complexes of interest, most notably perhaps the "magic number" serine octamer.[3] To demonstrate the current capabilities of the instrument, we extended previous studies on the gas-phase structures of protonated and sodiated asparagine monomers[4] into the IR regime between 3300 and 4000 cm–1. In addition, a theoretical re-assessment of the structural and spectroscopic properties of these species was undertaken with modern quantum-chemical approaches. We present this study as a stepping stone for further research into the structural and energetic preferences of small non-covalently bound amino acid aggregates.

[1] J. S. Page, K. Tang, R. T. Kelly, R. D. Smith, Anal. Chem. 2008, 80, 1800; I. Marginean, et al. Anal. Chem. 2012, 84, 9208. [2] N. C. Polfer, Chem. Soc. Rev., 2011, 40, 2211. [3] F. X. Sunahori, G. Yang, E. N. Kitova, J. S. Klassen, Y. Xu, Phys. Chem. Chem. Phys. 2013, 15, 1873. [4] A. L. Heaton, V. N. Bowman, J. Oomens, J. D. Steill, P. B. Armentrout, J. Phys. Chem. A 2009, 113, 5519.