

**1<sup>st</sup> June 2017 - 10:00 h**

**CFEL – Building 99, seminar room I+II (ground floor)**

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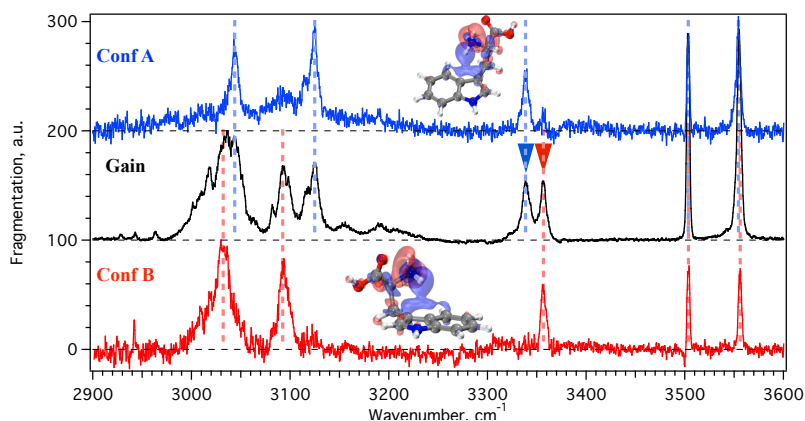
### IR-IR-(D)UV Hole-Burning Conformer-Selective Spectroscopy

Infrared-ultraviolet (IR-UV) double-resonance photofragmentation spectroscopy is a proven approach to conformer-selective vibrational spectroscopy of neutral and protonated biomolecules<sup>1</sup>. The conformer-selectivity of this method relies on the vibrational resolution in UV spectra, hence lifetime-broadening and high spectral congestion are crucial limiting factors of this technique<sup>2</sup>.

The IR-IR-UV hole burning technique combines the benefits of IR-IR tagging and IR-UV double-resonance gain techniques, enabling measurements of conformer-specific IR spectra with near-zero background<sup>3</sup>. This combination does not require tagging of the bare ion as it employs UV photofragmentation. Furthermore, since the conformational labelling employs IR transitions, this relaxes the need for vibrational resolution in the UV spectrum of the ion.

Another limiting factor of the gas-phase action spectroscopy is the necessary presence of a chromophore-containing amino acids in the peptide sequence. Excitation of peptides in the deep-UV spectral region allows the use of peptide bonds as chromophores, which makes IR-IR-DUV hole-burning spectroscopy the most general conformer-selective tool up to date.

The principles of the IR-IR-(D)UV hole-burning spectroscopy, as well as experimental results on conformer-specific vibrational spectra of protonated amino acids tryptophan and histidine, and several larger peptides will be presented.



1. T. R. Rizzo and O. V. Boyarkin, in *Gas-Phase IR Spectroscopy and Structure of Biological Molecules*, eds. A. M. Rijs and J. Oomens, Springer, 2015, vol. 364, pp. 43-98.
2. N. S. Nagornova, T. R. Rizzo and O. V. Boyarkin, *Angewandte Chemie International Edition*, 2013, 52, 6002-6005.
3. A. Y. Pereverzev, X. Cheng, N. S. Nagornova, D. L. Reese, R. P. Steele and O. V. Boyarkin, *The Journal of Physical Chemistry A*, 2016, 120, 5598-5608