

7th November 2013 – 10:00 a.m.
CFEL-bldg. 99, seminar room I and II (EG.076/078)

Oleg V. Boyarkin

Ecole Polytechnique Fédérale de Lausanne, Switzerland

Cold ion spectroscopy for structural determination of peptides and proteins

Spectroscopy of protonated biomolecules provides benchmarks for calculations of intrinsic three-dimensional structures of these large species. We employ double-resonance photo-fragmentation approach to measure UV and conformer-selective IR spectra of cryogenically cooled, protonated biomolecules as large as decapeptides, their water complexes and small proteins. Cooling of the molecules is essential to suppress thermal congestion and achieve vibrational resolution in the spectra, thus providing a significant number of details – a molecular fingerprint. These fingerprints reveal frequencies and, since recently, absolute intensities of vibrations, which must be reproduced by theory for validation of the correct ion structure. To view more details of such fingerprints, we are adding one more dimension to UV photofragmentation spectroscopy by combining it with high mass-resolution analysis of UV-induced fragments. We report on progress in coupling our cold ion instrument to a commercial Orbitrap mass-spectrometer.

