ESD2011: IR and UV Spectroscopy in Cold Ion Trap

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Three-dimensional structures of proteins and peptides and their heterogeneity in vivo reflect a fine balance between non-covalent intramolecular interactions and those with the surrounding solvent molecules. Decoupling intra- and intermolecular interactions and revealing the intrinsic structures of bio-molecules is crucial for understanding protein-peptide (-protein, -membrane) binding processes, protein folding, and can assist in silico drug design. We employ photo-fragmentation approach to measure UV and conformer-selective IR spectra of protonated biomolecules isolated in the gas phase. Our experiment combines electrospray ionization, mass-spectrometry, cryogenic cooling and laser spectroscopy.[1, 2] Cooling ions to ~10K in a 22-pole ion trap (Fig. 1) greatly suppresses thermal congestion and allows us to measure vibrationally resolved UV spectra and highly-resolved, conformer-specific IR spectra of proto-nated biomolecules as large as decapeptides. A measured "fingerprint" of vibrational transitions serves as a benchmark for structural calculations of a molecule.

We use conformer-selective Cold Ion Spectroscopy (CIS) for solving the 3D structure of a doubly protonated natural antibiotic, gramicidin S (GS), isolated in the gas phase. It is the largest molecule for which the gas phase structure has ever been accurately determined.[3] We also demonstrate application of CIS to the solvated complexes of GS with up to 50 water molecules, to phosphorylated peptides and to a multiply charged protein cytochrome-c.

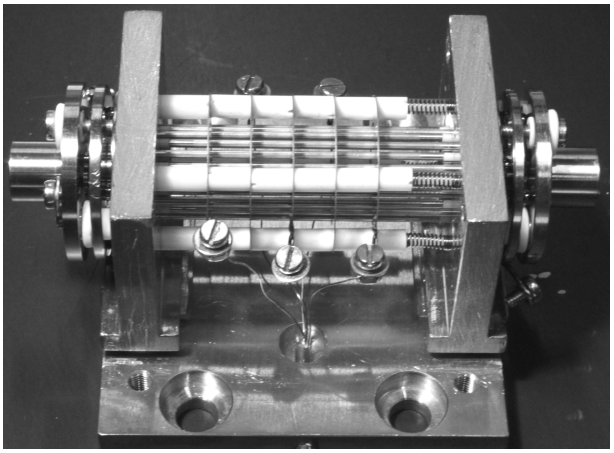

Figure 1. Opened view of the 22-pole ion trap cooled to 6K.

References

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