HOW CATION-PI INTERACTIONS ENHANCE AND STRUCTURE THE BINDING OF METAL IONS TO AMINO ACIDS AND PEPTIDES. DIALANINE PROBED BY IRMPD SPECTROSCOPY AS A PRIME EXAMPLE

ROBERT C. DUNBAR, *Chemistry Department, Case Western Reserve Univ., Cleveland, OH 44106*; JEFFREY STEILL, *FOM Institute for Plasma Physics, Nieuwegein, Netherlands*; JOS OOMENS, *FOM Institute for Plasma Physics, Nieuwegein, and University of Amsterdam, Netherlands.*

Spectroscopic examination of metalated amino acids and model peptides in the infrared region gives incisive conformational information. The role of cation-pi interactions of the metal ions with aromatic amino acids in structuring the complexes and enforcing particular architectures is being clarified by such experiments using IRMPD action spectroscopy as the experimental probe. The presence of multiple aromatic groups as in dialanine gives particularly stringent conformational stabilization. Comparing spectroscopic peak shifts across a range of alkali and alkaline earth metal ions, ranging from lithium to cesium, and from calcium to barium, allows us to view the systematic relations between normal mode frequencies and ion/peptide interactions. The spectra of the ions were acquired by irradiating the cell of the Fourier-transform ion cyclotron resonance mass spectrometer with infrared light from the FELIX free electron laser at wavelengths in the approximate range 500 to 1900 cm^{-1}.