CONFORMATIONS OF CATIONIZED PEPTIDES. DETERMINATION OF LIGAND BINDING GEOMETRIES BY IRMPD SPECTROSCOPY

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Spectroscopic study of the conformations of metalated amino acids has mapped out in some detail the preferences for canonical (charge solvated) versus zwitterionic (salt bridge) conformations. Corresponding studies of larger peptides are now possible. Here are described results for several singly and doubly charged metal ions with dipeptides and tripeptides. Factors including ion charge, size of cation, and side chain identity and sequence are found to be conformational determinants. IRMPD spectra of the ions were acquired by irradiating the cell with infrared light from the FELIX free electron laser at wavelengths in the approximate range 500 to 1900 cm^{-1}.