AMINO ACID COMPLEXES OF METAL IONS WITH +2 CHARGE. DETERMINATION OF SUCCESSIVE LIGAND CONFORMATIONS BY IRMPD SPECTROSCOPY

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Amino acid ligands can bind to metal ions in either the canonical (charge solvated) or the zwitterionic (salt bridge) conformation. Infrared multiple photon dissociation spectra are highly diagnostic for this structural feature, and have revealed that the conformation of the first ligand depends on the identities of the metal ion and the amino acid, as well as the charge of the complex. Attachment of a second amino acid ligand may give the same or a different conformation, and this choice will be examined for several different cases of complexes with doubly charged metal ions. The metal ion complexes of the amino acids were introduced by electrospray into the cell of the 4.7 T FT-ICR spectrometer interfaced to the free electron laser FELIX at the FOM Institute. IRMPD spectra of the ions were acquired by irradiating the cell with infrared from the laser at wavelengths in the approximate range 500 to 1900 cm^{-1}.