STRUCTURE INVESTIGATION OF CATION-PI COMPLEXES OF ALKALI METAL IONS WITH AROMATIC DIPEPTIDES BY IRMPD SPECTROSCOPY

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IRMPD spectroscopy has been used in the structural study of metal-ion complexes of aromatic dipeptides which combine aromatic rings, terminal amine and hydroxyl groups, and amide-derived binding points, as possible metal-ion attachment sites. Alkali metal complexes of the dipeptides were introduced by electrospray into the cell of the 4.9 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}. Sodium and potassium complexes of PheAla and AlaPhe were studied. The spectra of all four complexes were very similar, showing prominent IR peaks that were assigned as belonging to a free carbonyl stretch, a metal-bound carbonyl stretch, an N-H (amide) bend, and an OH bend. At least one weaker feature was also seen in the region of the phenyl out-of-plane bend. The consistency of the four spectra suggested that a similar chelation motif was adopted by all four systems. Preliminary comparison with the calculations gives three-fold chelated structures as the most probable.