

INFRARED SPECTRA OF $K^+(TRYPTAMINE)(H_2O)_{n=1-4}$ AND $K^+(TRYPTAMINE)(H_2O)_{n=0-2}Ar$

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A balance of competing electrostatic and hydrogen bonding interactions directs the structure of hydrated gas-phase cluster ions. In K^+ (Tryptamine) cluster ions, a favorable electrostatic interaction between the potassium cation and the tryptamine NH_2 lone pair stabilizes the high-energy Gph(in) and Gpy(in) conformers of neutral tryptamine. Previous studies of Tryptamine(H_2O) $_n$ clusters indicate that the hydrating water molecules stabilize the neutral minimum energy Gpy(out) tryptamine conformer. In this scheme, the first water molecule interacts directly with the NH_2 lone pair and is located to the side of the tryptamine monomer. By incorporating a potassium cation, however, the minimum energy tryptamine...water configuration is disrupted in order to maximize the electrostatic interactions with the cation, shifting so that the tryptamine...water interaction includes a π -hydrogen bond between the water and the phenyl ring of tryptamine. The infrared photodissociation spectra of K^+ (Tryptamine)(H_2O) $_{n=1-4}$ and K^+ (Tryptamine)(H_2O) $_{n=0-2}Ar$ will be presented along with parallel *ab initio* and thermodynamics calculations to assist with the identification of the isomers present in each experiment.