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$\cdots$water configuration is disrupted in order to maximize the electrostatic interactions with the cation, shifting so that the tryptamine$\cdots$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.