INFRARED SPECTRA OF M^+(2-AMINO-1-PHENYL ETHANOL)$(H_2O)_{n=0-2}$Ar (M=Na, K)

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A balance of competing electrostatic and hydrogen bonding interactions directs the structure of hydrated gas-phase cluster ions. Because of this, a biologically relevant model of cluster structures should include the effects of surrounding water molecules and metal ions such as sodium and potassium, which are found in high concentrations in the bloodstream. The molecule 2-amino-1-phenyl ethanol (APE) serves as a model for the neurotransmitters ephedrine and adrenaline. The neutral APE molecule contains an internal hydrogen bond between the amino and hydroxyl groups. In the M^+(APE) complex, the cation can either interrupt the internal hydrogen bond or position itself above the phenyl group, leaving the internal hydrogen bond intact. The former is preferred based on DFT calculations (B3LYP/6-31+G*) for both K^+ and Na^+ across the entire range from 0-400K, but infrared photodissociation (IRPD) spectra indicate a preference for the latter configuration at low temperatures. The IRPD spectra of $M^+(H_2O)_{n=1-2}$ and $M^+(H_2O)_{n=0-2}$Ar (M=Na, K) will be presented along with parallel DFT and thermodynamics calculations to assist with the identification of the isomers present in each experiment.