STRUCTURE AND PROPERTIES OF FORMANILIDE-WATER CLUSTERS IN A SUPERSONIC JET

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Electronic spectra of trans-formanilide clustered with water and ammonia have been obtained in a supersonic jet expansion. The observation of multiple origins for the single water species is consistent with the presence of two distinct hydrogen bonding sites in the trans-amide group capable of acting as either a hydrogen bond donor or acceptor. Structures have been assigned by comparison to the spectrum of trans-fromanilide ammonia cluster. Clusters of trans-formanilide with two and four water molecules have been observed and assigned to specific structures. These experimental observations are found to be in a good agreement with ab initio Hartree-Fock calculations.