WATER COMPLEXES OF AMINOPHENOL AND HYDROQUINONE

P. S. MEENAKSHI, N. BISWAS, and S. WATEGAONKAR, *Department of Chemical Sciences, Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai-400005, India*.

H-bonded water complexes of aminophenol and hydroquinone were studied in the supersonic jet by multiphoton ionization through the S_1 state. *Ab initio* calculations on both the systems were carried out in the S_0 and the S_1 states to determine the most stable structures of the complexes. Based on the spectroscopic signatures obtained from the excitation spectra and the calculations, structures for the observed complexes were proposed. A good correlation was shown to exist between the electronic red shift of the band origin of the complexes with respect to the corresponding monomers and the pKa* values (pKa in the excited state). A correlation was also drawn between the red shift in the band origin of the $1:1$ water complexes of various phenols with the relative decrease in the negative charge density on the phenolic oxygen atom upon excitation to the S_1 state.