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.