

MASS RESOLVED HOLE BURNING SPECTROSCOPY OF PHENOL(H₂O)₂₋₅ CLUSTERS AND ITS DEUTERATED ISOTOPOMERS: STRUCTURES AND INTERMOLECULAR VIBRATIONS IN THE S₁ - STATE

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Resonant two photon ionization spectra (R2PI) of hydrogen bonded Phenol-water clusters up to 10 H₂O were obtained in a supersonic jet expansion with ion detection via a special highly sensitive time of flight mass spectrometer. Using spectral hole burning (SHB) the unusually broad transitions to the intermolecular vibrations of Phenol(H₂O)₂ and Phenol-d₁ - (D₂O)₂ were observed for the first time. For Phenol(H₂O)₃₋₅ and Phenol-d₁ - (D₂O)₃₋₅ the observed intermolecular vibrational frequencies are compared with results from *ab initio* calculations based on cyclic or cage like minimum energy structures for the water moiety. Especially the very low frequencies in the range 10 - 60 cm⁻¹ which involve mutual ring motion („butterfly“, twisting, cogwheel movements of the phenol and water rings) turn out to depend quite sensitively on the cluster size and structure. Another „fingerprint“ region are the intermolecular OH...O stretch vibrations above 100 cm⁻¹. SHB is used to clear up the possibility of different isomers for the larger phenol-water clusters.