RESONANT ION-DIP INFRARED SPECTROSCOPY OF 2-HYDROXYPYRIDINE AND ITS SMALL WATER CLUSTERS

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The structures and dynamics of 2-hydroxypyridine-(water)$_n$ clusters (with n=1 and 2) have been investigated using resonant two-photon ionization time-of-flight mass spectroscopy (R2PI-TOFMS), IR-UV hole-burning, and resonant ion-dip infrared spectroscopy (RIDIRS). The double resonance technique of RIDIRS provides both wavelength and mass selectivity in recording the hydride stretch infrared spectrum (2200 to 3800 cm$^-$1) of a chosen cluster. The RIDIR spectrum of 2HOP monomer contains a narrow transition at 3598 cm$^-$1, about 55 cm$^-$1 lower in wavenumber than those of the corresponding hydroxy groups in phenol and cis/trans 2-naphthol. This suggests the presence of a weak intramolecular H-bond. The spectra of 2HOP-$(H_2O)_1 - 2$ contain sharp free OH stretch transitions near 3715 cm$^-$1 and H-bonded OH stretch transitions in the 3100-3500 cm$^-$1 region, which are remarkably broad (approaching 100 cm$^-$1 in 2HOP-$(H_2O)_2$) and show distinct sub-structure indicative of strong coupling to background states. A comparison with the results of density functional theory calculations indicates that the water molecules in 2HOP-$(H_2O)_1$ and 2HOP-$(H_2O)_2$ form bridges between the OH and N groups of 2HOP, accepting a H-bond from the OH group and donating a H-bond to the nitrogen lone pair. Possible reasons for the unusual breadth of these transitions will be put forward.