FLUORESCENCE-DIP INFRARED SPECTROSCOPY OF 2-PYRIDONE, ITS DIMER, AND WATER CLUSTERS

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Fluorescence-dip infrared spectroscopy (FDIRS) and IR-UV hole-burning spectroscopy have been used to probe the structures and dynamics of hydrogen bonding in the S_0 and S_1 states of 2-pyridone (2PYR), its dimer $(2PYR)_2$, and its water-containing clusters 2PYR-$(H_2O)_n$ (with n=1 and 2). This double resonance scheme combines the sensitivity of laser-induced fluorescence with the structure-resolving power of IR spectroscopy. 2-pyridone is the keto form of 2-hydroxypyridine (2HOP) and contains the same H-bonding sites that are found in the pyrimidine base, uracil (U). The pyridone dimer provides a first glimpse of an "improper" base pairing interaction in modeling the U-U dimer. The 2-pyridone dimer is known to be a cyclic, doubly H-bonded structure with C_2h symmetry. The infrared spectrum of this dimer has a single NH stretch which carries all the oscillator strength in this region. It produces an intense absorption with a maximum just below 2700 cm$^-$1, and a long tail stretching nearly 200 cm$^-$1 beyond this maximum. Distinct, sharp sub-structure with irregular spacing of about 5-10 cm$^-$1 and widths of 2-5 cm$^-$1 underlies this envelope. The implications of this sub-structure for the strong coupling present in the pyridone dimer will be discussed.