THE INFRARED SPECTROSCOPY OF STRONGLY H-BONDED DIMERS: A NEW LOOK AT AN OLD PROBLEM

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Fluorescence-dip infrared spectroscopy (FDIRS) has been used to record the infrared spectra of several strongly H-bonded dimers cooled in a supersonic jet. The strong hydrogen bonds present in these dimers are known to produce intense, extremely broad infrared bands, complete with sub-structure which has been the subject of much previous investigation. By cooling the dimers in the supersonic expansion, much of the breadth and sub-structure of the bands are removed, but the bands nevertheless retain significant breadth and partially resolvable sub-structure that has not been observed previously. In this talk we will present the fluorescence-dip infrared spectra of pyridone dimer and benzoic acid dimer, both with and without partial deuteration. The shape and sub-structure of these bands will be discussed in light of the strong anharmonic couplings present in the dimers. Density functional theory calculations have been used to model the hydride stretch potential and to isolate the strong anharmonic couplings that appear to dominate the appearance of the hydride stretch absorption.