COUPLING BETWEEN THE NH AND THE INTERMOLECULAR STRETCHING MODES OF 7-AZAINDOLE TAUTOMERIC DIMER

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Recently, couplings between the intramolecular OH/NH and the intermolecular stretching modes of double hydrogen-bonded dimers, such as benzoic acid and 7-azaindole dimers, are investigated by the two-dimensional IR spectroscopy in solution. Infrared OH/NH stretching bands of such species exhibit a very complicated pattern. This pattern is analyzed theoretically based on the anharmonic coupling between the OH/NH stretching and the other modes.

In the present study, we recorded infrared spectra of jet-cooled 7-AI tautomeric dimer by means of infrared-visible double resonance technique. This species is a product of the excited-state proton/hydrogen transfer reaction of 7-AI dimer and has the double hydrogen-bonded structure. Thus, the strong coupling between the intramolecular NH and the intermolecular stretching modes is expected as in the case of 7-AI normal dimer. In the IR spectrum observed in the present study, the NH stretching band exhibit a very broad width as expected. In addition, we have succeeded in recording the IR spectrum from the vibrational level involving an excitation of the intermolecular stretching mode. These results provide us with an effect of the coupling in the frequency-domain. The analysis of the vibrational coupling will be presented in the paper.