INFRARED SPECTROSCOPY OF 7-AZAINDOLE TAUTOMERIC DIMER: OBSERVATION OF THE ND STRETCH

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7-azaindole (7-AI) dimer is a very attractive species as a model system of nucleic-acid base pair. The 7-AI dimer is known to exhibit the excited-state double proton transfer (DPT) reaction. The tautomeric dimer produced in the DPT reaction goes back to normal form in the electronic ground state, in solution. In general, the proton-transfer reaction is a fundamental and an important elementary reaction in various chemical and biological systems. However, the ground-state reverse DPT reaction is not thoroughly studied, so far. Thus, we carry out infrared (IR) spectroscopy of the jet-cooled 7-AI tautomeric dimer. In our previous study, we measured IR spectra of the tautomeric dimer and its deuterated species in the NH stretch region and discussed the vibrational dynamic based on the band profiles[a]. In order to obtain more precise information about the deuteration effect, we have observed the ND stretch bands of the deuterated dimers in the present study.

The deuteration of the NH hydrogen provides three deuterated species, such as the NH-NH, NH-ND, and ND-ND dimers. The NH stretch band of the NH-NH dimer appears at 2680 cm^{-1}. It exhibits a less-structured and broad profile whose width is $\sim$245 cm^{-1}. On the contrary, the NH-ND dimer exhibits a narrower NH stretch band width. This difference is attributed to a change in the vibrational energy flow between the two monomer units in the dimer. In the present study, we have succeeded in measuring the ND stretch bands of the NH-ND and the ND-ND dimers. The ND stretch band of the ND-ND dimer appears at 2120 cm^{-1} and its width is found to be $\sim$90 cm^{-1}, whereas that of the NH-ND dimer is red-shifted and exhibits rather narrow width. Based on these observations, the single-deuteration effect on the vibrational dynamics and its relation to the DPT reaction is discussed in the paper.

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[a] H. Ishikawa, H. Yabuguchi, Y. Yamada, A. Fujihara, and K. Fuke, J. Phys. Chem. A, in press.