DEUTERATION EFFECT ON THE NH/ND STRETCH BAND OF THE JET-COOLED 7-AZAINDOLE AND ITS TAUTOMERIC DIMERS: RELATION TO THE GROUND-STATE DOUBLE PROTON-TRANSFER REACTION

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In order to investigate the deuteration effect on the vibrational dynamics of the NH and/or ND stretch excited levels of the 7-azaindole (7-AI) normal dimer and its tautomeric dimer, we have carried out infrared spectroscopy of three isotopic species for each dimers; undeuterated one (NH-NH) and one or two hydrogen atom(s) of the NH groups is deuterated ones (NH-ND and ND-ND, respectively). It is found that the ND stretch band profiles of the NH-ND and ND-ND tautomeric dimers are very similar with each other. This result is very distinct from the result of the comparison of the NH stretch band profiles of the NH-NH and NH-ND dimers in our previous study[a]. For a further discussion, we have examined the deuteration effect in the case of the 7-AI normal dimer. It is found that the NH stretch band profiles of the NH-NH and the NH-ND dimers and also the ND stretch band profiles of the NH-ND and the ND-ND dimers exhibit similar patterns, respectively. These facts indicates that the vibrational relaxation from the NH/ND stretch level of the normal dimer basically proceed within a monomer unit. The large deuteration effect of the NH stretch band profile observed previously is found to be characteristic of the tautomeric dimer. This behavior is related to a large anharmonicity of the potential energy surface originating from an existence of the double-proton transfer reaction barrier.

[a] H. Ishikawa, H. Yabuguchi, Y. Yamada, A. Fujihara, K. Fuke, *J. Phys. Chem. A* **114**, 3199 (2010).