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Final resolution of the step-wise versus concerted mechanism controversy for excited-state double proton transfer in the 7-azaindole dimer in the gas phase HIROSHI SEKIYA, KENJI SAKOTA, Department of Chemistry, Faculty of Science, Kyushu University, CHIE OKABE, NOBUYUKI NISHI, Institute for Molecular Science — The excited-state double-proton transfer (ESDPT) reaction in the 7-azaindole dimer has been extensively studied by spectroscopic methods in the gas phase and in solution. Two ESDPT mechanisms, stepwise and concerted mechanisms, have been proposed so far. However, a definite conclusion has not been provided due to a lack of clear evidence. We provide final resolution of the stepwise versus concerted mechanism controversy for the ESDPT reaction in the 7-azaindole dimer by electronic spectroscopy and picosecond-time resolved spectroscopy in the gas phase (K. Sakota, C. Okabe, N. Nishi, H. Sekiya, J. Phys. Chem. A, 109, 5245 (2005)). The ESDPT reaction in the 7-azaindole dimer proceeds via the concerted mechanism. We propose a dynamic cooperative effect, where the motions of the two transferring protons couple with each other through the electronic reorganization (K. Sakota ,H. Sekiya, J. Phys. Chem. A, 109, 2718 (2005); 109,2722 (2005)).

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