INFRARED SPECTROSCOPY OF 7-AZAINDOLE TAUTOMERIC DIMER AND ITS ISOTOPOMERS

HARUKI ISHIKAWA, HIROKI YABUGUCHI, YUJI YAMADA, AKIMASA FUJIHARA, KIYOKAZU FUKE, *Department of Chemistry, Graduate School of Science, Kobe University, Nada-ku, Kobe 657-8501, Japan*.

7-azaindole (7-AI) dimer is a very attractive species as a model system of neucleic-acid base pair. It is well-known that it exhibits the excited-state double proton transfer (DPT) reaction. In solution, the tautomeric dimer generated in the DPT reaction goes back to normal form in the electronic ground state. This ground-state inverse DPT reaction is not thoroughly studied, so far. Thus, we carry out infrared spectroscopy of the jet-cooled 7-AI tautomeric dimer and examine the possibility of the vibrational-excitation promoted inverse DPT reaction. In the IR spectrum of the 7-AI tautomeric dimer, a very strong and broad band appears at 2680 $cm^{-1}$ and is assigned as the anti-symmetric NH stretch mode. On the contrary, sharp bands around 3100 $cm^{-1}$ are assigned as the CH stretch modes. Such a large difference in the band profiles among these bands is related to the difference in the vibrational anharmonicity of these modes. To discuss the vibrational anharmonicity of the NH stretch mode and the relation to the DPT reaction, we have also recorded IR spectra of several deuterated dimers. Comparison among the IR spectra of isotopomers will be discussed in the paper.