IR INDUCED ISOMERIZATION AND ITS BACKWARD REACTION OF COLD PHENOL-METHANOL CLUSTER CATIONS

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Since gas-phase hydrogen-bonded clusters are treated as a microscopic model of hydrogen bond networks, a huge number of spectroscopic studies have been performed, so far. Structural fluctuations are one of features of hydrogen bond network. Such fluctuations correspond to isomerizations among isomers having distinct hydrogen bond structures in the cases of clusters. To elucidate dynamical aspects of microscopic hydrogen-bond networks, we have been investigating an IR-induced isomerization of phenol-methanol cluster cations, $[PhOH(MeOH_3)]^+$, trapped in a cold ion trap, and its backward reaction. In our experiment, we recorded UV-photodissociation (PD) spectra of $[PhOH(MeOH_3)]^+$ with and without IR excitation. An isomerization from the ring- to chain-type isomers can be observed as a decrease in the band intensity of the ring-type isomer and also an increase in that of the chain-type isomer in the UV-PD spectra. In the last symposium, we reported a clear evidence of the isomerization process and also its backward reaction.[a] In the present experiment, we carefully examined time propagations of the spectra. As a result, we observed a rapid generation of the chain-type isomers and a change in the UV-PD spectral profiles of the chain-type isomer in the order of 10 μs. This is due to the re-cooling and the backward reaction of the chain-type isomers within a cold trap. We estimated the temperatures of the chain-type isomers during the re-cooling process by referring to the UV-PD spectra of $[PhOH(MeOH_3)]^+$ measured at various temperatures.[b] Details of the observations are presented in the paper.

[a] M. Ozeki, *et al.* RM14, *International Symposium on Molecular Spectroscopy*, (2021).
[b] M. Orito, *et al.* RM13, *International Symposium on Molecular Spectroscopy*, (2021).