UV PHOTODISSOCIATION SPECTROSCOPY OF TEMPERATURE CONTROLLED HYDRATED PHENOL CLUSTER CATION

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Owing to various developments of spectroscopic techniques, microscopic hydration structures of various clusters in the gas phase have been determined so far. The next step for further understanding of the microscopic hydration is to reveal the temperature effect, such as a fluctuation of the hydration structure. Thus, we have been carrying out photodissociation spectroscopy on the hydrated phenol cation clusters, $[PhOH(H_2O)_n]^+$, trapped in our temperature-variable ion trap[a].

After the last symposium[b], we succeeded in improving our experimental condition and recorded the UV photodissociation spectra of $[PhOH(H_2O)_5]^+$ at the trap temperatures of 20, 50, and 100 K. We identified three groups of bands by their temperature dependence in the spectra. Based on the results of the DFT calculations, we estimated the temperature dependence of the relative populations among the isomers. As a results, the isomers were grouped into three groups having different motifs of the hydrogen-bond structures. Comparing the experimental with the theoretical results, we assigned the relation between the band carriers and the hydrogen-bond structure motifs. Details of the discussion will be presented in the paper.

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[a] H. Ishikawa, T. Nakano, T. Eguchi, T. Shibukawa, K. Fuke, *Chem. Phys. Lett.* **514**, 234 (2011).

[b] R. Yagi, Y. Kasahara, H. Ishikawa, WH12, the 70th International Symposium on Molecular Spectroscopy (2015)