STRUCTURE DETERMINATION AND EXCITED STATE PROTON TRANSFER REACTION OF 1-NAPHTHOL-AMMONIA CLUSTERS IN THE S_1 STATE STUDIED BY UV-IR-UV MID-IR SPECTROSCOPY

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1-naphthol ammonia clusters have been studied long time as a benchmark system of the excited state proton transfer (ESPT) reactions. Understanding the ESPT reaction in this system has still not been fully established. To detect the cluster size dependence of the S_1 state properties, many researcher extensively investigated such as emission spectra,[a] lifetime,[b] solvents (ammonia) evaporation pattern.[c] Curiously, cluster structure that is fundamental to discuss the reaction has not been determined for the system. Thus we applied an IR spectroscopy to the S_1 states of the system to determine the cluster structure and to discuss the minimum size inducing the ionic dissociation of the O-H bond in the S_1 state. IR spectra were recorded not only the O-H and N-H stretching region (3 μm) but also the skeletal vibrational region (5.5-10 μm). Though O-H and N-H stretching vibrations do not provide useful structural information due to the broadness, the skeletal vibrations hold the sharpness even in the S_1 states. Changes in the skeletal vibrations due to the ammonia solvation, e.g. C-O stretching and C-O-H bending, will be discussed based on a comparison with theoretical calculations.

[a] O. Cheshnovsky and S. Leutwylar, *J. Chem. Phys.* **1**, 4127 (1988).
[b] S. K. Kim et al., *Chem. Phys. lett.* **228**, 369 (1994).
[c] C. Dedonder-Lardeux et al., *Phys. Chem, Chem, Phys.* **3**, 4316 (2001).