REORIENTATION OF SOLVENT MOLECULES IN THE INTRAMOLECULAR CHARGE-TRANSFER REACTION OF SOLVATED CYANOPHENYLDISILANE CLUSTERS

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We have been investigating the intramolecular charge-transfer (ICT) process of jet-cooled phenyldisilanes by laser spectroscopic methods. In the previous study, we performed the transient IR absorption spectroscopy of (*p*-cyanophenyl)pentamethyldisilane (CPDS) and its solvated clusters. We determined the equilibrium structure of the charge-transfer(CT) state and confirmed the occurrence of the torsional deformation in the ICT process as expected by the TICT model[a]. Recently, we reported an observation of a reorientation of water molecule in the CT state of CPDS-water cluster by the transient IR spectroscopy[b].

In the present study, in order to obtain detailed information about the reorientation process in the ICT process, we have carried out the transient IR spectroscopy in the OH and CN stretching region of solvated CPDS cluster with various solvents, such as CH_3OH, CH_3CN, and CCl_4. In the case of 1:1 solvated clusters with CH_3OH and CH_3CN, reorientation process are clearly observed as in the case of water cluster. In addition to the 1:1 clusters, the transient IR spectra of CPDS-$(H2O)_2$ and CPDS-$(CH_3OH)_2$ clusters have been observed. In the former case, a large displacement of the water molecule is suggested by the transient IR spectrum. Possible orientations of the solvent molecules are examined based on theoretical calculations. Details will be presented in the paper.

[a] H. Ishikawa *et al*. *J. Phys. Chem. A* **109**, 8959 (2005).

[b] M. Sugiyam *et al.*, 59th Ohio State University International Symposium on Molecular Spectroscopy, WH10 (2005).