

LASER SPECTROSCOPIC STUDY ON PHENOL-ETHYLDIMETHYLSILANE DIHYDROGEN-BONDED CLUSTER

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Dihydrogen bond is a hydrogen bond which acts between two H atoms having opposite partial charges. Among various kinds of dihydrogen bond systems, we have been investigating the Si-H \cdots H-O type dihydrogen bond^{a,b}. On the course of our study, we found that the competition between the dihydrogen bond and dispersion interactions determines the structures of phenol-alkylsilane 1:1 dihydrogen-bonded clusters. However, since there are many isomers due to intermolecular orientation as well as conformation of alkyl groups, we have not yet determined their structures completely. In the present study, we have carried out a laser spectroscopic study on the phenol-ethyldimethylsilane (PhOH-EDMS) dihydrogen bonded clusters. Since EDMS has a simple structure, the number of the isomers is expected to be small. We recorded laser-induced fluorescence (LIF), UV-UV hole-burning, and IR spectra of jet-cooled PhOH-EDMS clusters. As a result, we identified two isomers, A and B, based on the UV-UV hole-burning spectra. The 0-0 band of the isomer A is redshifted by -83.3 cm^{-1} compared with that of the PhOH monomer and exhibits a simple and long progression of 16.6 cm^{-1} interval of the intermolecular vibration. On the other hand, the redshift of the 0-0 band of the isomer B is much smaller (-20.3 cm^{-1}) and exhibits rather congested band patterns. The redshifts of the OH stretching band of these isomers are -27 and -20 cm^{-1} for the isomers A and B, respectively. Based on the comparison of spectral features observed with those predicted by the DFT calculations, we determined the structure of the isomers A and B. Details will be presented in the paper.

^aH. Ishikawa, A. Saito, M. Sugiyama, N. Mikami, *J. Chem. Phys.* **123**, 224309 (2005).

^bH. Ishikawa, T. Kawasaki, R. Inomata, *J. Phys. Chem. A* **119**, 601 (2015).