INFRARED SPECTROSCOPY OF PHENOL$^+$-TRIETHYLSILANE DIHYDROGEN-BONDED CLUSTER: INTRINSIC STRENGTH OF THE Si-H⋯H-O DIHYDROGEN BOND

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Dihydrogen bond is known to be one of the unconventional hydrogen bonds. When a hydrogen atom is bonded to an electropositive atom, such as B, Al, and so on, the hydrogen atom has a partial negative charge. Then, a hydrogen-bond type interaction are formed between the oppositely charged two hydrogen atoms. This interaction is called a dihydrogen bond. In the previous study, we reported the infrared spectroscopy of neutral phenol (PhOH)-triethylsilane (TES) cluster$^a$. It was suggested that the Si-H⋯H-O dihydrogen bond should be as strong as the $\pi$-type hydrogen bond. In the present study, to investigate the intrinsic strength of the Si-H⋯H-O dihydrogen bond, infrared photodissociation spectroscopy on the PhOH$^+$-TES and PhOH$^+$-diethylmethysilane (DEMS) cationic cluster is was carried out$^b$.

Both of the clusters exhibit a very broad and intense band centered at about 2860 cm$^{-1}$. This band is assigned as the OH stretching band of the PhOH$^+$ moiety. Based on the amount of the red-shift of the OH stretching band and the results of the theoretical calculations, the intrinsic strength of the Si-H⋯H-O dihydrogen bond is evaluated to be stronger than that of the $\pi$-type hydrogen bond. The proton affinities of TES and DEMS estimated by the theoretical calculation are larger than those of benzene and ethylene. These results are consistent with our experimental observations.

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$^a$H. Ishikawa, T. Kawasaki, RJ02, the 68th International Symposium on Molecular Spectroscopy (2013)