FRANCK-CONDON-LIKE PATTERNS OBSERVED IN THE INFRARED SPECTRA OF PHENOL-ALKYLSILANE DIHYDROGEN-BONDED CLUSTERS IN THE EXCITED STATES

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We have been carrying out spectroscopic studies on the Si-H$\cdots$H-O type dihydrogen-bonded clusters. It was revealed that the strength of the Si-H$\cdots$H-O type dihydrogen bond is comparable to that of the dispersion interaction and that the cluster structure is determined by the balance between these two interactions. To examine an effect of a change in the balance between them, we recorded the IR spectra of phenol-alkylsilane clusters in the S_1 state. In the course of our study, we found that the OH stretching band profile consists of several bands involving the excitation of the intermolecular vibrational modes. These band profiles are referred to as the Franck-Condon-like patterns. In the case of the phenol-t-butyldimethylsilane cluster, the band patterns simulated based on the Franck-Condon factors for the intermolecular vibrational mode have reproduced the observed patterns very well. This behavior indicates the interaction between the OH stretch and intermolecular vibrational modes. On the other hand, the infrared spectra of the electronic excited states of phenol-ethyldimethylsilane dihydrogen-bonded cluster indicate the contribution of two intermolecular vibrational modes. In this case, we analyzed the band pattern involving effects of the Duschinsky rotation as well as the displacements of the equilibrium positions for the v_{OH} = 0 and 1 states. In the present paper, we report the details of the analysis of the Franck-Condon-like patterns.