REDUCTION OF THE ROTATIONAL CONSTANT OF SMALL MOLECULES IN HYDROGEN CRYSTALS INVESTIGATED BY FTIR SPECTROSCOPY

HIROMICHI HOSHINA, MIZUHO FUSHITANI and TAKAMASA MOMOSE, *Division of Chemistry, Graduate School of Science, Kyoto University, Kyoto 606-8502, JAPAN*.

We have been studying rotation-vibration transitions of molecules embedded in solid hydrogen by high-resolution Fourier-transform infrared spectroscopy. Some small molecules such as methane and methyl radical show clear rotational branches in their vibrational transitions. The observed rotation-vibration spectra were fully analyzed by assuming that the guest molecule is rotating almost freely at an substitutional site of the hexagonal close-packed lattice of solid hydrogen. The effective rotational constants obtained from the analysis of the spectra were found to be slightly smaller than the rotational constants in the gas phase, but the reduction varies 70 - 90 % of the gas phase values depending on molecules. It is also found that the reduction is larger in solid $ortho$-D_2 than in solid $para$-H_2. The origin of the reduction of the rotational constant of molecules embedded in hydrogen crystals will be discussed in terms of the interaction between the rotational motion of the guest molecules and crystal phonon.