INFRARED SPECTROSCOPY OF THE HCN- $(H_2/D_2)_n$ CLUSTERS IN THE SUPERFLUID HELIUM DROPLETS

MASAZUMI ISHIGURO, ROGER E. MILLER, Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599.

The Superfluid He droplet is an ideal matrix for making large sized molecular clusters, because of its extremely low temperature (T < 0.5 K) and very weak interaction with molecules. In this study, we observed vibrational spectra for the CH stretching band of the HCN-(H₂/D₂)_n clusters in the He droplets under a strong electric field (30 kV/cm).

For the HCN- $(H_2)_n$ system, HCN- $(o-H_2)_n$ (n = 1-5), HCN- $(p-H_2)_n$ (n = 1-3), and HCN- $(o-H_2)_1(p-H_2)_1$ have been observed. Since $o-H_2$ (j = 1) has a quadrupole moment, it is supposed that the interaction between $o-H_2$ and HCN is stronger than that between $p-H_2(j = 0)$ and HCN. Nevertheless, the observed red-shift of the CH-stretching band for HCN- $(o-H_2)_n$ is much smaller than that of HCN- $(p-H_2)_n$. This phenomenon strongly suggests that the geometrical structure for HCN- $(o-H_2)_n$ and that for $(p-HCN)_n$ are distinctly different. That is, in HCN- $(o-H_2)_n$, the H₂ molecules are bonding to the N site of HCN. Contrastedly in HCN- $(p-H_2)_n$, the H₂ molecules are bonding to the H site of HCN, and affect strongly to the CH-stretching vibration. For the HCN- $(D_2)_n$ system, we obtained the same conclusion. In addition to the vibrational spectra under the strong electric field, we mention vibrational-rotational spectra for HCN- $(H_2/D_2)_1$ clusters under the field-free condition.