MILLIMETER-WAVE SPECTROSCOPY OF THE vdW BANDS OF He-HCN NEAR THE DISSOCIATION LIMIT.

KENSUKE HARADA and KEIICHI TANAKA, *Department of Chemistry, Faculty of Science, Kyushu University, Hakozaki, Higashiku, Fukuoka, 812-8581 Japan.*

The He-HCN complex is a weakly bound complex with binding energy of about 9 cm^{-1}. We have measured the internal rotation bands (to the j = 1 and 2 states) and intermolecular stretching bands of the He-HCN complex by millimeter-wave absorption spectroscopy combined with a pulsed-jet expansion technique, and reported the potential energy surface (PES) to reproduce the observed transition frequencies.[a] The PES obtained has a global minimum in the linear configuration with a depth of 30.3 cm^{-1} and has a saddle point at the anti-linear configuration with a depth of 20.3 cm^{-1}. The intermolecular stretching level and the second excited (j = 2) level of the internal rotation state are determined to be located 9.1407 and 9.0529 cm^{-1}, respectively, above the ground state, very close to the calculated dissociation limit (D_0) of 9.33 cm^{-1} .

In the present study, we have extended the measurement to the transitions to the bound states above the "dissociation limit" (D_0) and observed several such transitions for the first time in the ground state of the molecular complex. The rovibrational levels of He-HCN with e label dissociate to the HCN molecule with $J = 0$ and the He atom (D_0), while those with f label, due to the parity conservation, to the HCN molecule with $J = 1$ and the He atom which is higher in energy by about $2B_{\mathrm{HCN}} \sim 2.96$ cm^{-1} than D_0, as discussed in the infrared study of He-HF.[b] The PES obtained in the present analysis indicates that four f levels in the j = 1 and 2 excited states are bound above the "dissociation limit" (D_0) due to the parity conservation. In addition five levels (both of e and f labels) are predicted to be bound by centrifugal barrier with finite life times but not yet observed.

---

[a] K. Harada, K. Tanaka, T. Tanaka, S. Nanbu, and M. Aoyagi, J. Chem. Phys. **117**, 7041 (2002).
[b] C. M. Lovejoy and D. J. Nesbitt, J. Chem. Phys. **93**, 5387 (1990).