MILLIMETER-WAVE SPECTROSCOPY OF He-HCN AND He-DCN: ENERGY LEVELS NEAR THE DISSOCIATION LIMIT.

KENSUKE HARADA, KEIICHI TANAKA, *Department of Chemistry, Kyushu University, Fukuoka, Japan*.

The He-HCN complex is a weakly bound complex with binding energy of about 9 cm^{-1}. We have measured the the $j = 1 \leftarrow 0$ internal rotation fundamental band of the He-HCN complex by millimeter-wave absorption spectroscopy and reported the potential energy surface (PES) to reproduce the observed transition frequencies.[a]

In the present study, we have extended the measurement to the $j = 2 \leftarrow 1$ internal rotation hot bands of the He-HCN and He-DCN complexes. In the analysis, the upper state of several observed transitions are found to be located above the "dissociation limit" (D_0). The rovibtrational levels 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 2.96 cm^{-1} ($2B_{\rm HCN}$) than D_0. The f levels are bound up to $D_0 + 2B_{\rm HCN}$.

The revised PES of He-HCN has a global minimum in the linear He–HCN configuration with a depth of 29.9 cm^{-1} and has a saddle point at the anti-linear He–NCH configuration with a depth of 20.9 cm^{-1}. The ν_s intermolecular stretching first excited state and the $j = 2$ internal rotation second excited state are determined to be located 9.1405 and 9.0530 cm^{-1} above the ground state and very close to the calculated dissociation limit (D_0) of 9.32 cm^{-1}. Life times of several quasi-bound levels (both of e and f labels) and line widths of the related transitions are predicted for He-HCN and He-DCN from the revised PESs.

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[a] K. Harada, K. Tanaka, T. Tanaka, S. Nanbu, and M. Aoyagi, J. Chem. Phys. **117**, 7041 (2002).