

## INTERMOLECULAR POTENTIAL OF He-HCN AND He-DCN.

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The He-HCN complex is a weakly bound complex with a binding energy of only  $9\text{ cm}^{-1}$ .<sup>a</sup> We have measured the internal rotation<sup>a</sup> and intermolecular stretching bands of the He-HCN and He-DCN complexes by millimeter-wave absorption spectroscopy combined with a pulsed-jet expansion technique.

In the present study, the transition frequencies of the  $\nu_s$ ,  $\nu_s \leftarrow j = 1$ ,  $j = 2 \leftarrow 1$ , and  $j = 2 \leftarrow 0$  bands of He-HCN and He-DCN were fitted using the intermolecular potential function, where  $\nu_s$  refers to the intermolecular stretching first excited state and  $j$  denotes the quantum number for the HCN internal rotation. The combined potential of the Born-Mayer type repulsive term, asymptotic long range interaction term, and the general expansion terms were used for the fitting of the transition frequencies. The transition frequencies were fitted within the experimental uncertainties of 70kHz. The potential energy surfaces obtained has a global minimum in the linear configuration with a depth of  $30.3\text{ cm}^{-1}$ . The potential surface has a saddle point at the anti-linear configuration with a depth of  $20.3\text{ cm}^{-1}$ . The intermolecular stretching frequency is  $9.1405\text{ cm}^{-1}$ , while the dissociation energy ( $D_0$ ) is  $9.3183\text{ cm}^{-1}$  for He-HCN. The average distance and the root mean square amplitude are  $6.209\text{ \AA}$  and  $2.840\text{ \AA}$  for the intermolecular stretching first excited state ( $\nu_s$ ,  $J=1$ ), which are much larger than those for the ground state ( $4.306\text{ \AA}$  and  $0.577\text{ \AA}$ ). The wavefunction of the  $\nu_s$ ,  $J=1$  state has a node along the radial coordinate and has finite probability density even at  $14\text{ \AA}$ . The difference of the energy level structure between normal and deuterated species will be discussed.

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<sup>a</sup>K. Harada, K. Tanaka, T. Tanaka, S. Nanbu, and M. Aoyagi, *J. Chem. Phys.* **117**, 7041 (2002).