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 cm^{-1}.[a] We have measured the internal rotation[a] 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 ν_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 ν_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 cm^{-1}. The potential surface has a saddle point at the anti-linear configuration with a depth of 20.3 cm^{-1}. The intermolecular stretching frequency is 9.1405 cm^{-1}, while the dissociation energy (D_0) is 9.3183 cm^{-1} for He-HCN. The average distance and the root mean square amplitude are 6.209 Å and 2.840 Å for the intermolecular stretching first excited state (ν_s, J=1), which are much larger than those for the ground state (4.306 Å and 0.577 Å). The wavefunction of the ν_s, J=1 state has a node along the radial coordinate and has finite probability density even at 14 Å . The difference of the energy level structure between normal and deuterated species will be discussed.

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