MILLIMETER WAVE SPECTROSCOPY OF THE INTERNAL ROTATION BANDS OF 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 bands,[a] and intermolecular stretching band of the He-HCN complex and determined intermolecular potential energy surface. In the present study, the internal rotation fundamental band (j=1-0), hot band (j=2-1), and overtone (j=2-0) of the deuterated species (He-DCN) were observed by millimeter-wave absorption spectroscopy combined with a pulsed-jet expansion technique. 13, 6, and 2 transitions were assigned to the internal rotation fundamental band (j=1-0), hot band (j=2-1), and overtone (j=2-0) in the frequency region of 85–205 GHz. Combination differences were used to confirm the assignment. The observed transition frequencies were analyzed to improve an empirical intermolecular potential energy surface. No level of the intermolecular stretching first excited state (ν_s) was predicted below the dissociation limit for the deuterated species, while the normal species has two energy levels in the intermolecular stretching first excited state below the dissociation limit. 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).