MILLIMETER WAVE SPECTROSCOPY OF THE VAN DER WAALS BENDING BANDS OF Ne-HCN AND Ne-DCN

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The millimeter wave absorpion spectroscopy have been applied to the observation of the van der Waals bending bands of ^{20}Ne-HCN, ^{22}Ne-HCN, ^{20}Ne-DCN, and ^{22}Ne-DCN. The band origins of the Σ_1-Σ_0 and Π_1-Σ_0 bands were observed at 133 and 107 GHz for Ne-HCN, and at 134 and 103 GHz for Ne-DCN. Most lines were split into the hyperfine components of the nitrogen nucleus. The observed frequencies were analyzed to determine an empirical intermolecular potential energy surface. The potential surface thus determined has a global minimum at the linear configuration (Ne$\cdots$H–C–N) with a well depth of 62.9 cm^{-1}. The anti-linear configuration (H–C–N$\cdots$He) is higher in energy than the global minimum by 16.6 cm^{-1}. The center-of-mass distance $R_{\rm m}$ of Ne and HCN along the minimum energy path shows a large angular dependence; $R_{\rm m}$ is 4.242 Å and 4.012 Å in the linear and anti-linear forms, respectively, and has a minimum value of 3.475 Å in a T-shaped configuration. The present empirical potential energy surface gives the average intermolecular distance $< R >$ of 3.970 Å in the ground state. The calculated $< R >$ for the Ne-HCN is shorter than those for He-HCN and Ar-HCN by 0.34 and 0.40 Å in accordance with the recent spectroscopic results.[a] The empirical potential energy surfaces are compaired with the recent *ab initio* potential energy surface.[b]

[a] H. S. Gutowski, J. D. Keen, T. C. Germann, T. Emilsson, J. D. Augspurger, and C. E. Dykstra, J. Chem. Phys. 98, 6801(1993).

[b] G. Murdachaew, A. J. Misquitta, R. Bukowski, and K. Szalewicz, J. Chem. Phys. 114, 764(2001).