MILLIMETER WAVE SPECTROSCOPY OF THE INTERNAL ROTATION BANDS OF ^{20}Ne-HCN AND ^{22}Ne-HCN

KENSUKE HARADA and KEIICHI TANAKA, *Department of Chemistry, Faculty of Science, Kyushu University, Hakozaki, Higashiku, Fukuoka, 812-8581 JAPAN*; SHINKO NANBU, *Institute for Molecular Science, Okazaki, 444-8585, JAPAN*.

The millimeter wave absorpion spectroscopy have been applied to the observation of the internal rotation bands of ^{20}Ne-HCN and ^{22}Ne-HCN. The band origins of the Σ_1-Σ_0 and Π_1-Σ_0 bands of j=1-0 were observed at 133 and 107 GHz, where j denotes the quantum nomber for the HCN internal rotation. Most lines were split into hyperfine components due to the nuclear quadrupole interaction of the nitrogen nucleus. The observed frequencies were analyzed to improve an intermolecular potential energy surface (PES) by adding the parameters to the *ab initio* PES and fitting them to the experimental data. Especially, the long range attractive terms of the PES were determined by the simultaneous analysis of the internal rotation bands of the both isotopic species. The PES thus obtained has a global minimum in the linear configuration (Ne$\cdots$H–C–N) with a well depth of 62.8 cm^{-1}, and a saddle point located in the anti-linear configuration (H–C–N$\cdots$Ne) which is higher by 16.50 cm^{-1} than the global minimum. The ground rotation-internal rotation state (zero point energy level) is 6.5 cm^{-1} higher than the well depth at the saddle point. The distance between the Ne atom and the center of mass of HCN along the minimum energy path is 4.243, 3.474, and 3.985 Å in the linear, T-shaped, and anti-linear forms. The Σ_2-Σ_1, Σ_2-Π_1, Π_2-Σ_1, Π_2-Π_1, and Δ_2-Π_1 bands of j=2-1 of ^{20}Ne-HCN were also observed and assigned based on the prediction from the modified PES, which was accurate within 100 MHz.