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

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The Ne-HCN cluster is a weakly bound complex with the binding energy (D_0) of 39 cm^{-1}.[a] In the present work, we have observed the vdW bending bands of Ne-HCN. A pulsed jet millimeter-wave spectrometer was used for the experiment. The millimeter wave radiation passed twenty times through the jet expansion using a White type optical path to attain high sensitivity. The 14 and 22 vdW transitions were observed for the Σ_1-Σ_0 and Π_1-Σ_0 bands in the frequency region of 79-201 GHz. Most lines were split into the hyperfine components of nitrogen nucleus. From the eQq constants, the root mean square amplitudes $\langle\theta^2\rangle^{1/2}$ of the HCN part were estimated to be 47°, 56°, and 63° for the Σ_0, Σ_1, and Π_1 states. The center of mass distance of the intermolecular bond were derived from the rotational constants to be 3.89, 3.85, and 3.66 Å for those states.

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