MILLIMETER-WAVE SPECTROSCOPY OF THE HCN-H_2 CLUSTER

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Millimeter-wave absorption spectroscopy combined with a pulsed-jet expansion technique was applied to the measurement of the rotational and rovibrational transitions of the HCN-H_2 cluster in the frequency region of 75−150 GHz. So far, four rotational lines for the ground Σ_0 state of the HCN-(o-H_2) cluster split into hyperfine structure due to the nitrogen nucleus were observed. Rotational constant $B_0 = 12899.718(20)$ MHz and centrifugal distortion constant $D_0 = 12.2470(16)$ MHz were derived together with its higher constants. The hyperfine constants determined $eqQ = -2.830(33)$ MHz which is smaller than that of HCN molecule means a large amplitude motion of HCN of $< \theta >$ = 31.1 degree in the ground linear form. The bond length between HCN and H_2 parts is derived to be 3.90 Å. Some lines belonging to the $\Sigma_1 - \Sigma_0$ van der Waals bending band of HCN-(o-H_2) were also observed. The $\Sigma_1 - \Sigma_0$ van der Waals bending frequency 136.831 GHz of HCN-(o-H_2) is larger than that of He-HCN 98.70 GHz, but much smaller than that of Ar-HCN 164.89 GHz. The hyperfine constant in the Σ_1 state indicate the cluster has T-shape in the excited state of the vdW bending mode.
A search of the rotational lines of the ground Σ_0 state of HCN-(p-H2) and the Π_0 state of HCN-(o-H_2) are now in progress as well as the vdW mode rovibrational lines for both HCN-(o-H_2) and -(p-H_2) clusters.