ROTATIONAL SPECTRA OF THE H_2-HCN CLUSTER OBSERVED BY MILLIMETER-WAVE SPECTROSCOPY AND FOURIER-TRANSFORM MICROWAVE SPECTROSCOPY. EVIDENCE OF THE (p)H_2-HCN AND (o)H_2-NCH CONFIGRATIONS IN THE GROUND STATE.

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Millimeter-wave spectroscopy and Fourier-Transform microwave spectroscopy were applied to observe the $J = 1-0 \sim 6-5$ rotational lines of the H_2-HCN and H_2-DCN cluster containing the $ortho$ as well as $para$ hydrogen molecule. The Σ symmetry in the ground state was confirmed for the both species. The isotope effect on rotational lines confirms the totally different configurations in the ortho and para species in accordance with the recent infrared spectroscopy in He-droplet: H_2 is attached to the hydrogen end of HCN in the para species, while to the nitrogen end in the ortho species. From the observed rotational constants, the average distance between the center of mass of H_2 and that of HCN was derived to be 3.9613 (35) Å for the ortho species and 4.229 (11) Å for the para species. The hyperfine splitting due to the hydrogen nuclear spin ($I_{\mathrm{H_2}} = 1$) internal rotation interaction of the H_2 part was observed for the ortho species, indicating the almost free rotation of H_2 in the cluster, but not for the para species. The nuclear quadrupole interaction constants due to nitrogen nuclear spin ($I_{\mathrm{N}} = 1$) show that the HCN part executes a floppy motion with a large mean amplitude in the ortho as well as para species.