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 CONFIGURATIONS IN THE GROUND STATE.

MASAZUMI ISHIGURO, K. HARADA, T. TANAKA and K. TANAKA, Department of Chemistry, Faculty of Science, Kyushu University, Fukuoka, 812-8581 Japan; Y. SUMIYOSHI and Y. ENDO, Department of Pure and Applied Sciences, Graduate School of Arts and Sciences, The University of Tokyo, Komaba, Meguroku, Tokyo, 153-8902, Japan.

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 $\Sigma$ 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 ($I_{H_2} = 1$) 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 ($I_N = 1$) show that the HCN part executes a floppy motion with a large mean amplitude in the ortho as well as para species.