# ROTATIONAL SPECTRA OF THE $H_2$-HCN COMPLEX OBSERVED BY FOURIER-TRANSFORM MICROWAVE SPECTROSCOPY. THE INTERNAL ROTATION OF $H_2$ IN THE $H_2$-HCN COMPLEX.

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Fourier-Transform Microwave (FTMW) spectroscopy has been applied to the observation of the $J = 1 - 0$ rotational lines of the $H_2$-HCN and $H_2$-DCN complexes for the $ortho$- and $para$-$H_2$ species. The rotational constants derived for the HCN/DCN complexes support definitely that $H_2$ is attached to the N end of HCN for the $ortho$-$H_2$ species, while $H_2$ is attached to the H end of HCN for the $para$-$H_2$ species, consistent with the recent vibrational spectra in the He-droplet [a]. The nuclear quadrupole interaction constants of the nitrogen nucleus ($I_N = 1$) show that the HCN/DCN part executes a floppy motion with a large mean amplitude.
The splitting due to the magnetic hyperfine interaction of the $H_2$ part was observed for ortho-$H_2$-HCN ($j = 1$ for $H_2$ internal rotation) thanks to the high resolution of FTMW spectroscopy, but not for para-$H_2$-HCN ($j = 0$ for $H_2$ internal rotation). Because of $\Sigma$ symmetry of the ortho-$H_2$-HCN complex in the ground state, nuclear spin-nuclear spin interaction contributes to the hydrogen hyperfine interaction, but not the nuclear spin-rotation intraction. The magnetic interaction constant $d_H$ for ortho-$H_2$-HCN was determined to be 54.6(38) kHz. The value corresponds to 94.7% of that of free hydrogen molecule 57.671(24) kHz [b], indicating almost free rotation of the $H_2$ part in the complex. The spectrum of ortho-$H_2$-DCN shows also the splitting due to the magnatic hyperfine interaction of $H_2$, but the hyperfine partern is more complicated because of the nuclear quadrupole interaction of the D atom ($I_D = 1$). The magnetic interaction constant for ortho-$H_2$-DCN indicates that $H_2$ is rotating almost freely in the complex as well.

[a] D. T .Moore, M. Ishiguro, and R. E. Miller, *J. Chem. Phys.* 115, 5144 (2001)
[b] H. G. Kolsky and N. F. Ramsey, *Phys. Rev.* 87, 395 (1952)