# REASSIGNMENT OF MILLIMETERWAVE SPECTRUM OF THE HCN INTERNAL ROTATION BANDS OF $H_2$-HCN

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The $H_2$-HCN complex is a weakly bound molecular complex and we have reported the pure rotational transitions of $H_2$-HCN in the MMW region.[a] According to the results, ortho- and para-$H_2$ complexes have different structures in the ground state, $H_2$ is attached to the nitrogen and hydrogen end of HCN, respectively, for ortho- and para-$H_2$ complexes and the $\Sigma$ symmetry has been confirmed for both species.

We also reported the MMW spectroscopy of $j$=1-0 internal rotation band of $H_2$-HCN in 2006 [b], where $j$ is the quantum number for the HCN internal rotation. Although we assigned most of intense lines to the $\Sigma_1 - \Sigma_0$ and $\Pi_1 - \Sigma_0$ bands of (ortho)$H_2$-HCN, some intense lines are unidentified. To confirm their assignments, we performed the MMW-MMW double resonance spectroscopy in the present study and came to the conclusion that our previous assignments of $\Sigma_1 - \Sigma_0$ and $\Pi_1 - \Sigma_0$ bands should be changed, and then all of the intense lines are finally assigned to the $\Pi_1 - \Sigma_0$ ($R_0$, $R_1$,$R_2$, $Q_1$, $Q_2$, and $P_2$) and $\Sigma_1 - \Sigma_0$ ($R_0$, and $P_2$) bands.

The band origins of the $\Sigma_1 - \Sigma_0$ and $\Pi_1 - \Sigma_0$ bands of (ortho)$H_2$-HCN newly determined are 187 and 165 GHz, respectively. They are larger than those of Ne-HCN (133 and 107 GHz) but comparable with those of Ar-HCN (165 and 182 GHz, their order is reversed) indicating that the potential anisotropy of (ortho)$H_2$-HCN is larger than that of Ne-HCN but comparable with that of Ar-HCN. The mean square amplitudes of HCN for excited states ( $57^\circ$ and $51^\circ$ for $\Sigma_1$ and $\Pi_1$), given by the analysis of hyperfine structure of the nitrogen nucleus, are much larger than that ($33^\circ$) of the ground $\Sigma_0$ state.

A plenty of weak lines in the 100-300 GHz region are still unassigned, possibly due to the higher internal rotation bands of ortho-$H_2$ complex, such as the $\Delta_1 - \Pi_0$ band, as well as the fundamental bands ($\Sigma_1 - \Sigma_0$ and $\Pi_1 - \Sigma_0$) of para-$H_2$ complex. Analysis of these weak bands and survey in the region with pure para-$H_2$ sample are now in progress.

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[a] M. Ishiguro, T. Tanaka, K. Harada, C. J. Whitham and K. Tanaka, *J. Chem. Phys.* **115**, 5155 (2001).

[b] M. Hagi, K. Harada, and K. Tanaka, *The 61st International Symposium on Molecular Spectroscopy*, **TE01**, (2006).