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 Σ 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° and 51° for Σ_1 and Π_1), given by the analysis of hyperfine structure of the nitrogen nucleus, are much larger than that (33°) of the ground Σ_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).