MILLIMETERWAVE SPECTROSCOPY 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 including molecular hydrogen. The hydrogen molecule attaches to the nitrogen end of HCN for (ortho)H_2-NCH, while to the hydrogen end for (para)H_2-HCN in the ground state according to the recent study of the pure rotational transitions of H_2-HCN[a]. The Σ symmetry of the internal rotation ground state has been confirmed for both ortho and para H_2-HCN.

In the present study, we have observed the $\Sigma_1 - \Sigma_0$ band of the j=1-0 internal rotation band of (ortho)H_2-HCN, where j denotes the quantum number for the HCN internal rotation. Observed lines split into hyperfine structure due to the nuclear quadrupole interaction of the nitrogen nucleus. The assignments of the internal rotation transitions were confirmed by the combination differences of the transition frequencies for the *P* and *R* branch lines. The band origin of the $\Sigma_1 - \Sigma_0$ band of (ortho)H_2-HCN has been determined to be 150 GHz. This value is larger than that of Ne-HCN, 133 GHz, but smaller than that of Ar-HCN, 165 GHz.The rotational constant in the Σ_1 state is 14255 MHz, by 1355 MHz larger than that in the Σ_0 state, 12900 MHz.

A survey of other internal rotation bands, such as the $\Pi_1 - \Sigma_0$ band of (ortho)H_2-HCN and the $\Sigma_1 - \Sigma_0$ and $\Pi_1 - \Sigma_0$ bands of (para)H_2-HCN, is now in progress. Observations of these internal rotation bands are important to determine the intermolecular potential energy surface of H_2-HCN.

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