EXPERIMENTAL DETERMINATION OF INFRARED TRANSITION DIPOLE MOMENTS FOR HNC FROM HERMAN-WALLIS EFFECT

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The transition dipole moments for the fundamental bands of HNC were obtained from analyses of Herman-Wallis effect on the absorption intensities. All the fundamental bands were measured using a Fourier transform infrared spectrometer (Bruker IFS 120HR) at Nobeyama Radio Observatory. A glow discharge in a mixture of CH$_3$CN (\(\sim 50\) mTorr), H$_2$ (\(\sim 150\) mTorr), and Ar (\(\sim 100\) mTorr) was used for production of HNC. The spectra were recorded with resolution of 0.01 cm$^{-1}$ and the absorption path length was 24 m.

The experimentally determined first order Herman-Wallis coefficients for the \(\nu_1\) and \(\nu_3\) bands, combined with the relative value of the transition dipole moments for the \(\nu_2\) and \(\nu_3\) bands derived from the relative intensity measurements, yielded the following values for the transition dipole moments (in Debye), using the expressions for Herman-Wallis coefficients given by Watson\(^a\),

\[
R_1 = 0.194(13), \quad R_2 = -0.886(13), \quad R_3 = -0.169(11).
\]

These values are considerably larger than the corresponding values for HCN\(^b\) and are in reasonable agreement with \textit{ab initio} values\(^c\)^d.

\(^a\)J. K. G. Watson, J. Mol. Spectrosc. 125, 428(1987)