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_3CN($\sim$ 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 ν_1 and ν_3 bands, combined with the relative value of the transition dipole moments for the ν_1 and ν_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 $ab\ initio$ values[cd].

[a] J. K. G. Watson, J. Mol.Spectrosc. 125, 428(1987)
[b] A. G. Maki $et\ al$, J. Mol.Spectrosc. 174, 365(1995)
[c] P. Botschwina $et\ al$, Chem. Phys. 190, 345(1995)
[d] T. J. Lee and A. P. Rendell, Chem. Phys. Lett. 177, 491(1991)