

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 CH₃CN (~ 50 mTorr), H₂ (~ 150 mTorr), and Ar (~ 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}.

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