The Inversion Spectrum of Cyanamide

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Twelve Q branch lines and four R branch lines in the inversion spectrum of cyanamide are reported for the first time together with the μ_c component of the dipole moment of cyanamide and a double-minimum potential function that describes the inversion motion.

The microwave spectrum of cyanamide has been extensively studied[1—4] and together with its i.r. spectrum[5] has led to the conclusion that the equilibrium structure of cyanamide has a pyramidal amino group. The analysis of Coriolis-type perturbations in the microwave spectrum has led to a value of about 49 cm^{-1} for the inversion splitting.[4] With an A rotational constant of about[4,5] 10 cm^{-1}, c-type inversion lines between the $K_{-1} = 2$ (0^-) and $K_{-1} = 3$ (0^+) levels are predicted to fall in the microwave region. However, hitherto these direct inversion transitions have not been observed. In the process of a more extensive measurement and analysis of the microwave spectrum of cyanamide,[6] including various isotopic species, we were able to predict a ^cQ-branch starting above 50 GHz and we now report the detection and

Table 1. Observed direct inversion transitions of cyanamide.[a]

(a)	[c]Q-branch transitions 0^+–0^-	
	10_{38}–10_{28}	55 607.347
	10_{37}–10_{29}	55 683.173
	11_{39}–11_{29}	56 259.931
	11_{38}–11_{210}	56 369.495
	12_{310}–12_{210}	56 958.929
	12_{39}–12_{211}	57 112.386
	13_{311}–13_{211}	57 701.310
	13_{310}–13_{212}	57 910.620
	14_{312}–14_{212}	58 483.908
	14_{311}–14_{213}	58 763.136
	15_{313}–15_{213}	59 303.641
	15_{312}–15_{214}	59 668.931
(b)	[c]R-branch transitions 0^- –0^+	
	5_{24}–4_{32}	46 932.477
	5_{23}–4_{31}	46 937.625
	6_{25}–4_{33}	66 557.926
	6_{24}–5_{32}	66 568.575

[a] In kHz. The estimated uncertainty of frequencies is ±20 kHz.

identification of these transitions. We subsequently could also find a series of [c]R-branch lines with a separation of *ca.* 20 GHz. Table 1 lists the observed frequencies.

Inclusion of [a]Q-lines with $K_{-1} = 2$ and $K_{-1} = 3$, found in the progress of this work, allowed us to fit the rotation–inversion spectrum of cyanamide to a 2-vibrational level Hamiltonian similar to the one used by Johnson *et al.*[4] 15 Rotational constants, the inversion frequency, and a matrix element, representing vibrational angular momentum in the *b* direction, could be determined.

Table 2. Observed and calculated energy levels in cm^{-1}.

	Observed	Calculated
0^+	0	0
0^-	49.279 ± 0.013[a]	49.279
1^+	413.6 ± 2.0[b]	415.4
1^-	714.1 ± 0.4[b]	713.9

[a] This work. [b] Ref. 5.

The inversion frequency was found to be 49.279 ± 0.013 cm^{-1}. This value and two additional i.r. frequencies[5] were fitted to a simple double minimum potential $V = 45.09 \times (Q^4 - 6.461 \times Q^2)$ cm^{-1}, where Q is a dimensionless co-ordinate and the reduced mass was assumed to be fixed. The barrier to inversion is 470 cm^{-1}. Table 2 shows the good agreement between observed and calculated frequencies.

The application of electric fields leads to very strong mixing of vibrational–rotational wavefunctions and the appearance of forbidden Stark effects at higher fields. Investigation into the Stark effect of the J = 12 Q-branch inversion doublet led to a value of 1.04 ± 0.15 Debye for μ_c.

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