

## Rotational measurements on (4-6), (5-7) bands of CN ( $B^2\Sigma^+ - X^2\Sigma^+$ ) transition

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**Abstract.** Rotational analysis of (4-6), (5-7) bands of CN ( $B^2\Sigma^+ - X^2\Sigma^+$ ) transition extending to high  $J$  and emitted from the chemiluminescent reaction involving pink afterglow of nitrogen is presented.

**Keywords.** Nitrogen pink afterglow; microwave discharge; chemiluminescent reaction; Rotational analysis.

### 1. Introduction

CN bands have been widely studied and rotational analysis of many bands belonging to  $A^2\Pi - X^2\Sigma^+$  and  $B^2\Sigma^+ - X^2\Sigma^+$  transitions have been reported (Rosen 1970). (4-6) and (5-7) bands are difficult to analyse since they are heavily overlapped by other bands. Schoonveld and Sundaram (1979) has recently reported an analysis of these bands. In one of our experiments with pink afterglow of nitrogen we obtained these bands without much overlapping because of the anomalous population distribution in vibrational states. An additional advantage is that high rotational excitation was observed enabling detection of high  $J$  lines. The data presented in this paper extend the results of Schoonveld (1979) to high  $J$  values and are expected to be of relevance in astrophysical studies since CN is an important molecule in that respect.

### 2. Experimental

The experimental set-up consisted a discharge tube and a chamber for mixing the discharge products of nitrogen with organic vapours. The discharge tube and the reaction chamber were made of quartz tubing of bore 10 mm and length 20 cm and 30 cm respectively and were connected to the rest of the glass assembly through graded sales. Ultrapure nitrogen (Indian Oxygen Ltd.) was passed through a liquid nitrogen trap before admitting it to the discharge region. A microwave (2450 MHz) discharge in the flowing nitrogen produced a pink afterglow about 10 to 15 cm in length in the mixing chamber next to the discharge tube. The pre-cooling of the nitrogen was found to be essential for producing the pink afterglow. To this glow were added  $C_2H_2$  and  $BrCN$  in small quantities. These chemicals were of reagent purity. The resulting luminescent reaction was photographed using 3.4 meter

**Table 1.** Wave-numbers of rotational lines of the (4-6) band of CN ( $B^2\Sigma^+ - X^2\Sigma^+$ ).

<i>J</i>	Observed	Calculated	Schoonveld and Sundaram (1979)
<i>R</i> -branch			
0	22186·41	22186·47	22186·50
1	190·49	190·38	—
2	194·53	194·44	1944·4
3	199·07	198·68	198·67
4	203·26	203·08	203·10
5	207·31	207·64	207·72
6	212·43	212·37	212·40
7	217·52	217·26	217·36
8	22222·60	22222·32	22222·42
9	226·46	227·54	227·66
10	232·05	232·92	—
11	238·87	238·47	238·69
12	244·07	244·18	244·39
13	250·50	250·05	—
14	255·70	256·09	256·40
15	262·69	262·28	—
16	267·60	268·64	268·92
17	275·88	275·16	—
18	282·69	281·85	—
19	288·75	288·67	—
20	295·85	295·82	—
21	302·27	302·82	—
22	310·44	310·14	—
23	317·80	317·61	—
24	324·93	325·24	—
25	333·96	333·03	—
26	341·84	340·97	—
27	349·08	349·06	—
28	358·08	357·31	—
29	366·69	365·71	—
30	374·45	374·27	—
31	—	382·98	—
32	391·19	391·84	—
33	401·42	400·85	—
34	410·41	410·02	—
35	—	419·33	—
36	429·01	428·79	—
37	438·18	438·39	—
<i>P</i> -branch			
1	22179·52	22179·17	22179·18
2	175·82	175·76	175·77
3	172·68	172·53	172·56
4	169·58	169·46	169·48
5	166·63	166·55	166·59
6	163·93	163·81	163·90
7	161·42	161·24	161·33
8	159·01	158·84	158·95
9	156·80	156·60	156·70
10	154·74	154·53	—
11	152·88	152·63	152·72
12	151·16	150·89	151·12
13	149·69	149·32	149·60
14	148·22	147·91	148·23
15	146·06	146·67	—
16	145·23	145·60	*146·01
17	—	144·69	*145·17
18	143·46	143·95	*144·48

\*—To be decreased by one unit.

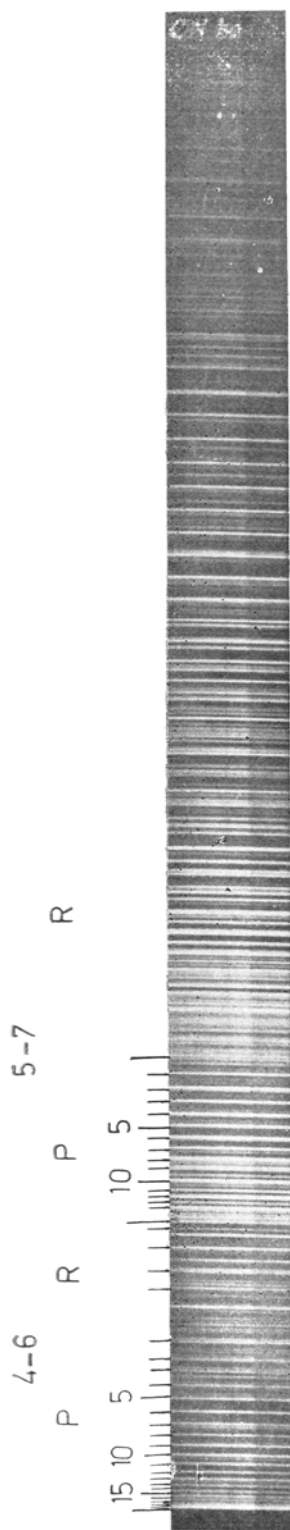


Figure 1. Rotational spectra of CN ( $B^2\Sigma^+ \rightarrow X^2\Sigma^+$ ) bands.



Table 2. Wave-numbers of the rotationals of (5-7) band of CN ( $B^2\Sigma^+ - X^2\Sigma^+$ ).

<i>J</i>	Observed	Calculated	Schoonveld and Sundaram (1979)
<i>R</i> -branch			
0	22250.50	22250.48	—
1	254.12	254.31	254.26
2	258.57	258.34	258.31
3	262.69	262.52	262.49
4	267.61	266.87	266.87
5	271.47	271.37	271.34
6	275.89	276.03	275.91
7	280.65	280.86	280.70
8	285.57	285.85	285.76
9	290.67	290.99	290.76
10	295.86	296.29	296.00
11	301.92	301.76	301.38
12	307.35	307.38	306.98
13	313.72	313.16	312.61
14	319.35	319.09	318.42
15	324.94	325.19	324.30
16	331.07	331.44	330.42
17	337.26	337.84	—
18	344.30	344.41	—
19	—	351.12	—
20	358.09	357.99	—
21	—	365.02	—
22	372.54	372.20	—
23	379.81	379.53	—
24	—	387.00	—
25	394.69	394.64	—
26	402.73	402.42	—
27	410.41	410.38	—
28	418.10	418.42	—
29	427.00	426.65	—
30	435.45	435.03	—
31	443.56	443.34	—
<i>P</i> -branch			
1	22243.47	22243.25	—
2	239.86	239.85	239.80
3	236.79	236.63	236.65
4	233.33	233.58	233.58
5	230.86	230.70	230.70
6	227.99	227.97	227.92
7	225.47	225.42	225.30
8	222.61	223.01	222.88
9	220.73	220.78	220.52
10	218.56	218.70	218.47
11	216.73	216.79	216.52
12	214.81	215.05	214.66
13	213.28	213.46	212.99
14	212.44	212.04	211.44
15	210.61	210.77	**210.15
16	210.11	209.68	**208.94
17	208.98	208.74	**207.89
18	207.85	207.96	—
19	207.31	207.34	—

\*\*To be increased by one unit.

Jarrel-Ash, Ebert-mount plane grating spectrograph with a reciprocal linear dispersion of about 1.25 Å/mm in the second order. Kodak 103 aF plates were used.

### 3. Results

The reaction flame of C<sub>2</sub>H<sub>2</sub> and BrCN obtained with pink afterglow was brighter compared to that obtained with Lewis Rayleigh glow. The main emissions from these reactions were the CN red (A<sup>2</sup>π—X<sup>2</sup>Σ<sup>+</sup>) and violet (B<sup>2</sup>Σ<sup>+</sup>—X<sup>2</sup>Σ<sup>+</sup>) bands. The CN violet bands were most intense and showed anomalously high intensities at high v-values and high rotational excitation with rotational temperature 2500 K (Gorbali and Savadatti 1980) (see figure 1). The J-values have been assigned on comparison with calculated wave-numbers using equation (1) (Herzberg 1950).

$$\nu = \nu_0 + (B_{v'} + B_{v''})m + (B_{v'} - B_{v''} - D_{v'} + D_{v''})m^2 - 2(D_{v'} + D_{v''})m^3 - (D_{v'} - D_{v''})m^4 \quad (1)$$

$$m = -J \text{ for } P \text{ — branch}$$

$$= (J + 1) \text{ for } R \text{ — branch}$$

The molecular constants  $\nu_0$  and  $B_{v'}$ ,  $B_{v''}$  are from Schoonveld and Sundaram (1979) as they are the latest and  $D_{v'}$  and  $D_{v''}$  are from Engleman (1974). All the rotational lines measured and calculated are listed in tables 1 and 2 along with those of Schoonveld and Sundaram for comparison. From the tables it appears that the assignment of J-values by Schoonveld and Sundaram for some rotational lines in P-branch needs to be modified by one unit.

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### References

- Engleman R Jr 1974 *J. Mol. Spectros.* **49** 106  
 Gorbali M R and Savadatti M I 1980 *J. Quant. Spectrosc. Radiat. Transfer.* **24** 471  
 Herzberg G 1950 *Molecular spectra and molecular structure* Vol. I. Spectra of diatomic molecules (D Von Nostrand)  
 Rosen B 1970 *Spectroscopic data relative to diatomic molecules* (Oxford: Pergman Press)  
 Schoonveld L and Sundaram S 1979 *Astrophys. J. Suppl.* **41** 669