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Ultraviolet Emission Spectrum of CaBr Molecule

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Using a high frequency source, the emission band spectrum of CaBr molecule in the ultraviolet region has been photographed at a dispersion of 3·5 and 1·8 Å/mm with a plane grating spectrograph. Twenty-eight additional bandheads have been measured. Vibrational constants have been evaluated and the assignments of quantum numbers are confirmed by isotopic calculations. The vibrational constants (in cm^{-1}) determined are: $\nu_e = 30190{\cdot}64$, $\omega_e'' = 285{\cdot}15$, $\omega_e''x_e'' = 0{\cdot}865$, $\omega_e' = 327{\cdot}64$ and $\omega_e'x_e' = 1{\cdot}245$.

THE band spectrum of CaBr molecule has been studied by several workers[1-5]. Recently a new system of bands has been reported by Reddy and Rao[5] in the region λ 3025-2900 Å. They have also reported some additional bands of the previously reported $D \rightarrow X$ system in the region λ 3300-3100 Å. Because of the isotopic Ca^{81}Br and Ca^{79}Br heads and low dispersion used by them the constants derived from their analysis give wide discrepancies in the values of $\nu_0 - \nu_c$ for a number of bandheads. The aim of the present study has been to carry out a complete vibrational analysis of the $D \rightarrow X$ system, using better dispersion and support it by measurement of isotopic effect which is measurable for most of the bands. The results obtained are presented in this note.

The spectrum of CaBr molecule was excited in a high frequency discharge and was photographed in the second and third orders of a plane grating spectrograph at a dispersion of 3·5 and 1·8 Å/mm respectively.

About 63 bandheads have been measured, out of which 35 were reported earlier. For most of the bandheads isotopic separations have been observed and are compared with the theoretically calculated values. The wavenumbers of the bandheads and their assignments are given in Table 1. The values reported by the earlier workers have also been given (column 2) for the sake of comparison. In columns 4 and 5 are given the values of isotopic shifts observed experimentally and calculated theoretically by using the standard relations. The close agreement between these values confirms the correctness of the analysis. The following bandhead equation was derived:

$$\nu_H = 30190{\cdot}64 + [327{\cdot}64(v'+\tfrac{1}{2}) - 1{\cdot}245(v'+\tfrac{1}{2})^2] - [285{\cdot}15(v''+\tfrac{1}{2}) - 0{\cdot}865(v''+\tfrac{1}{2})^2]$$

A few of these bands have been recorded at higher dispersions and simple rotational structure having two branches has been observed. This, therefore, confirms that the system arises due to an electronic transition of the type $^2\Sigma \rightarrow {}^2\Sigma$. A detailed fine structure analysis of these bands will be reported later.

Table 1 — Wavenumbers of the Bandheads and Their Assignments of the $D \rightarrow X$ System of CaBr

Wavenumber, cm^{-1}		v', v''	Isotope shift	
Present work	Observed by earlier workers		Obs.	Calc.
30130·2	—	1, 5 (79)		
30134·1	—	1, 5 (81)	3·9	4·2
30178·4	—	2, 6 (79)		
30182·5	—	2, 6 (81)	4·1	4·1
30224·4	—	3, 7 (79)		
30228·3	—	3, 7 (81)	3·9	3·8
30362·5	30365·1	0, 3 (79)		
30365·9	—	0, 3 (81)	3·4	3·4
30408·7	30410·4	1, 4 (79)		
30411·9	—	1, 4 (81)	3·2	3·2
30454·2	30456·7	2, 5 (79)		
30457·8	30462·3	2, 5 (81)	3·6	3·0
30499·5	—	3, 6 (79)		
30502·3	—	3, 6 (81)	2·8	2·8
30543·3	—	4, 7 (79)		
30545·1	—	4, 7 (81)	1·8	2·5
30644·2	30645·3	0, 2 (79)		
30646·4	—	0, 2 (81)	2·2	2·2
30688·6	30690·6	1, 3 (79)		
30691·0	—	1, 3 (81)	2·4	2·0
30732·7	—	2, 4 (79)		
30734·7	30742·6	2, 4 (81)	2·0	1·8
30755·0	—	3, 5 (79)		
30776·9	—	3, 5 (81)	1·9	1·7
30927·0	30927·8	0, 1 (79)		
30927·9	30928·8	0, 1 (81)	0·9	1·1
30970·0	30970·0	1, 2 (79)		
30970·9	30970·9	1, 2 (81)	0·9	0·9
31012·7	—	2, 3 (79)		
31013·5	—	2, 3 (81)	0·8	0·7
31211·8	31211·7	0, 0		
31293·9	31293·3	2, 2		
31333·5	31333·1	3, 3		
31372·0	31371·4	4, 4		
31411·1	—	5, 5		
31535·6	31534·6	1, 0 (81)		
31537·4	31535·6	1, 0 (79)	1·8	1·4
31574·4	31573·5	2, 1 (81)		
31575·9	31575·5	2, 1 (79)	1·5	1·6
31613·4	—	3, 2 (81)		
31615·0	—	3, 2 (79)	1·6	1·7
31650·0	—	4, 3 (81)		
31652·7	—	4, 3 (79)	2·7	1·9
31857·4	31856·3	2, 0 (81)		
31860·2	—	2, 0 (79)	2·8	2·7
31894·1	31892·8	3, 1 (81)		
31897·1	31895·8	3, 1 (79)	3·0	3·0
31930·1	31929·4	4, 2 (81)		
31933·4	31932·5	4, 2 (79)	3·3	3·0
31964·2	31965·3	5, 3 (81)		
31969·4	—	5, 3 (79)	5·2	5·4
32000·1	32000·1	6, 4 (81)		
32003·2	—	6, 4 (79)	3·1	3·2
32178·0	32175·9	3, 0 (81)		
32182·3	—	3, 0 (79)	4·3	4·1
32210·2	32210·2	4, 1 (81)		
32214·4	32214·4	4, 1 (79)	4·2	4·2
32243·7	32244·5	5, 2 (81)		
32247·3	32248·7	5, 2 (79)	3·6	4·2
32277·6	32277·8	6, 3 (81)		
32282·0	32282·0	6, 3 (79)	4·4	4·4
32314·5	32314·4	7, 4 (79)		
32342·3	32341·5	8, 5 (81)		

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A band system of the SrI molecule in the region λ3350–λ3560 Å

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Abstract. The spectrum of the SrI molecule has been excited in a high frequency discharge source and photographed in the fourth order of a plane grating spectrograph at a reciprocal dispersion of 1 8 Å mm^{-1} The existence of a new band system in the region λ3350–λ3560 Å has been established and the analysis has been carried out The nature of the electronic transitions involved have been discussed

1. Introduction

The spectrum of the SrI molecule was first reported by Olmsted (1906) in flames and later by Walters and Barratt (1928) in absorption. It consists of three groups of bands in the regions λ6150–λ7100, λ4200–λ4500 and λ3350–λ3450 Å. Mesnage (1939) investigated the spectrum of this molecule in emission in the range λ4250–λ4485 Å and assigned the bands to two separate systems A and B. Later Reddy *et al* (1971) reinvestigated the above group of bands at a higher dispersion (1·25 Å mm^{-1}) and assigned these bands to a transition of the type C $^2\Pi$–X $^2\Sigma$ and established the correlations with the corresponding systems observed in the spectra of Sr F, Sr Cl and Sr Br. They also photographed the bands of this molecule in the region λ6150–λ7100 Å and assigned them two different systems namely A $^2\Pi$–X $^2\Sigma$ and B $^2\Sigma$–X $^2\Sigma$. The group of bands of the SrI molecule in the region λ3350–λ3450 Å as reported by Walters and Barratt is known to consist of three bands at 3378 Å, 3406 Å and 3439 Å. No analysis has been offered so far for these bands and it was thought desirable to investigate the spectrum in this region. The results obtained are reported in this communication.

2. Experiment

The spectrum of the SrI molecule has been excited in a high frequency discharge source of conventional type. A capillary discharge was found most suitable and the spectrum was recorded in the fourth order of a plane grating spectrograph at a reciprocal dispersion of 1·8 Å mm^{-1} on Ilford N-40 plates with an exposure of 10 to 20 minutes. The plates were measured with an Abbey Comparator against iron-arc standard lines.

3. Results and analysis

The spectrogram of the group of bands in the region λ3300–λ3500 Å (as seen on the negative) has been reproduced in figure 1 (plate). It reveals seven sharp and single

Table 1. Band head data of the D $^2\Sigma$–X $^2\Sigma$ system of SrI molecule

Intensity	Wavenumber in vacuum ν (cm^{-1})	v', v''	$\Delta\nu = \nu_{obs} - \nu_{cal}$ (cm^{-1})
2	29 813·5	7, 3	−0·3
2	29 790·1	6, 2	−2·3
3	29 771·9	5, 1	1·2
4	29 747·5	4, 0	−1·2
2	29 620·1	6, 3	−0·3
2	29 599·4	5, 2	1·4
3	29 574·0	4, 1	−1·3
6	29 552·9	3, 0	0·6
1	29 449·1	6, 4	0·0
2	29 427·2	5, 3	1·2
2	29 403·1	4, 2	0·5
8	29 378·2	3, 1	−0·7
8	29 354·3	2, 0	−0·6
3	29 254·2	5, 4	−0·5
3	29 230·7	4, 3	0·1
3	29 206·4	3, 2	0·2
7	29 180·7	2, 1	−0·8
9	29 156·3	1, 0	−0·2
2	29 060·5	4, 4	1·2
5	29 034·5	3, 3	0·3
7	29 009·2	2, 2	0·4
2	28 983·7	1, 1	0·6
10	28 957·1	0, 0	0·0
1	28 915·6	5, 6	1·4
2	28 889·3	4, 5	0·6
2	28 862·9	3, 4	−1·5
2	28 835·9	2, 3	−0·9
3	28 810·3	1, 2	−0·1
9	28 783·5	0, 1	−0·2
1	28 744·7	5, 7	−0·3
2	28 720·5	4, 6	1·7
3	28 691·1	3, 5	−1·2
3	28 665·5	2, 4	0·0
8	28 637·9	1, 3	−0·5
7	28 610·3	0, 2	−0·7
1	28 574·7	5, 8	−1·8
1	28 550·6	4, 7	1·0
2	28 522·4	3, 6	0·0
4	28 494·1	2, 5	−0·8
2	28 466·5	1, 4	−0·6
2	28 437·5	0, 3	−1·5
1	28 381·1	4, 8	0·0
4	28 352·5	3, 7	−0·7
2	28 323·9	2, 6	−1·1
1	28 296·4	1, 5	−0·1
1	28 268·8	0, 4	1·1
1	28 154·4	2, 7	−1·4
1	28 127·4	1, 6	0·8
1	28 097·0	0, 5	−0·1

headed bands. Their wavenumbers in vacuum, visually estimated intensities, vibrational assignments and the difference between observed and calculated wavenumbers of the bands are given in table 1.

The most intense band at 28957·1 cm^{-1} has been taken as $\Delta v = 0$ sequence and the vibrational analysis has been carried out in the usual way and the following equation representing the band heads was derived

$$\nu_{\text{head}} = 28943{\cdot}99 + \{200{\cdot}4(v'+\tfrac{1}{2}) - 0{\cdot}50(v'+\tfrac{1}{2})^2\} - \{174{\cdot}1(v''+\tfrac{1}{2}) - 0{\cdot}35(v''+\tfrac{1}{2})^2\}.$$

The value of lower state frequency 174·1 ± 0·05 cm^{-1} observed from the system agrees very well with the ground state frequency 173·9 cm^{-1} of the other systems and it may therefore be attributed to the X $^2\Sigma$ state of this molecule. At the dispersion used in the present work it is not possible to resolve the rotational structure of the bands; however the heads are single and sharp. This leads to a conclusion that the upper state involved in this system may also be of the type $^2\Sigma$.

A comparison of the region of occurrence of this system with D $^2\Sigma$–X $^2\Sigma$ systems of Sr F, Sr Cl and Sr Br molecules indicates that the system occurs in the expected region and may therefore be attributed to electronic transition of the type D $^2\Sigma$–X $^2\Sigma$.

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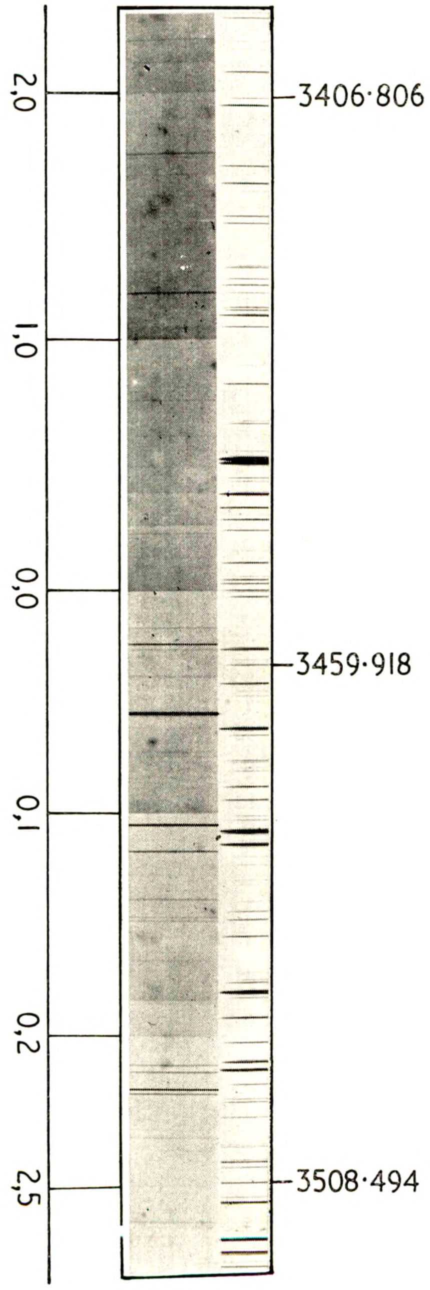

Figure 1. Grating spectrogram of Sr I bands in the region λ3350–λ3560 Å (dispersion 1·8 Å mm^{-1}).