PART II

CHAPTER IV

VIBRATIONAL ANALYSES OF CALCIUM IODIDE AND ZINC IODIDE MOLECULES

This chapter deals with the experimental observations and the study of vibrational structures of the band systems of CaI and ZnI molecules in emission, carried out during present investigation.

A preliminary survey of the spectra of CaI and ZnI molecules in the visible as well as in the ultra-violet regions was made on an E_2-glass spectrograph and on a medium quartz spectrograph respectively. The spectra of these molecules were excited in a conventional type of a quartz discharge tube with external electrodes by means of a high frequency (10-15 MH_z) oscillator. Continuous evacuation of the discharge tube by a high vacuum pump and strong external heating by a burner were found necessary to maintain characteristic colour of discharge which wes dark pink in case of CaI molecule and golden yellow in case of ZnI molecule. Under these conditions of excitation, the band systems for these molecules developed strong in intensity without any impurity bands. As the molecules under investigation are highly hygroscopic, in first few attempts impurity bands of CaH and ZnH were developed. The occurrence of these impurity bands was completely eliminated by using dehydrated substances. The substances were dehydrated by heating them in atmosphere. Throughout the course of present investigation dehydrated substances have been used.

Having established the conditions of excitation the spectra were photographed on a 2 meter plane grating spectrograph. Ilford N-40 and Astra-3 plates were employed to record the spectra in the ultraviolet and visible (red) regions respectively. Measurements of the bands were made on an Abbe Comparator against iron arc lines or internal atomic lines asstandards. In what follows will now be given the details regarding the work carried out on the grating spectra of CaI and ZnI molecules.

4.1 CaI BANDS

Bands in the region λλ 6600-6175 A°

A group of CaI bands in the region λλ 6600-6175A° has been recorded. The spectrum was photographed in the first and second order of a 2 meter plane grating spectrograph at reciprocal dispersions of 7.5 A°/mm and 3.38 A°/mm respectively. A spectrum with reasonable intensity and clarity could be recorded in second order on Astra-3 plates in about an hour. The bands in the region $\lambda\lambda$ 6600-6175 A° have been analysed into two different systems which may be attributed to electronic transitions $A\,^2\Pi$ —— $X\,^2\Sigma^+$ and $B\,^2\Sigma^+$ —— $X\,^2\Sigma^+$ showing the $A\,^2\Pi$ separation of about 59 cm^{-1} and the spin splitting in the $B\,^2\Sigma^+$ state of about 3.4 cm^{-1} respectively. The spectra are reproduced in plates (1 and 2). Plate 1 reveals two kinds of groups of violet degraded bands. One of them having two sub heads (P_1 and P_2) with equal intensity and a separation between them of about 3.4 cm^{-1} while the other having intense Q heads and corresponding weak P heads. In tables 4, 5 and 6 corresponding to A - X and B - X systems, respectively, visually estimated intensities wave numbers in vacuum, vibrational assignments and differences between observed and calculated wave numbers of the band heads are given. The bands of the A - X and B - X systems have been arranged in the Deslandress Tables (7, 8, 9 and 10).

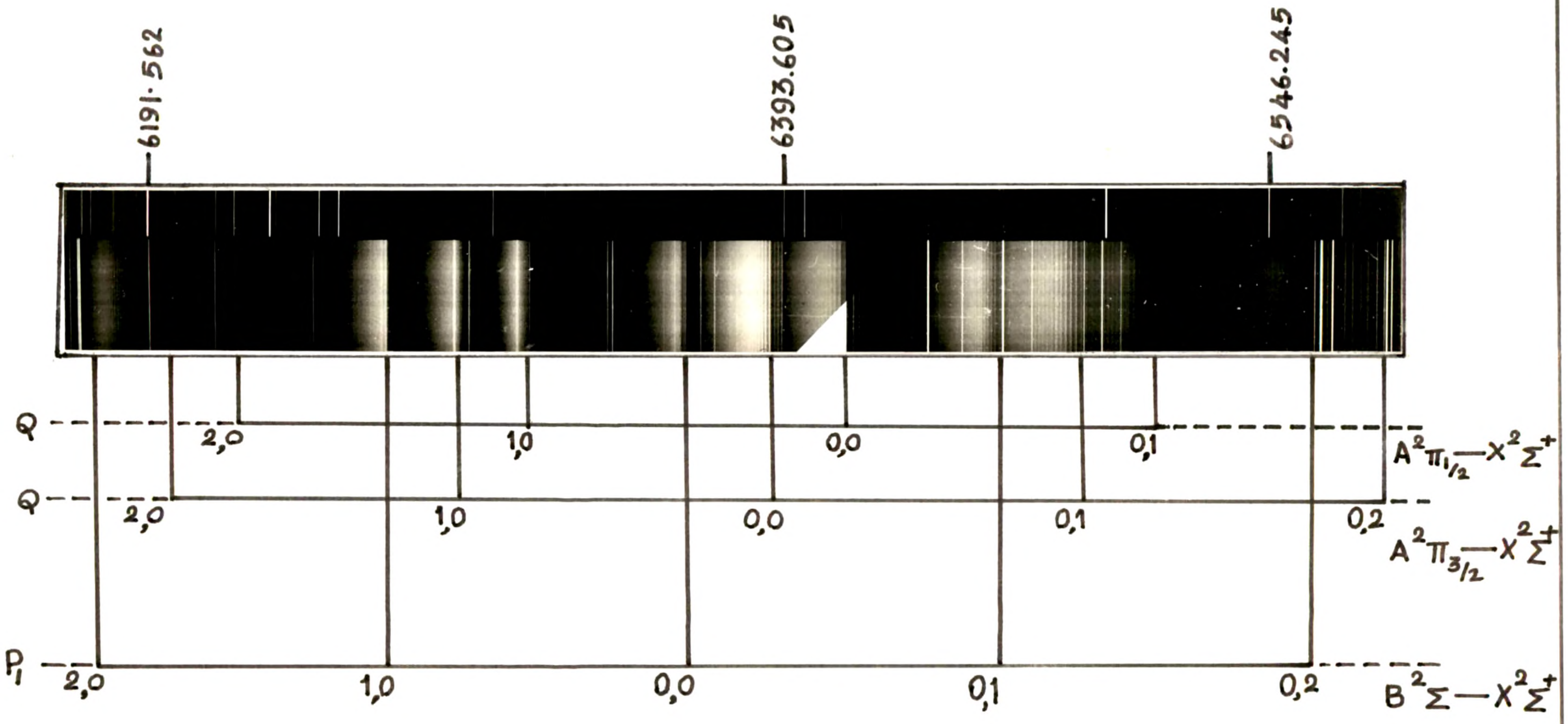

PLATE 1.

GRATING SPECTROGRAM OF CaI MOLECULE (A–X & B–X SYSTEMS) IN THE

REGION λλ 6600 — 6175 Å (7.25 Å/mm.)

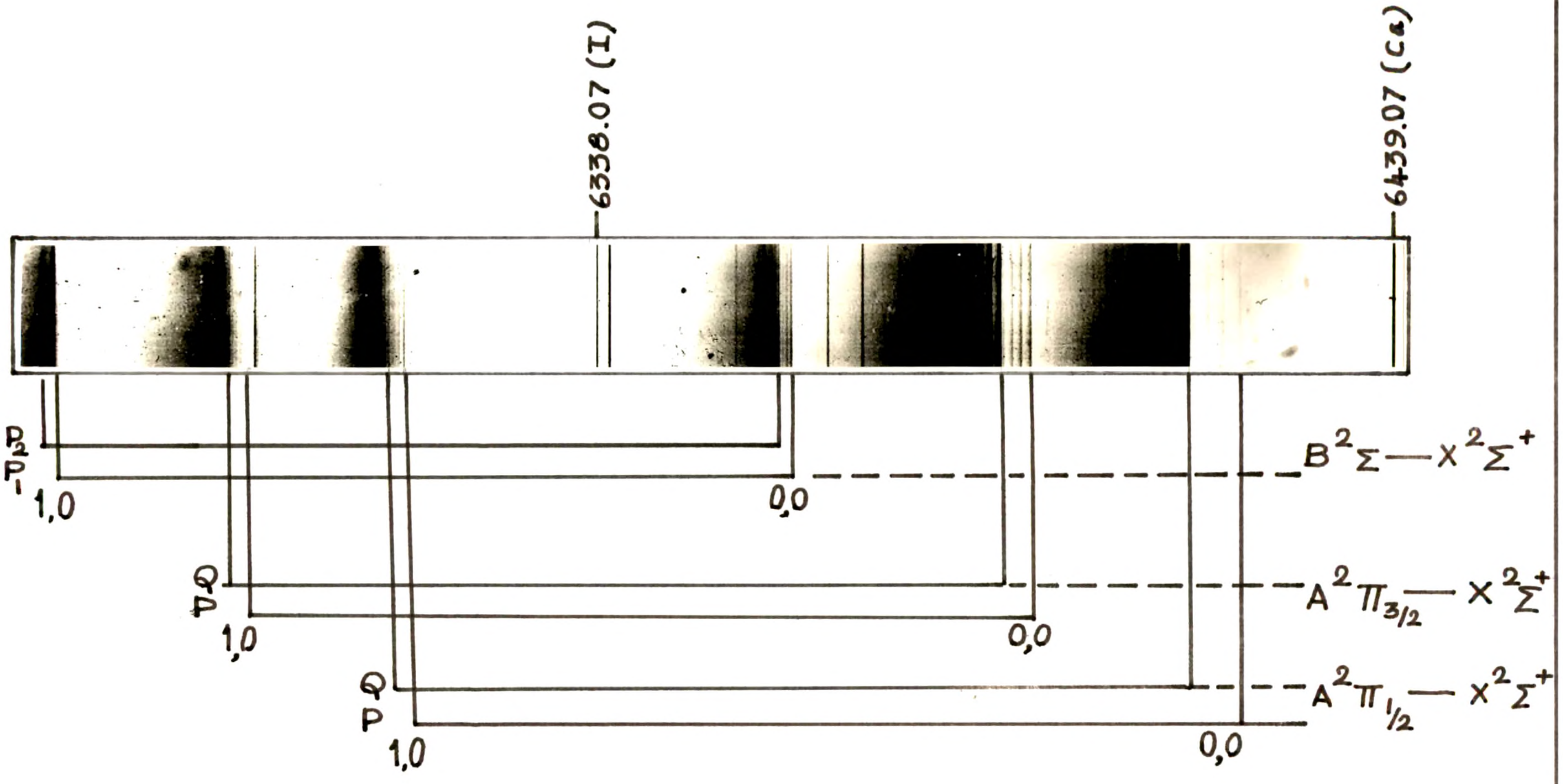

PLATE 2.

A PART OF GRATING SPECTROGRAM OF CaI MOLECULE AT 3.38 Å/mm SHOWING SUB-HEADS R_1 AND R_2 OF THE BANDS OF $B^2\Sigma — X^2\Sigma^+$.

TABLE 4

Band head data of the A $^2\Pi_{3/2}$ —— X $^2\Sigma^+$ system of CaI molecule.

Visual Intensity	Wave Length A°	Wave number in Vacuum (cm^{-1}) ν	Assignment v' - v"	Difference $\nu_{obs}-\nu_{cal}$ cm^{-1}
3	6588.6	15173.5	0, 2 (Q)	-1.6
2	6586.0	15179.5	1, 3 (Q)	-1.6
4	6577.8	15198.4	4, 6 (Q)	-1.7
3	6571.7	15212.5	6, 8 (Q)	+0.4
5	6487.5	15410.0	0, 1 (Q)	-0.3
4	6485.2	15415.3	1, 2 (Q)	+0.1
5	6483.7	15419.1	2, 3 (Q)	-0.7
6	6481.0	15425.4	3, 4 (Q)	+0.9
6	6479.3	15429.4	4, 5 (Q)	+0.3
4	6477.4	15434.1	5, 6 (Q)	+0.6
4	6476.3	15436.5	6, 7 (Q)	-0.9
9	6389.1	15647.2	0, 0 (Q)	0.0
5	6393.1	15637.5	0, 0 (P)	
8	6387.9	15650.2	1, 1 (Q)	-0.2
4	6391.6	15641.2	1, 1 (P)	

Table 4 (Cont)

Visual Intensity	Wave Length A°	Wave number in Vacuum (cm^{-1}) ν	Assignment $v'-v''$	Difference $\nu_{obs}-\nu_{cal}$ cm^{-1}
7	6386.7	15653.1	2, 2 (Q)	-0.4
4	6390.7	15643.5	2, 2 (P)	
6	6385.8	15655.3	3, 3 (Q)	-1.2
6	6384.9	15657.7	4, 4 (Q)	-1.8
8	6292.8	15886.7	1, 0 (Q)	-0.5
6	6291.7	15889.6	2, 1 (Q)	+0.9
4	6290.2	15893.4	4, 3 (Q)	+1.8
3	6289.1	15896.0	6, 5 (Q)	+1.9
4	6200.3	16123.8	2, 0 (Q)	+1.8
2	6199.6	16125.6	3, 1 (Q)	+0.1
2	6199.1	16127.0	4, 2 (Q)	+1.7

TABLE 5

Band head data of the A $^2\Pi_{\frac{1}{2}}$ —— X $^2\Sigma^+$ system of CaI molecule.

Visual Intensity	Wave Length A°	Wave number in Vacuum (cm^{-1}) ν	Assignment v' - v"	Difference $\nu_{obs}-\nu_{cal}$ cm^{-1}
3	6607.3	15130.6	2, 4 (Q)	-0.7
2	6603.3	15139.7	3, 5 (Q)	+0.5
3	6600.0	15147.3	4, 6 (Q)	0.0
2	6596.5	15155.4	5, 7 (Q)	-0.1
2	6592.6	15164.4	6, 8 (Q)	+0.4
2	6512.4	15251.1	0, 1 (Q)	-0.5
2	6510.0	15356.6	1, 2 (Q)	-1
2	6508.0	15361.5	2, 3 (Q)	-1.5
3	6505.8	15366.5	3, 4 (Q)	-1.7
10	6413.2	15588.5	0, 0 (Q)	+0.1
6	6416.7	15580.1	0, 0 (P)	
9	6411.4	15592.9	1, 1 (Q)	-0.1
7	6414.9	15584.4	1, 1 (P)	
9	6410.0	15596.4	2, 2 (Q)	-1.4
6	6413.7	15587.2	2, 2 (P)	

Table 5 (Cont)

Visual Intensity	Wave Length A°	Wave number in Vacuum (cm^{-1}) ν	Assignment $v' - v''$	Difference $\nu_{obs} - \nu_{cal}$ cm^{-1}
6	6315.6	15829.4	1, 0 (Q)	-0.4
5	6314.2	15832.9	2, 1 (Q)	-0.2
7	6313.0	15835.9	3, 2 (Q)	-0.8
4	6221.7	16068.3	2, 0 (Q)	-1.7
3	6220.1	16072.4	3, 1 (Q)	+0.3

Table 6 (Cont)

Visual Intensity	Wave Length A°	Wave number in Vacuum (cm^{-1}) ν	Assignment $v' - v''$	Difference $\nu_{obs}-\nu_{cal}$ cm^{-1}
7	6361.3	15716.8	0, 0 (P_2)	0.0
6	6362.2	15713.4	1, 1 (P_1)	0.0
5	6360.8	15717.0	1, 1 (P_2)	+0.3
7	6361.7	15714.6	2, 2 (P_1)	+0.4
6	6360.3	15718.2	2, 2 (P_2)	+0.5
6	6267.6	15950.7	1, 0 (P_1)	-0.3
6	6266.4	15953.6	1, 0 (P_2)	-0.8
6	6266.7	15952.9	2, 1 (P_1)	+1.1
6	6265.5	15955.9	2, 1 (P_2)	-1.6
4	6179.4	16178.3	8, 6 (P_1)	+1.3
5	6178.5	16180.7	7, 6 (P_1)	+0.3
2	6177.7	16182.6	6, 4 (P_1)	+0.8
3	6177.1	16184.3	5, 3 (P_1)	+0.6
3	6176.5	16185.9	4, 2 (P_1)	+0.5
3	6175.7	16188.0	3, 1 (P_1)	+0.9

TABLE 7

DESLANDRES TABLE FOR Q HEADS OF A ${}^2\Pi_{3/2} \longrightarrow X\ {}^2\Sigma^+$ SYSTEM OF CaI MOLECULE

v' \ v"	0		1		2		3		4		5		6		7
0	15647.2	237.2	15410.0	236.5	15173.5										
	239.5		240.2		241.8										
1	15886.7	236.5	15650.2	234.9	15415.3	235.8	15179.5								
	237.1		239.4		237.8		239.6								
2	16123.8	234.2	15889.6	236.5	15653.1	234.0	15419.1								
			236.0				236.2								
3			16125.6				15655.3	229.9	15425.4						
							238.1		232.3						
4					16127.0	233.6	15893.4	235.7	15657.7	228.3	15429.4	231.0	15198.4		
													235.7		
5													15434.1		
6											15896.0				15436.5

TABLE 8

DESLANDRES TABLE FOR Q HEADS OF A $^2\Pi_{1/2} \longrightarrow$ X $^2\Sigma^+$ SYSTEM OF CaI MOLECULE

v' \ v"	0	1	2	3	4	5	6	7
0	15588.5$^{237.4}$	15351.1						
	240.9	241.8						
1	15829.4$^{236.5}$	15592.9$^{236.3}$	15356.6					
	238.9	240.0	239.4					
2	16068.3$^{235.4}$	15832.9$^{236.5}$	15596.4$^{234.9}$	15361.5$^{230.9}$	15130.6			
		239.5	239.5		235.9			
3		16072.4$^{236.5}$	15835.9		15366.5$^{226.8}$	15139.7		
4							15147.3	
5								15155.4

TABLE 9

DESLANDRES TABLE FOR P_1 HEADS OF B $^2\Sigma^+ \longrightarrow$ X $^2\Sigma^+$ SYSTEM OF CaI MOLECULE

v'' v'	0		1		2		3		4		5		6		7		8		9
0	15712.4	238.2	15474.2																
	238.3		239.2																
1	15950.7	237.3	15713.4	237.6	15475.8														
			239.5		238.8														
2			15952.9	238.3	15714.6	237.6	15477.0												
			235.1																
3			16188.0								15246.9								
											235.4								
4					16185.9						15482.3	231.7	15250.6						
													234.1						
5							16184.3						15484.7	231.6	15253.1				
															232.1				
6									16182.6						15485.2	231.0	15254.2		
7											16180.7								15257.7
8													16178.3						

TABLE 10

DESLANDRES TABLE FOR P_2 HEADS OF $B\ ^2\Sigma^+ \longrightarrow X\ ^2\Sigma^+$ SYSTEM OF CaI MOLECULE

v″ v′	0		1		2		3
0	15715.8	238.2	15477.6				
	237.8		239.4				
1	15953.6	236.6	15717.0	237.4	15479.6		
			238.9		238.6		
2			15955.9	237.7	15718.2	237.6	15480.6

In the present investigation about thirty bands have been recorded in addition to those already reported by earlier workers (Walters and Barrat 1928; Hedfeld 1931). From the group of bands having equal intensity of two sub heads the most intense bands at 15712.4 cm^{-1} and 15715.8 cm^{-1} were taken as P_1 and P_2 heads of the 0,0 band and a vibrational analysis was carried out in the usual way. The following vibrational quantum equation satisfactorily represents P_1 and P_2 heads.

$$\nu_{head} = \begin{matrix} (P_1)\ 15711.8 \\ (P_2)\ 15715.2 \end{matrix} + 239.95\,(v' + \tfrac{1}{2}) - 0.62\,(v' + \tfrac{1}{2})^2 - 238.8\,(v'' + \tfrac{1}{2}) + 0.55\,(v'' + \tfrac{1}{2})^2 \qquad (31)$$

The lower state frequency of 238.8 cm^{-1} observed in the present work agrees very well with the ground state frequency 238.3 cm^{-1} of CaI molecule as reported by earlier workers. Moreover the system has also been observed in absorption by E. Morgan (1970) which confirms that the lower state involved in this system is the ground state X $^2\Sigma^+$. The upper state shows a splitting of 3.4 cm^{-1} which may be considered as a spin splitting in the upper state B $^2\Sigma^+$. Such a spin splitting has been observed in the B $^2\Sigma^+$ states of CaF, SrF, BaF and SrCl molecules. A comparision of region of occurrence of this system with B$^2\Sigma$ - X $^2\Sigma$ systems of CaF, CaCl and CaBr molecules indicates that the system may be attributed to an electronic transition B$^2\Sigma^+$ - X$^2\Sigma^+$ showing a spin splitting of 3.4 cm^{-1} in the upper state, considering the spin splitting in the ground state X $^2\Sigma^+$ to be very very small.

The spectrogram also reveals a large number of bands having intense Q heads and corresponding weak P heads with a separation between them about 9 cm^{-1}. Amongst these 15647.2 cm^{-1} and 15588.2 cm^{-1} were taken as the 0,0 bands of the sub systems A $^2\Pi_{3/2}$ —— X$^2\Sigma^+$ and A $^2\Pi_{1/2}$ —— X $^2\Sigma^+$ respectively and the vibrational analysis was carried out in the usual way.

The following vibrational quantum equations satisfactorily represent 43 Q heads.

$$A\ {}^2\Pi_{3/2} — X\ {}^2\Sigma^+ \quad \text{system :}$$

$$\nu_{\text{head}} = 15645.57 + 241.69\ (v' + \tfrac{1}{2}) - 0.83\ (v' + \tfrac{1}{2})^2$$

$$- 238.40\ (v'' + \tfrac{1}{2}) + 0.79\ (v'' + \tfrac{1}{2})^2 \quad (32)$$

$$A\ {}^2\Pi_{1/2} — X\ {}^2\Sigma^+ \quad \text{system :}$$

$$\nu_{\text{head}} = 15586.20 + 242.65\ (v' + \tfrac{1}{2}) - 0.62\ (v' + \tfrac{1}{2})^2$$

$$- 238.26\ (v'' + \tfrac{1}{2}) + 0.73\ (v'' + \tfrac{1}{2})^2 \quad (33)$$

The nature of the bands and a comparision of region of occurence of this system with A $^2\Pi$- X $^2\Sigma^+$ systems of CaF, CaCl and CaBr molecules indicate that the system may be attributed to an electronic transition A $^2\Pi$ — X $^2\Sigma^+$ with a $^2\Pi$ separation of about 59 cm^{-1}.

The identity of the emitter of the band system was confirmed by standard methods. Which leads us to believe that the bands in the region λλ6600-6175 A° observed in the present investigation belong to CaI molecule.

4.2 ZnI BANDS

The near ultraviolet bands in the region λλ3392.5-3260 A°.

A group of ZnI bands in the region λλ3392.5-3260 A° has been recorded. The spectrum was photographed in the fourth order of a 2 meter plane grating spectrograph at a reciprocal dispersion of 1.88 A°/mm. A spectrum with reasonable intensity and clarity could be recorded on Ilford N-40 plates in about an hour. The bands in the region λλ 3392.5-3260 A° were reported by Wieland (1929). These bands were considered as one of the components of a $^2\Pi - {}^2\Sigma$ transition and later Rao and Rao (1946) observed the second component in the region λλ 3278-3123 A°. The longer and shorter wave length components were designated as C $^2\Pi_{\frac{1}{2}}$ - X $^2\Sigma$ and D $^2\Pi_{3/2}$ - X $^2\Sigma$ systems respectively. The bands of the system C - X are very intense and show a clear degradation towards violet where as those of the system D - X are diffuse and are probably degraded to red.

The maximum dispersion availed by Wieland to photograph the C - X system of ZnI bands was 10 A°/mm. The photograph of this system is obtained in the present work at a dispersion of 1.88 A°/mm with the help of the plane grating spectrograph, and it is reproduced in plate 3. Only a part of the D - X system (below 3278 A°) is shown and in that region the bands belonging to both systems are overlapping.

The aim of the present study is to reinvestigate a complete vibrational analysis of C - X system using a higher dispersion and support it by vibrational isotopic effect due to Zn^{64}, Zn^{66} and Zn^{68} which is measurable for most of the bands. The results obtained are presented in this section.

Contrary to what is reported by earlier workers

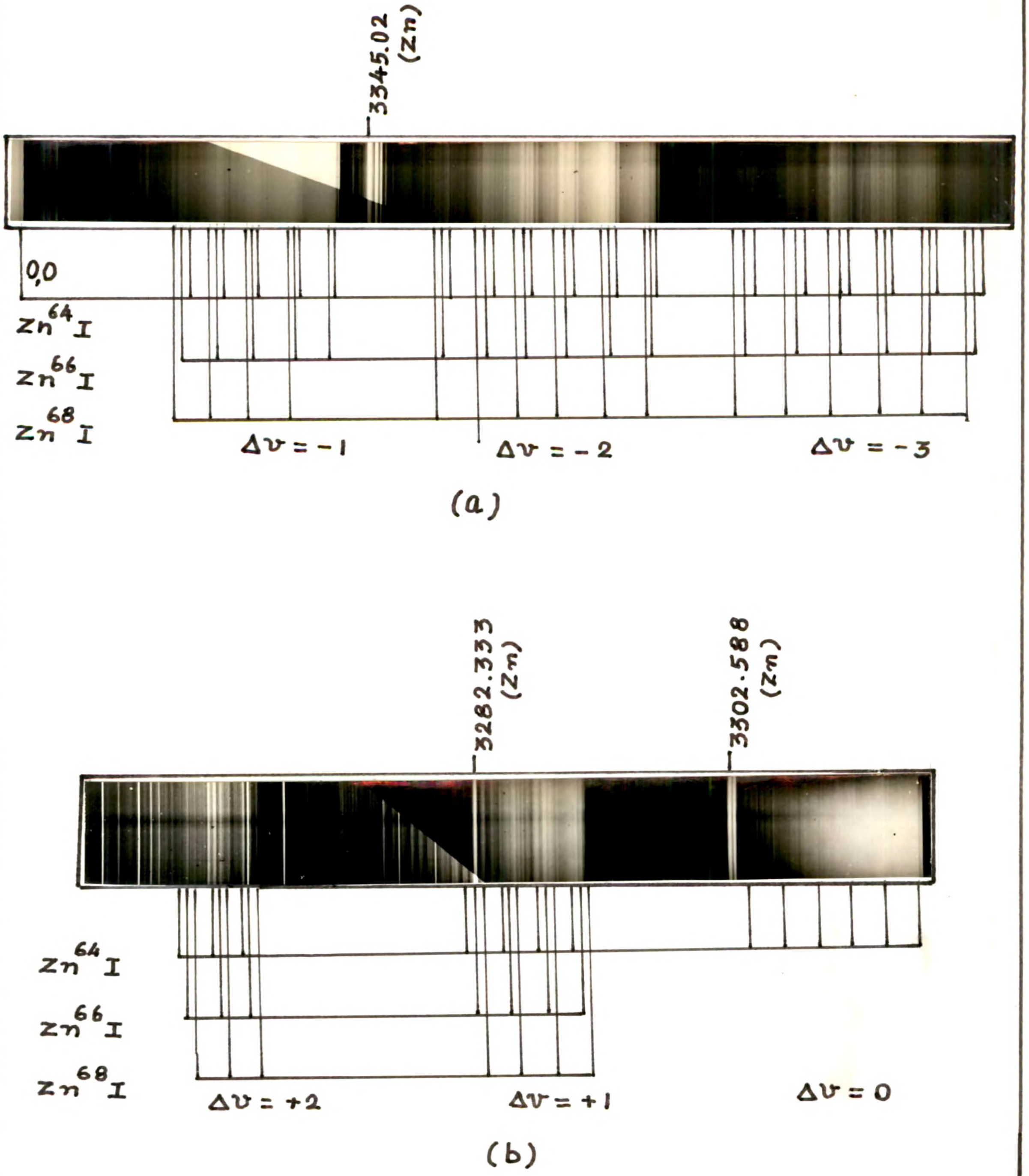

PLATE 3.

GRATING SPECTROGRAM OF ZnI MOLECULE (C-X SYSTEM) REVEALING THE VIBRATIONAL ISOTOPIC EFFECT.

(Wieland 1929), the present study using higher dispersion reveals that each band is distinctly seen to be accompanied by ancillary heads on longer and shorter wavelength sides whose intensities and separations from the main heads indicate to consider them as Q heads of the isotopic bands due to Zn^{66} I and Zn^{68} I. All the bands are measured against iron arc standards and the observed wave numbers in vacuum, vibrational assignments and the observed and calculated isotopic shifts for $Zn^{66}I^{127}$ and $Zn^{68}I^{127}$ with respect to $Zn^{64}I^{127}$ are given in Table 11. The isotopic shifts were calculated using the usual formula.

$$\begin{aligned}\Delta\nu &= \nu^{i} - \nu \\ &= (\rho-1)\left[\omega'_e(v'+\tfrac{1}{2}) - \omega''_e(v''+\tfrac{1}{2})\right] \\ &\quad -(\rho^2-1)\left[\omega'_e x'_e(v'+\tfrac{1}{2})^2 - \omega''_e x''_e(v''+\tfrac{1}{2})^2\right]\end{aligned} \qquad (34)$$

The abundance ratio of Zn^{64} and Zn^{66} is approximately 1.8:1 and that between Zn^{64} and Zn^{68}

TABLE 11

Band head data for Q heads of the C $^2\Pi_{\frac{1}{2}} \longrightarrow X\ ^2\Sigma$ system of ZnI molecule

Wavelength A°	Wave number in vacuum ν cm^{-1}	Assignment v', v"	Isotope shift for $Zn^{66}I^{127}$ and $Zn^{68}I^{127}$ w.r.t. $Zn^{64}I^{127}$	
			Obs. cm^{-1}	Cal. cm^{-1}
3392.52	29468.62	0,3(64)	-	-
3391.71	29475.12	0,3(66)	6.50	6.39
3391.03	29481.27	0,3(68)	12.65	12.79
3389.12	29498.01	1,4(64)	-	-
3388.43	29503.91	1,4(66)	5.90	6.06
3387.76	29510.21	1,4(68)	12.20	12.12
3385.78	29527.66	2,5(64)	-	-
3385.01	29533.46	2,5(66)	5.80	5.72
3384.32	29539.32	2,5(68)	11.66	11.44
3382.34	29557.26	3,6(64)	-	-
3381.76	29562.68	3,6(66)	5.42	5.37
3381.12	29567.88	3,6(68)	10.62	10.74
3378.91	29587.20	4,7(64)	-	-

contd..

Table 11 (contd..)

Wavelength A°	Wave number in vacuum ν cm^{-1}	Assignment v', v''	Isotope shift for $Zn^{66}I^{127}$ and $Zn^{68}I^{127}$ w.r.t. $Zn^{64}I^{127}$	
			Obs. cm^{-1}	Cal. cm^{-1}
3378.33	29592.20	4,7(66)	5.00	5.02
3377.74	29597.44	4,7(68)	10.24	10.04
3375.52	29616.89	5,8(64)	-	-
3375.02	29621.39	5,8(66)	4.50	4.67
3374.42	29626.41	5,8(68)	9.92	9.34
3372.14	29646.80	6,9(64)	-	-
3371.63	29651.0	6,9(66)	4.20	4.33
3371.12	29655.62	6,9(68)	8.82	8.66
3367.51	29687.12	0,2(64)	-	-
3367.03	29691.42	0,2(66)	4.30	4.25
3366.67	29695.42	0,2(68)	8.30	8.50
3364.36	29715.35	1,3(64)	-	-
3363.85	29719.55	1,3(66)	4.20	3.94
3363.42	29722.97	1,3(68)	7.62	7.88
3361.21	29742.76	2,4(64)	-	-

Contd..

Table 11 (Contd..)

Wavelength A°	Wave number in vacuum ν cm^{-1}	Assignment v', v"	Isotope shift for $Zn^{66}I^{127}$ and $Zn^{68}I^{127}$ w.r.t. $Zn^{64}I^{127}$	
			Obs. cm^{-1}	Cal. cm^{-1}
3360.83	29746.26	2,4(66)	3.50	3.61
3360.42	29750.16	2,4(68)	7.40	7.22
3358.01	29771.10	3,5(64)	-	-
3357.64	29774.61	3,5(66)	3.51	3.32
3357.32	29777.52	3,5(68)	6.42	6.64
3354.91	29798.61	4,6(64)	-	-
3354.51	29801.82	4,6(66)	3.21	3.0
3354.22	29804.41	4,6(68)	5.80	6.0
3351.64	29828.21	5,7(64)	-	-
3351.32	29830.73	5,7(66)	2.52	2.68
3351.01	29833.72	5,7(68)	5.51	5.36
3342.82	29906.47	0,1(64)	-	-
3342.61	29908.47	0,1(66)	2.00	2.08
3339.53	29936.02	1,2(64)	-	-
3339.31	29938.02	1,2(66)	2.00	1.8

Contd..

Table 11 (Contd..)

Wavelength A°	Wave number in vacuum ν cm^{-1}	Assignment v', v"	Isotope shift for $Zn^{66}I^{127}$ and $Zn^{68}I^{127}$ w.r.t. $Zn^{64}I^{127}$	
			Obs. cm^{-1}	Cal. cm^{-1}
3339.11	29939.84	1,2(68)	3.82	3.6
3336.62	29962.04	2,3(64)	-	-
3336.44	29963.66	2,3(66)	1.62	1.51
3336.26	29965.25	2,3(68)	3.21	3.03
3334.18	29984.50	3,4(64)	-	-
3333.91	29985.92	3,4(66)	1.42	1.23
3333.82	29987.0	3,4(68)	2.50	2.46
3330.81	30014.31	4,5(64)	-	-
3330.71	30015.41	4,5(66)	1.10	0.95
3330.62	30016.31	4,5(68)	2.00	1.89
3327.84	30041.11	5,6(64)	-	-
3327.73	30041.81	5,6(66)	0.70	0.66
3327.61	30042.52	5,6(68)	1.48	1.32
3318.07	30129.09	0,0(64)P	-	-
3317.71	30132.70	0,0(64)Q	-	-

Contd..

Table 11 (Contd..)

Wavelength A°	Wave number in vacuum ν cm^{-1}	Assignment v', v"	Isotope shift for $Zn^{66}I^{127}$ and $Zn^{68}I^{127}$ w.r.t. $Zn^{64}I^{127}$	
			Obs. cm^{-1}	Cal. cm^{-1}
3315.30	30154.53	1,1(64)P	-	-
3314.95	30158.17	1,1(64)Q	-	-
3312.52	30179.91	2,2(64)P	-	-
3312.10	30183.66	2,2(64)Q	-	-
3309.67	30205.30	3,3(64)Q	-	-
3307.34	30227.4	4,4(64)Q	-	-
3291.12	30376.25	1,0(64)	-	-
3291.33	30374.02	1,0(66)	-2.23	-2.57
3291.63	30371.10	1,0(68)	-5.15	-5.15
3288.84	30397.50	2,1(64)	-	-
3289.02	30395.15	2,1(66)	-2.35	-2.80
3289.41	30391.70	2,1(68)	-5.80	-5.60
3286.12	30422.47	3,2(64)	-	-
3286.43	30419.47	3,2(66)	-3.00	-3.02
3286.72	30416.66	3,2(68)	-5.81	-6.04

Contd..

Table 11 (Contd..)

Wavelength A°	Wave number in vacuum ν cm^{-1}	Assignment v', v"	Isotope shift for $Zn^{66}I^{127}$ and $Zn^{68}I^{127}$ w.r.t. $Zn^{64}I^{127}$ Obs. cm^{-1}	Cal. cm^{-1}
3283.43	30447.50	4,3(64)	-	-
3283.81	30444.05	4,3(66)	-3.45	-3.25
3284.12	30441.09	4,3(68)	-6.41	-6.50
3264.71	30622.21	2,0(64)	-	-
3265.22	30617.41	2,0(66)	-4.80	-5.0
3265.71	30612.10	2,0(68)	-10.11	-10.0
3262.32	30644.41	3,1(64)	-	-
3262.92	30639.11	3,1(66)	-5.30	-5.20
3263.42	30633.79	3,1(68)	-10.62	-10.4
3260.01	30666.51	4,2(64)	-	-
3260.52	30661.09	4,2(66)	-5.42	-5.39
3261.11	30655.51	4,2(68)	-11.0	-10.79

is 2.6:1. The calculated values of mass factors $(\rho-1)$ & (ρ^2-1) are -0.01 and -0.02 for Zn^{66} and Zn^{68} with respect to Zn^{64} respectively.

The close agreement between calculated and observed isotopic shifts (Table 11) confirm the correctness of the vibrational analysis of C – X system. The lower state frequency (223.4 cm^{-1}) of this system agrees with the previously reported ground state frequency of ZnI molecule. (Wieland 1929). The identity of the emitter is confirmed by the standard methods.