Vibrational analysis of Fourier transform spectrum of the A 3 Π 0 −X 1 Σ + and B 3 Π 1 −X 1 Σ + transitions of indium monobromide

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Vibrational analysis of Fourier transform spectrum of the $A^3\Pi_0$–$X^1\Sigma^+$ and $B^3\Pi_1$–$X^1\Sigma^+$ transitions of indium monobromide

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Abstract. The emission spectrum of InBr molecule has been recorded in the region 350–400 nm on BOMEM DA8 Fourier transform spectrometer at an apodized resolution of 0.06 cm^{-1} using microwave excitation technique. About 61 violet degraded and single headed bands have been recorded and are classified into two band systems, viz. $A^3\Pi_0$–$X^1\Sigma^+$ and $B^3\Pi_1$–$X^1\Sigma^+$. A few new bands have been observed and are fitted in the vibrational schemes of the two systems. Revised vibrational constants have been determined. The vibrational assignments have been confirmed by observing isotope effect due to InBr^{81} in the 30 bands of the $A^3\Pi_0$–$X^1\Sigma^+$ system and 19 bands of the $B^3\Pi_1$–$X^1\Sigma^+$ system. The analysis is further supported by calculating the Franck–Condon factor for InBr^{79} and InBr^{81} molecules. The following vibrational constants (in cm^{-1}) have been determined from the analysis:

$A^3\Pi_0$–$X^1\Sigma^+$ system: $\nu_{00} = 26599.1$ $\omega_e' = 226.42$, $\omega_e'x_e' = 1.24$ cm^{-1},
     $\omega_e'' = 221.19$, $\omega_e''x_e'' = 0.528$ cm^{-1}.
$B^3\Pi_1$–$X^1\Sigma^+$ system: $\nu_{00} = 27380.52$ $\omega_e' = 223.086$, $\omega_e'x_e' = 1.446$ cm^{-1},
     $\omega_e'' = 221.19$, $\omega_e''x_e'' = 0.528$ cm^{-1}.

Keywords. Fourier transform spectroscopy; vibrational analysis; isotope effect; Franck–Condon factor.

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1. Introduction

There is renewed interest in the study of indium monobromide molecule (InBr) due to its peculiar properties like low volatility at reasonable temperature, fast recombination rate and low dissociation energies. Nowadays they are widely used in the production of efficient atomic laser, nonresonant and Stokes–Raman laser,

Table 1. Spectroscopic constant (cm^{-1}) for the $A^3\Pi_0$, $B^3\Pi_1$ and $X^3\Sigma^+$ states of $InBr^{79}$.

Constants	Lakshminarayana and Harnath [3]	Vempati and Jones [9]	Singh *et al* [5]	Singh *et al* [8]	Burnecka and Zyrnicki [10]	Present study
			$A^3\Pi_0$			
ν_{00}	26598.4	26600.26	26601.40	26599.13	26597.846	26599.10
ω_e'	229.2	229.2	229.4	227.99	228.163	226.42
$\omega_e x_e'$	1.42	1.42	1.09	1.14	1.195	1.24
			$B^3\Pi_1$			
ν_{00}	27379.44	27381.73			27381.247	27380.52
ω_e'	225.0	225.0			224.328	223.086
$\omega_e x_e'$	1.53	1.53			1.273	1.446
			$X^1\Sigma^+$			
ω_e''	223.1	223.0		223.0	222.927	221.19
$\omega_e x_e''$	0.56	0.58		0.58	0.549	0.528

light industry and semiconductor devices which provides a further impetus for the study of molecular electronic states of these halides.

The electronic spectrum of indium monohalides (InF, InCl, InBr and InI) consists of mainly three band systems in visible and ultraviolet region of the spectrum, viz. A–X, B–X and C–X. In InBr molecule, A–X and B–X systems were observed in 350–400 nm region in emission as well as in absorption. The vibrational analyses of the A–X and B–X systems were first reported by Pertrikaln and Hochberg [1]. Later, Wehrli and Miescher [2] studied the absorption spectrum of InBr in second order of 3 m grating and reported red degraded bands. The spectrum was further extended by Lakshminarayana and Harnath [3] by photographing in first order of 21 ft concave grating spectrograph having a dispersion of 1.25 Å/mm. Nampoori and Patel [4] recorded the spectra on 2 m plane grating spectrograph (PGS-2) at a dispersion of 0.5 Å/mm. Vibrational constants reported by Singh *et al* [5] agree with those of Lakshminarayana and Harnath [3] but their reported values of vibrational heads do not match with each other. They also reported predissociation in $A^3\Pi_0$ state.

The early rotational studies on InBr molecule were performed by Wehrli and Miescher [2]. Later, Barrett and Mendel [6] determined spectroscopic constants for the ground state using microwave technique. Barrow [7] obtained the dissociation energy of InBr molecule. The rotational analyses of a few bands of the A–X and B–X systems were reported by Nampoori and Patel [4]. Singh *et al* [8] recorded both emission and absorption spectra of InBr molecule and reported rotational constants. Since their spectrum is not well-resolved, the assignments seem to be ambiguous. Vempati and Jones [9] recorded high resolution spectra of InBr molecule at a reciprocal linear dispersion of 0.13 Å/mm. In lower region of the spectrum of A–X system, P and R branches overlapped. Burnecka and Zyrnicki's [10] study
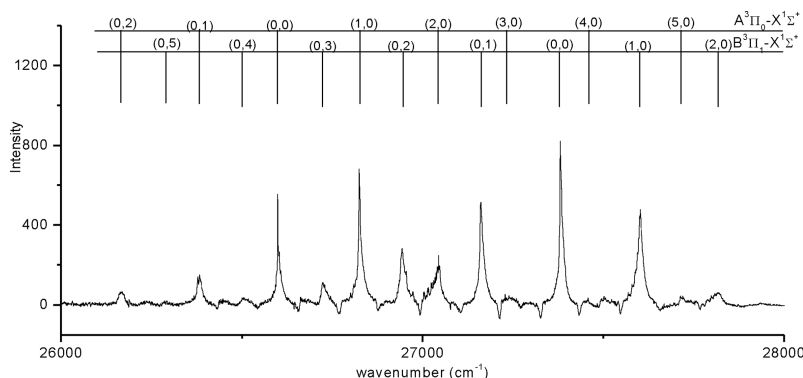
Figure 1. Vibrational spectra of $A^3\Pi_0$–$X^1\Sigma^+$ and $B^3\Pi_1$–$X^1\Sigma^+$ transitions of InBr.
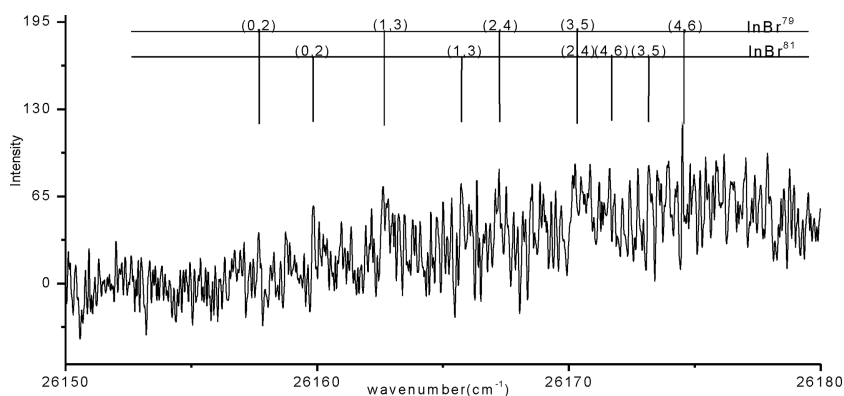

Figure 2. Vibrational spectra of bands of $\Delta\nu = -2$ sequence of $A^3\Pi_0$–$X^1\Sigma^+$ transition.

shows that the data obtained from their constants do not match with the reported spectrum. Apart from this, the rotational structure of $A^3\Pi_0$–$X^1\Sigma^+$ and $B^3\Pi_1$–$X^1\Sigma^+$ systems, the Rydberg–Klein–Rees (RKR) curve and the Franck–Condon factor [11,12], rotational [13–15] and nuclear quadrupole [16] coupling constants of the ground state of InBr were determined.

In addition to the $A^3\Pi_0$–$X^1\Sigma^+$ and $B^3\Pi_1$–$X^1\Sigma^+$ systems, Wehrli and Miescher [17] observed the bands of $C^1\Pi$–$X^1\Sigma^+$ system. In the absorption spectrum of InBr, Haraguchi and Fuwa [18] found six vibrational levels in C–X system. Moreover, Singh *et al* [15] observed a green emission in the region of 480–530 nm with the maximum at 520 nm and assigned it to a transition from a certain higher state to the $C^1\Pi$ state. Recently, Yang *et al* [19] studied the laser-induced fluorescence spectra of InBr molecule. They recorded the bands of the $A^3\Pi_0$–$X^1\Sigma^+$, $B^3\Pi_1$–$X^1\Sigma^+$ and $C^1\Pi$–$X^1\Sigma$ systems and reported spectroscopic constants of the $C^1\Pi$ state. Apart from these studies, ionization energy and spectroscopic constants of the ground state as well as the excited states of InBr molecule were calculated theoretically
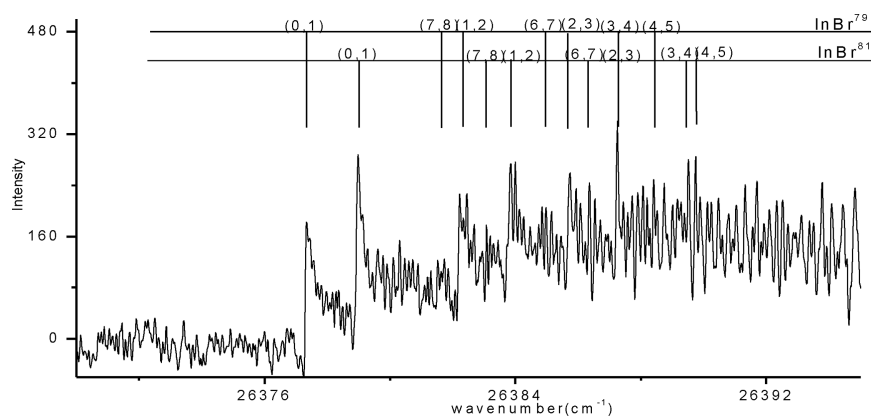
Figure 3. Vibrational spectra of bands of $\Delta\nu = -1$ sequence of $A^3\Pi_0$–$X^1\Sigma^+$ transition.
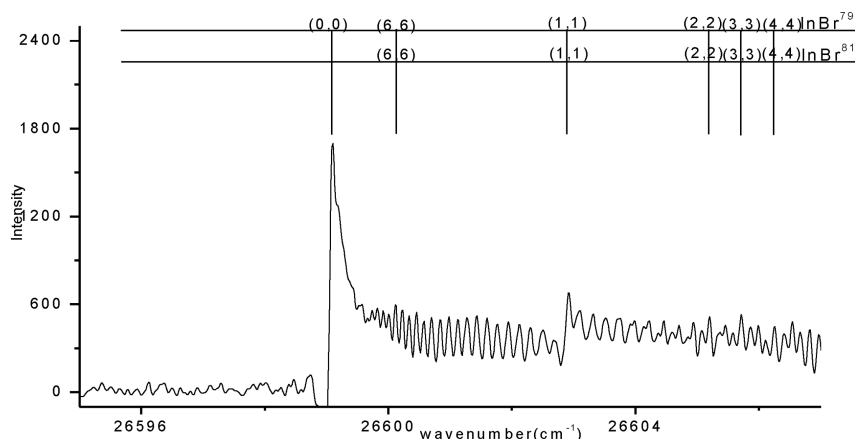

Figure 4. Vibrational spectra of bands of $\Delta\nu = 0$ sequence of $A^3\Pi_0$–$X^1\Sigma^+$ transition.

using various methods such as coupled-cluster single and double linear response theory [20–22].

The scrutiny of the available literature about InBr molecule reveals that different workers have reported different constants for the different systems even for the ground state as well as band head data, viz. table 1. In addition, the Fourier transform study of the isovalent molecule InCl by Saksena and Deo [23] yielded fruitful information. Because of the additional advantage of Fourier transform spectrometer such as fast scanning rate, low signal-to-noise ratio, free from stray light, high resolution and high sensitivity, we have decided to investigate this molecule using Fourier transform spectrometer and microwave excitation technique.

In this article, we present the Fourier transform (FT) high resolution spectrum of InBr molecule excited by microwave discharge technique and the vibrational

Figure 5. Vibrational spectra of bands of $\Delta\nu = +1$ sequence of $A^3\Pi_0$–$X^1\Sigma^+$ transition.

Figure 6. Vibrational spectra of bands of $\Delta\nu = +2$ sequence of $A^3\Pi_0$–$X^1\Sigma^+$ transition.

analysis of the bands of the $A^3\Pi_0$–$X^1\Sigma^+$ and $B^3\Pi_1$–$X^1\Sigma^+$ systems supported by isotopic shift study and Franck–Condon factor.

2. Experimental

The spectrum of indium monobromide molecule was excited using microwave power. A few grams of spec-pure sample of $InBr_3$ substance (Aldrich 99.99%), was placed in a quartz boat of length 8 cm and diameter 6 mm, which was kept in the side arm of a quartz discharge tube. This boat was heated to about 400°C by an electrical furnace of nichrome wire. The discharge tube was evacuated by means of a rotary vacuum
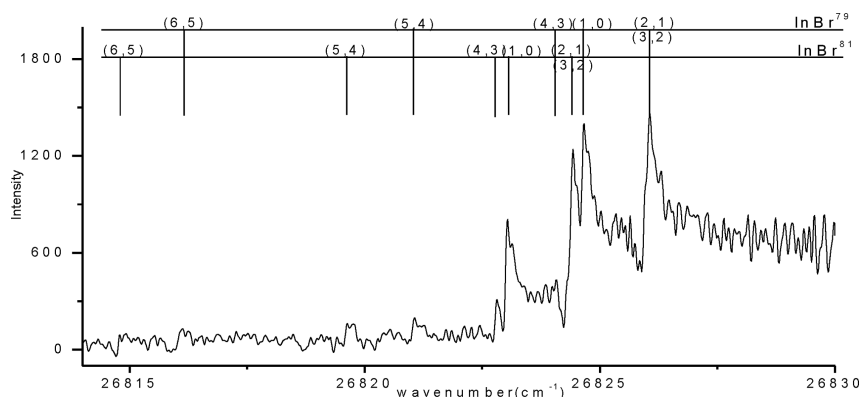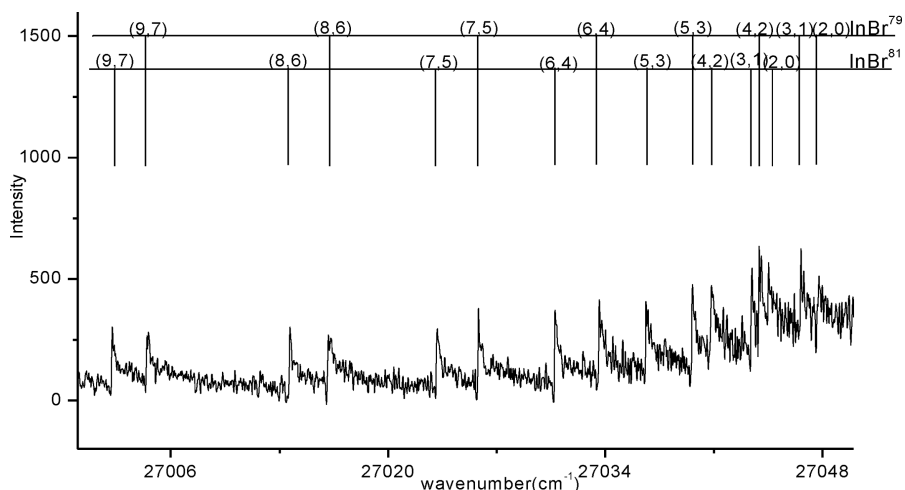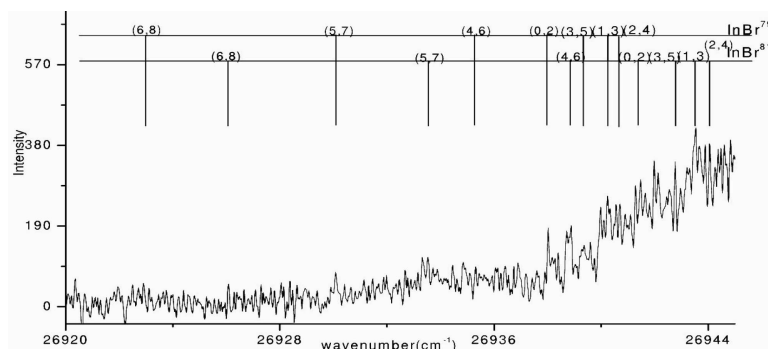
Figure 7. Vibrational spectra of bands of $\Delta\nu = -2$ sequence of $B^3\Pi_1$–$X^1\Sigma^+$ transition.
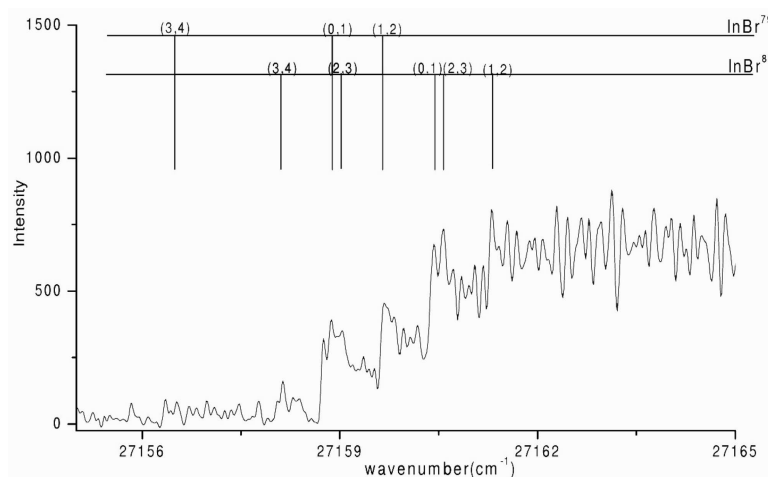

Figure 8. Vibrational spectra of bands of $\Delta\nu = -1$ sequence of $B^3\Pi_1$–$X^1\Sigma^+$ transition.

pump. Along with the $InBr_3$ vapour, buffer gas argon, at a pressure of about 5 Torr was let into the microwave discharge region. Hundred and twenty Watts of power at 2.45 GHz was applied to the microwave cavity. By optimizing the pressure of argon, a characteristic intense blue–violet colour is observed in the microwave discharge. To maintain this characteristic intense blue–violet colour, constant external heating was found necessary during the experiment. The discharge glow was focussed onto the emission port of the Fourier transform spectrometer using a spherical lens. The spectra were recorded in the region 25,000–30,000 cm^{-1} on BOMEM DA 8 Fourier transform spectrometer at an apodized resolution of 0.06 cm^{-1} using a quartz UV beam splitter, photomultiplier detector and appropriate filter. Sixty-four scans (integration time $\sim$60 min) were co-added to improve the signal-to-noise ratio.
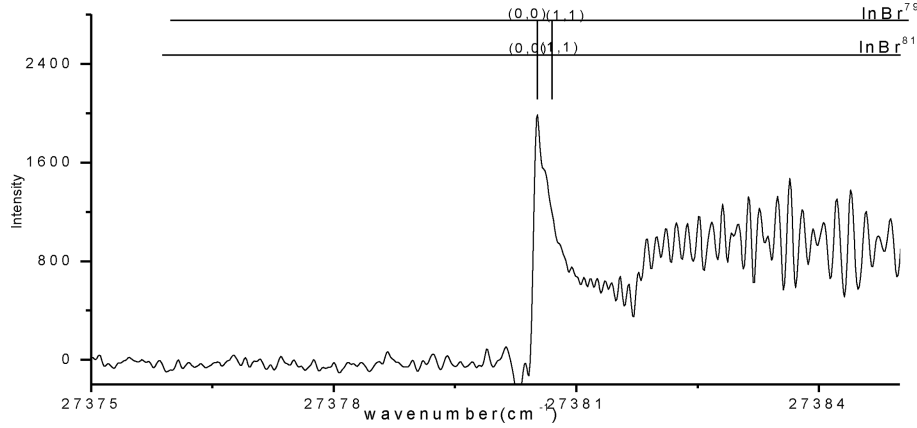
Figure 9. Vibrational spectra of bands of $\Delta\nu = 0$ sequence of $B^3\Pi_1$–$X^1\Sigma^+$ transition.
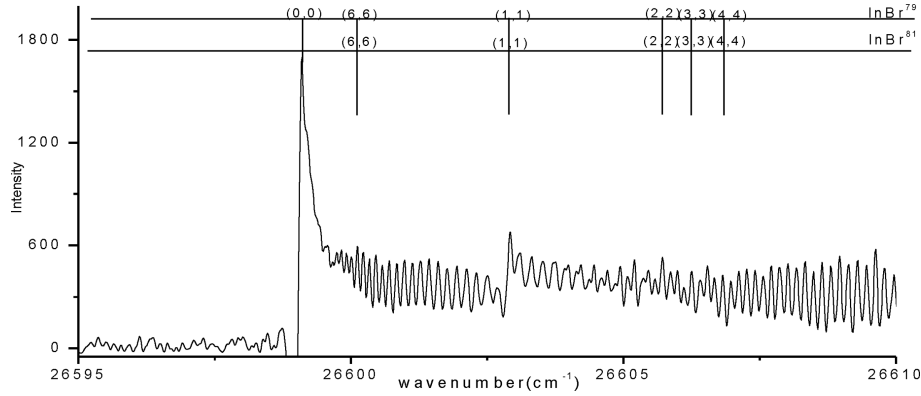
Figure 10. Vibrational spectra of bands of $\Delta\nu = +1$ sequence of $B^3\Pi_1$–$X^1\Sigma^+$ transition.

3. Results and discussion

The Fourier transform emission spectrum of InBr molecule has been recorded in the spectral region 350–400 nm. In general, the spectrum is free from overlap of atomic lines and about sixty-one bands, degraded to violet have been observed. They have been classified into two systems: $A^3\Pi_0$–$X^1\Sigma^+$ and $B^3\Pi_1$–$X^1\Sigma^+$. Figure 1 shows the gross spectrum of $A^3\Pi_0$–$X^1\Sigma^+$ and $B^3\Pi_1$–$X^1\Sigma^+$ band systems while figures 2–11 display the enlarged spectrum of different sequence bands of the $A^3\Pi_0$–$X^1\Sigma^+$ and $B^3\Pi_1$–$X^1\Sigma^+$ systems. The vibrational bands of both the transitions can be represented by the expression

$$\nu = T_e + \omega'_e(v'+1/2) - \omega'_e x'_e(v'+1/2)^2 - \omega''_e(v''+1/2) + \omega''_e x''_e(v''+1/2)^2,$$

where ω_e is the vibrational frequency, $\omega_e x_e$ is anharmonicity constant of the molecule, T_e is the term value. Single prime and double prime indicate the upper state
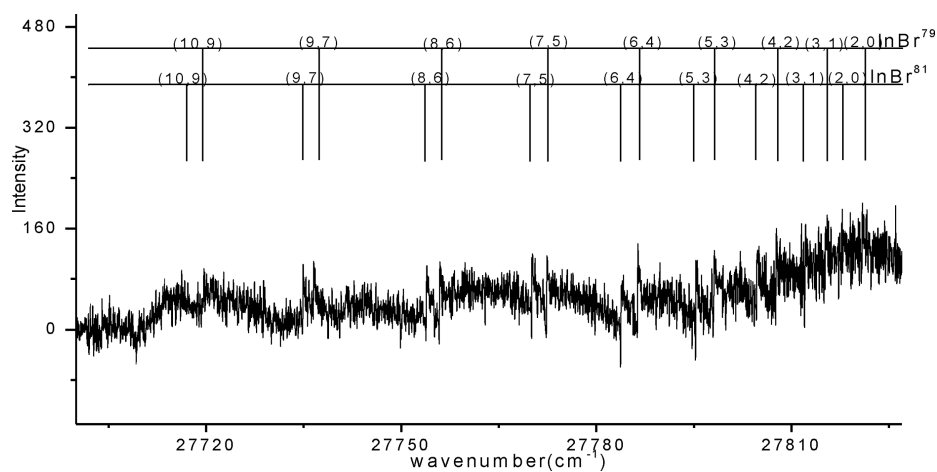
Figure 11. Vibrational spectra of bands of $\Delta\nu = +2$ sequence of $B^3\Pi_1$–$X^1\Sigma^+$ transition.
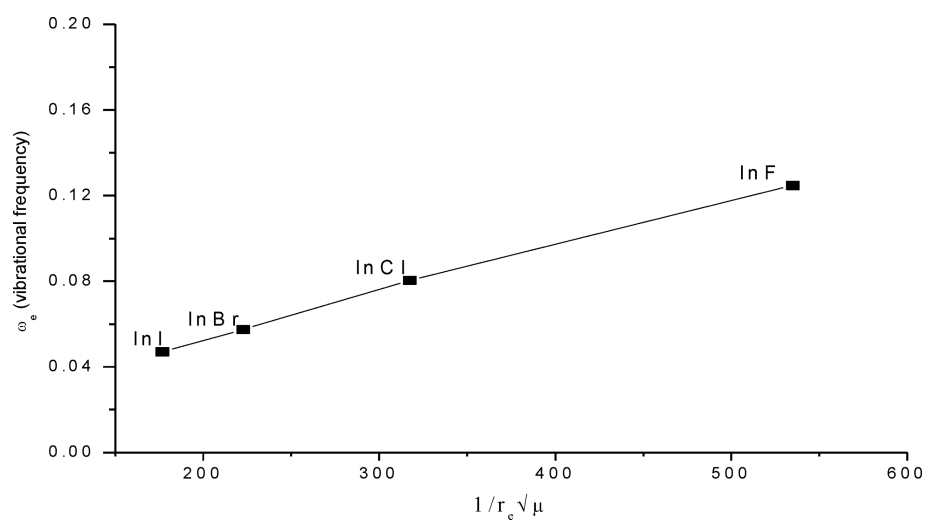
Figure 12. Plot between ground state vibrational frequency and $1/r_e\sqrt{\mu}$ for the InF, InCl, InBr and InI molecules.

and lower state constants of the molecule. The various spectroscopic constants obtained from band head measurements of the A–X and B–X systems and Deslandre's table is given below:

For $A^3\Pi_0$–$X^1\Sigma^+$ system:

$$\nu_{00} = 26599.1: \quad \omega_e' = 226.42, \quad \omega_e'x_e' = 1.24 \text{ cm}^{-1},$$
$$\omega_e'' = 221.19, \quad \omega_e''x_e'' = 0.528 \text{ cm}^{-1}.$$

For $B^3\Pi_1$–$X^1\Sigma^+$ system:

$$\nu_{00} = 27380.52: \quad \omega'_e = 223.086, \quad \omega'_e x'_e = 1.446 \text{ cm}^{-1},$$
$$\omega''_e = 221.19, \quad \omega''_e x''_e = 0.528 \text{ cm}^{-1}.$$

Table 2. Isotopic shift study of $A^3\Pi_0$–$X^1\Sigma^+$ band system of InBr molecule.

	InBr^{81}				InBr^{79}				Isotopic shift	
(v', v'')	ν_{obs}	ν_{cal}	$\Delta\nu$	FCF	ν_{obs}	ν_{cal}	$\Delta\nu$	FCF	$\Delta\nu_{obs}$	$\Delta\nu_{cal}$
(0,2)	26159.89	26159.84	0.05	0.0973	26156.68	26156.67	0.01	0.0970	3.21	3.17
(1,3)	26165.81	26165.74	0.07	0.1605	26162.65	26162.65	0.02	0.1607	3.16	3.09
(2,4)	26170.30	26170.26	0.04	0.1697	26167.17	26167.17	0	0.1705	3.13	3.08
(3,5)	26173.37	26173.16	0.21	0.1413	26170.24	26170.14	0.10	0.1427	3.13	3.02
(4,6)				0.0979	26171.88	26171.63	0.25	0.0994		
(0,1)	26378.97	26378.97	0	0.2846	26377.36	26377.33	0.03	0.2848	1.61	1.64
(1,2)	26383.83	26383.83	0	0.2582	26382.26	26382.28	−0.02	0.2594	1.57	1.55
(2,3)	26387.27	26387.24	0.03	0.1554	26385.71	26385.74	−0.03	0.1567	1.56	1.50
(3,4)	26389.28	23689.36	−0.08	0.0667	26387.71	26387.25	0.46	0.0678	1.57	2.11
(4,5)	26389.87	26389.75	0.12	0.0162	26388.27	26388.39	−0.12	0.0167	1.60	1.36
(5,6)				0.0001	26387.39	26387.25	0.14	0.0002		
(6,7)	26386.28	26386.78	−0.50	0.0069	26385.06	26385.14	−0.08	0.0067	1.22	1.63
(7,8)	26383.10	26383.08	0.02	0.0246						
(8,9)	26377.99	26377.98	0.01	0.0445						
(0,0)	26599.10	26599.10	0	0.5781	26599.12	26599.10	0.02	0.5790	−0.02	0
(1,1)	26599.10	26599.10	0	0.1244	26599.12	26599.10	0.02	0.1250	−0.02	0
(2,2)	26602.91	26602.91	0	0.0045	26602.94	26602.94	0	0.0046	−0.03	−0.03
(3,3)	26605.29	26605.22	0.07	0.0160	26605.32	26605.22	0.09	0.0158	−0.03	−0.01
(4,4)	26606.25	26606.24	0.01	0.0625	26606.25	26606.24	0.01	0.0623	0	0
(6,6)	26605.78	26605.78	0	0.1259	26605.74	26605.78	−0.04	0.1258	0.04	0
(7,7)	26600.58	26599.10	1.48	0.1299						
(8,8)	26595.84	26596.14	−0.30	0.1201	26595.53	26595.37	0.16	0.1198	0.31	0.77
(1,0)	26589.68	26589.72	−0.04	0.3492	26589.24	26589.19	0.05	0.3484	0.44	0.53
(2,1)	26823.04	26823.04	0	0.4217	26824.69	26824.64	0.05	0.4207	−1.65	−1.59
(3,2)	26824.37	26824.43	−0.06	0.3748	26826.00	26826.05	−0.05	0.3734	−1.63	−1.63
(4,3)	26824.27	26824.30	−0.03	0.2887	26825.86	26825.95	−0.09	0.2872	−1.59	−1.66
(5,4)	26822.75	26822.81	−0.06	0.2019	26824.28	26824.30	−0.02	0.2004	−1.53	−1.49
(6,5)	26819.80	26819.63	0.17	0.1300	26821.25	26821.05	0.20	0.1286	−1.45	−1.42
(2,0)	26815.43	26814.86	0.57	0.0680	26816.78	26816.12	0.66	0.0680	−1.35	−1.26
(3,1)	27044.50	27044.54	−0.04	0.1540	27047.76	27047.76	0.00	0.1540	−3.26	−3.22
(4,2)	27043.35	27043.45	−0.10	0.2345						
(5,3)	27040.77	27040.83	−0.06	0.3007	27043.89	27043.79	0.10	0.3003	−3.12	−2.96
(6,4)	27036.77	27036.84	−0.07	0.3506	27039.79	27039.76	0.03	0.3497	−3.02	−2.92
(7,5)	27031.34	27030.87	0.47	0.3858	27034.25	27033.66	0.59	0.3845	−2.91	−2.79
(3,0)	27024.49	27023.12	1.37	0.0047	27027.26	27025.66	1.60	0.0048	−2.77	−2.54
(4,1)	27263.61	27263.48	0.13	0.0150	27268.36	27268.30	0.06	0.0152	−4.75	−4.82
(5,2)	27259.92	27259.85	0.07	0.0302	27264.57	27264.51	0.06	0.0307	−4.65	−4.66
(6,3)	27254.79	27254.62	0.17	0.0490	27259.17	27259.40	−0.23	0.0498	−4.38	−4.78
(7,4)	27248.39	27248.31	0.08	0.0702	27252.97	27252.78	0.19	0.0712	−4.58	−4.47
(8,5)	27239.05	27240.40	−1.35	0.0924	27243.24	27244.72	−1.48	0.0937	−4.19	−4.32

ν_{obs} = wavenumber of the observed band head (in cm^{-1}), ν_{cal} = wavenumber of the calculated band head (in cm^{-1}), $\Delta\nu$ ($\nu_{obs} - \nu_{cal}$) (in cm^{-1}), $\Delta\nu_{obs}$ = ($\nu_{cal} - \nu_{obs}$) InBr^{81} (in cm^{-1}) and $\Delta\nu_{cal}$ = ($\nu_{cal} - \nu_{obs}$) InBr^{79} (in cm^{-1}).

Table 3. Isotopic shift study of $B^3\Pi_1$–$X^1\Sigma^+$ band system of InBr molecule.

(v', v'')	InBr^{81}				InBr^{79}				Isotopic shift	
	ν_{obs}	ν_{cal}	$\Delta\nu$	FCF	ν_{obs}	ν_{cal}	$\Delta\nu$	FCF	$\Delta\nu_{\text{obs}}$	$\Delta\nu_{\text{cal}}$
(0,2)	26941.31	26941.29	0.02	0.0840	26938.09	26938.03	0.06	0.0832	3.22	3.26
(1,3)	26943.48	26943.54	−0.06	0.1458	26940.27	26940.24	0.03	0.1453	3.21	3.30
(2,4)	26943.82	26943.76	0.06	0.1634	26940.60	26940.71	−0.11	0.1639	3.22	3.05
(3,5)	26942.32	26942.77	−0.45	0.1462	26939.07	26939.00	0.07	0.1478	3.25	3.77
(4,6)	26938.98	26938.88	0.10	0.1111	26935.67	26935.31	0.36	0.1132	3.31	3.57
(5,7)	26933.81	26933.54	0.27	0.0723	26930.40	26930.08	0.32	0.0745	3.41	3.46
(6,8)	26926.80	26926.09	0.71	0.0391	26923.28	26923.12	0.16	0.0410	3.52	2.97
(0,1)	27160.39	27160.58	−0.19	0.2663	27158.77	27158.87	−0.10	0.2659	1.62	1.71
(1,2)	27161.50	27161.29	0.21	0.2633	27159.87	27159.67	0.20	0.2647	1.63	1.62
(2,3)	27160.78	27160.58	0.20	0.1785	27159.14	27159.67	−0.53	0.1810	1.64	0.91
(3,4)	27158.22	27158.14	0.08	0.0932						
(0,0)	27380.52	27380.52	0	0.6174	27380.52	27380.52	0	0.6193	0	0
(1,1)	27380.58	27380.52	0.06	0.1733	27380.57	27380.52	0.05	0.1758	0.01	0
(1,0)	27600.71	27600.64	0.07	0.3281	27602.33	27602.01	0.32	0.3265	−1.62	−1.37
(2,1)	27597.88	27597.64	0.24	0.4296	27599.44	27599.23	0.21	0.4283	−1.56	−1.59
(3,2)	27593.21	27593.15	0.06	0.4198	27594.69	27594.58	0.11	0.4193	−1.48	−1.43
(4,3)	27586.71	27586.73	−0.02	0.3629	27588.07	27588.09	−0.02	0.3632	−1.36	−1.36
(5,4)	27578.37	27578.40	−0.03	0.2929	27579.59	27579.77	−0.18	0.2938	−1.22	−1.37
(6,5)	27568.19	27567.97	0.22	0.2263	27569.25	27569.03	0.22	0.2275	−1.06	−1.06
(7,6)	27556.18	27556.37	−0.19	0.1699	27557.05	27556.07	0.98	0.1712	−0.87	0.30
(8,7)	27542.33	27543.01	−0.68	0.1254	27542.98	27544.02	−1.04	0.1268	−0.65	−1.01

ν_{obs} = wavenumber of the observed band head (in cm^{-1}), ν_{cal} = wavenumber of the calculated band head (in cm^{-1}), $\Delta\nu = (\nu_{\text{obs}} - \nu_{\text{cal}})$ (in cm^{-1}), $\Delta\nu_{\text{obs}} = (\nu_{\text{cal}} - \nu_{\text{obs}})$ InBr^{81} (in cm^{-1}) and $\Delta\nu_{\text{cal}} = (\nu_{\text{cal}} - \nu_{\text{obs}})$ InBr^{79} (in cm^{-1}).

The observed wave number of the bands along with their vibrational assignments are listed in tables 2 and 3. The determined constants are in close agreement with the earlier reported values [3,5,8,10]. The comparison between reported values and present study is given in table 1. The vibrational assignments are also confirmed by the study of bromine isotope effect. The calculated and observed isotopic shifts due to bromine isotope are given in tables 2 and 3. As the spectrum is recorded at apodized resolution of 0.06 cm^{-1}, band head exhibits well-resolved isotope effect. Isotopic shift of band head due to InBr^{81} molecule from those of the slightly more abundant InBr^{79} molecule agrees well with the calculated values. A natural sample of indium monobromide contains 48.37% InBr^{79} and 47.30% InBr^{81}. As a result, the two InBr isotopic species have similar abundance. Therefore, the vibrational bands of these isotopic molecules would be similar in intensities and lie close to each other. The observed features of the spectrum support these facts. This has also been supported by calculating the Franck–Condon factor (FCF) of both the species. The calculated values of FCF are given in tables 2 and 3. The plot of the ground state vibrational frequency (ω_{e}) and $1/r_{\text{e}}\sqrt{\mu}$ for the InF, InCl, InBr and InI molecules [24] is a straight line (figure 12) which shows the accuracy of the determined constants for the InBr molecule. This fact is also in agreement with the criteria suggested by Zavitas [25].

Acknowledgements

References

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