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Rotational analysis of the B→X system of indium monochloride molecule

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Emission spectrum of InCl was photographed in the seventh order of a two metre plane grating spectrograph at a dispersion of 0.5 Å/mm 1,0 0,0 and 0,1 bands of B——X system were resolved and rotational analyses of these bands have been carried out. Results of the analysis are as follows:

$r'_e = 2.342$ Å° $\quad r''_e = 2.405$ Å°

$B'_e = 0.1140$ cm^{-1} $\quad B''_e = 0.1083$ cm^{-1}

$\alpha'_e = 6.4 \times 10^{-4}$ cm^{-1} $\quad \alpha''_e = 5.3 \times 10^{-4}$ cm^{-1}

$D' = 4.5 \times 10^{-8}$ cm^{-1} $\quad D'' = 3.9 \times 10^{-8}$ cm^{-1}

The spectrum of indium monochloride molecule was first reported by Wehrli & Meisher (1934). They observed two band-systems in the region 3500 3800 Å and one system in the region 2500- -2800 A°. They were designated as A——X, B— -X and C - —X respectively. The C— X system was analysed by Froslie & Winans (1947). The ground state of this molecule was studied in microwave aborption by Battet & Mandel (1955) and molscular constants were obtained for the groundstate only. A partial rotational analysis of A——X and B——X systems has also been carried out by Youngner & Winans (1960) In the B——X system only the 0,0 band was attempted: The band was not properly resolved for rotational analysis and hence the rotational assignments were given using the head to origin distance and the second difference between the rotational lines in the resolved region. Since no other band could be resolved in this system, the rotational assignment could not be checked using any common states It was therefore decided to photograph the B——X system of this molecule at higher dispersion and resolution so as to carry out a detailed rotational analysis.

The spectrum of InCl molecule was excited in a high frequency discharge working in the frequency range of 10—15 MHz having an output of 125 watts. Diatomic InCl was formed when the discharge was established in vapours of

pure indium metal in presence of chlorine. The spectrum was photographed in the seventh order of a 2-metre plane grating spectrograph at a dispersion of 0.5 Å°/mm. It was not difficult to maintain the deep blue colour of the discharge for fairly long time. About two hours of exposure was sufficient to get a satisfactory spectrogram on Ilford N-40 plates. Measurements were made on an Abbe comparator against iron arc standards.

The 0,1 0,0 and 1,0 bands were found suitable for carrying out the rotational analysis. Reproduction of the 0,0 band is given in the plate. As is could be seen on the plate, the 0,0 band of B——X system is well resolved up to the origin. At low J values. R branch lines and the returning R branch lines merge together but get resolved at high J values. The structure of 0,1 and 1,0 bands appear similar to the 0,0 band except for the appearance of vibrational isotopic effect. The band heads due to $InCl^{37}$ were weak due to its low abundance.

J numbering of the R branch and a few P branch lines of the 0,0 band was made by observing the origin. The J numbering of Q branch lines and the returning R branch lines were fixed by the combination difference method The J assignments and the analysis of 1,0 and 0,1 bands was carried out by comparing the common states involved in these transitions. α_e and $\Delta G_{1/2}$ for the upper and lower states were calculated graphically and are given in the table.

The ground state of InCl molecule is $^1\Sigma^+$ arising from the configuration $z\sigma^2\ y\sigma^2\ \omega\pi^4\ x\sigma^2$ The exicited state configuration $z\sigma^2\ y\sigma^2\ \omega\pi^4\ x\sigma\ v\pi$ gives two states $^3\pi$ and $^1\pi$. The $^1\pi$—$X^1\Sigma$ transition corresponds to C——X system. $^3\pi$ in InCl is nearer to Hunds case (a) and $^3\pi_0$, $^3\pi_1$ and $^3\pi_2$ states are similar to $^1\Sigma$, $^1\pi$ and $^1\Delta$ states. B——X system corresponds to $^3\pi_1$—$X^1\Sigma$ transition.

Table 1. Results of Rotational analysis for B——X system of $InCl^{35}$

(a)

	Origin cm^{-1}	B′ cm^{-1}	B″ cm^{-1}	10^8 D′ cm^{-1}	10^8 D″ cm^{-1}
0,1	28258.82	0.1142	0.1080	4.5	3.9
0,0	28574.01	0.1143	0.1085	4.6	4.0
1,0	28910.58	0.1137	0.1084	4.4	3.9

(b)

	B_e cm^{-1}	r_e Å	$\Delta G_{1/2}$ cm^{-1}	α_e cm^{-1}
$B^3\pi_1$	0.1140	2.342	338.2	6.4×10^{-4}
$X^1\Sigma$	0.1083	2.405	315.4	5.3×10^{-4}

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