LETTERS TO THE EDITOR

THERMAL EMISSION SPECTRUM OF H → X AND I → X SYSTEMS OF NiBr MOLECULE

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EARLY studies of the band spectrum of nickel monobromide were made by Mesnage[1] and Krishnamurty[2]. Later Reddy and Rao[3], using heavy current discharge, photographed the emission spectrum in the region $\lambda\lambda$ 4700–4050 Å. A few additional bands in the region $\lambda\lambda$ 4525–4060 Å were reported by Sundarachary[4], using the same technique. All the previous workers[1–4] were confronted with a large number of atomic lines due to nickel and superimposition of these atomic lines over bands had in its turn rendered the distinction between bands and lines uncertain. Recently authors[5] obtained some fruitful results while investigating thermal emission spectrum of NiBr in the region $\lambda\lambda$ 5540–4720 Å. This spectrum was free from atomic lines. Therefore it was thought interesting to reinvestigate thermal emission spectrum lying in the region $\lambda\lambda$ 4350–4060 Å.

A small quantity of anhydrous nickel bromide of high purity mixed with spec-pure nickel powder was heated to about 2200° C, using vacuum graphite furnace. The rest of the experimental conditions were the same as described earlier by the authors[5].

Thermal emission spectrum of the NiBr molecule has been photographed for the first time in the region $\lambda\lambda$ 4350–4060 Å. A total of 57 double head and red degraded bands has been recorded out of which 80 heads have been observed for the first time. All these bands have been classified into six sub-systems, *viz.*, $H_1 \rightarrow X_2$, $H_1 \rightarrow X_1$, $H_2 \rightarrow X_2$, $I_1 \rightarrow X_2$, $I_1 \rightarrow X_1$ and $I_2 \rightarrow X_2$ out of which three sub-systems are new ones. A completely revised analyses have been proposed for two fragmentary systems and a partial modification has been made in the case of one system. The vibrational constants derived by the authors for these sub-systems have been enlisted in Table I.

It has been established by the authors[5] that the *ground state of* NiBr *molecule is a* $^2\Delta$ *with* an electronic separation of 533 cm^{-1} and probable electronic transitions responsible for NiBr spectrum are $\Phi^2 - {}^2\Delta$, $^2\Delta - {}^2\Delta$ and $^2\Pi - {}^2\Delta$. In all these sub-systems R heads. have been found to be stronger than the Q heads which is expected in $\Phi^2 - {}^2\Delta$ and $^2\Delta - {}^2\Delta$ transitions. In the absence of any rotational data the excited states of these systems could not be decided unambiguously. The presence of the two pairs of band sub-systems $H_1 \rightarrow X_1$ and $H_1 \rightarrow X_2$ and $I_1 \rightarrow X_1$

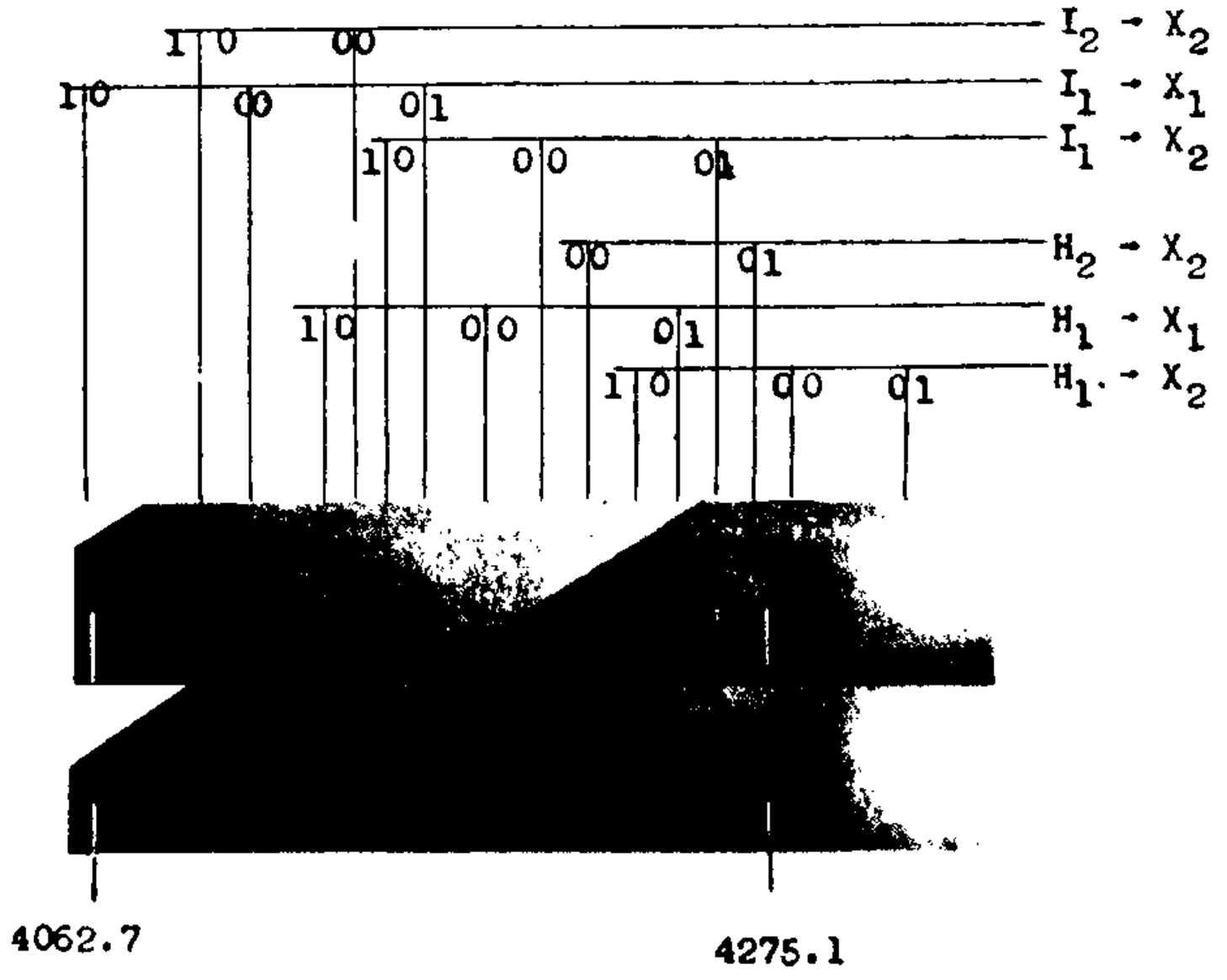

FIG. 1. Thermal emission spectrum of NiBr *molecule*.

TABLE I

Virbational constants for $H \rightarrow X$ and $I \rightarrow X$ systems of NiBr molecule

Sub-systems	$\nu^0_{,}{}^0$ cm^{-1}	ω_e'	$\omega_e' x_e'$	ω_e''	$\omega_e'' x_e''$	No. of bands
$H_1 \rightarrow X_2$*	23369 23361	294·0	2 00	310·0	1·20	13
$H_2 \rightarrow X_2$*	23744 23736	289·0	2·00	310·0	1·20	6
$H_1 \rightarrow X_1$	23905 2389·4	294·0	2·00	322·8	1·10	9
$I_1 \rightarrow X_2$	23791 23786	299 0	2·20	310·5	1·10	9
$I_2 \rightarrow X_2$*	24141 24132	277·0	1·50	310·0	1·20	5
$I_1 \rightarrow X_1$	24321 24313	300·0	2·00	322·4	1·20	15

* New sub-systems.

TABLE II

Band head data for $H \rightarrow X$ system of NiBr molecule

$\nu_{abs.}$	Int.	(v', v'')	$\nu_{abs.}$	Int.	(v', v'')
	$H_1 \rightarrow X_2$		23721	3	1,1 R
23658	4	1,0 R	23712	2	1,1 Q
23651	3	1,0 Q	23696	2	2,2 R
23636	3	2,1 R	23687	1	2,2 Q
23629	2	2,1 Q	23437	3	0,1 R+
23613	2	3,2 R+	23429	2	0,1 Q+
23605	1	3,2 Q	23418	2	1,2 R+
23369	4	0,0 R	23406	1	1,2 Q
23361	3	0,0 Q	23394	1	2,3 R
23351	3	1,1 R	23384	1	2,3 Q
23343	2	1,1 Q			
23333	3	2,2 R		$H_1 \rightarrow X_1$	
23323	2	2,2 Q	24195	3	1,0 R
23310	2	3,3 R	24183	2	1,0 Q
23302	1	3,3 Q	24160	2	2,1 R
23289	1	4,4 R	24150	1	2,1 Q
23280	1	4,4 Q	23905	5	0,0 R+
23061	4	0,1 R	23894	3	0,0 Q
23054	3	0,1 Q	23874	4	1,1 R+
23046	3	1,2 R	23863	2	1,1 Q
23037	2	1,2 Q	23842	3	2,2 R
23030	2	2,3 R	23831	1	2,2 Q
23020	1	2,3 Q	23808	2	3,3 R
23010	2	3,4 R	23796	1	3,3 Q
23003	1	3,4 Q	23584	4	0,1 R+
22991	1	4,5 R	23572	2	0,1 Q
22981	1	4,5 Q	23555	3	1,2 R+
			23546	2	1,2 Q
	$H_2 \rightarrow X_2$		23526	2	2,3 R
23744	4	0,0 R	23513	1	2,3 Q+
23736	3	0,0 Q			

\+ Bands reported by Reddy and Rao[8].

TABLE III

Band head data for $I \rightarrow X$ system of NiBr molecule

$\nu_{abs.}$	Int.	(v', v'')	$\nu_{abs.}$	Int.	(v', v'')
	$I_1 \rightarrow X_2$			$I_1 \rightarrow X_1$	
24086	3	1,0 R	24618	5	1,0 R
24080	2	1,0 Q*	24609	4	1,0 Q+*
24067	2	2,1 R	24590	4	2,1 R
24061	1	2,1 Q	24582	3	2,1 Q+*
24047	1	3 2 R	24559	3	3,2 R+
24041	1	3,2 Q	24552	2	3,2 Q
23791	5	0,0 R	24528	3	4,3 R+
23786	4	0,0 Q+*	24520	2	4,3 Q
23777	4	1,1 R+*	24495	2	5,4 R
23770	3	1,1 Q+*	24488	1	5,4 Q
23760	3	2,2 R*	24462	2	6,5 R
23754	2	2,2 Q	24454	1	6,5 Q
23481	3	0,1 R*	24321	8	0,0 R+*
23476	2	0,1 Q*	42313	6	0,0 Q+*
23471	3	1,2 R+*	24298	6	1,1 R+*
23465	2	1,2 Q+*	24291	4	1,1 Q+*
23457	2	2,3 R+*	24271	4	2,2 R+*
23449	1	2,3 Q+*	24263	3	2,2 Q
			24246	3	3,3 R
	$I_2 \rightarrow X_2$		24235	2	3,3 Q+
24415	4	1,0 R	24215	2	4,4 R
24406	3	1,0 Q	24208	1	4,4 Q
24377	3	2,1 R	24002	5	0,1 R+*
24368	2	2,1 Q	23994	4	0,1 Q+*
24342	2	3,2 R	23978	4	1,2 R+*
24333	1	3,2 Q	23970	3	1,2 Q*
24141	5	0,0 R	23956	3	2,3 R
24132	4	0,0 Q	23949	2	2,3 Q+
24107	3	1,1 R	23931	2	3,4 R
24097	2	1,1 Q	23924	1	3,4 Q

+ Bands reported by Reddy and Rao[3]. * Bands reported by Sundarachary[4].

and $1_1 \rightarrow X_2$ confirms that the electronic interval of 533 cm^{-1} has rightly been attributed to the ground state $^2\Delta$ by the authors[5].

The authors are grateful to Prof. Vachaspati for his keen interest in the work. R. G. expresses his thanks to C.S.I.R., New Delhi, for the award of Post-Doctoral fellowship.

March 9, 1981.

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