PRAMANA
— journal of
physics

Vol. 42, No. 3,
March 1994
pp. 239–243

New band system of YbI molecule

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MS received 19 October 1993; revised 5 February 1994

Abstract. Thermal emission spectrum of YbI molecule has been photographed for the first time in the spectral region $\lambda\lambda$ 6100–6400 Å using Saha's high temperature furnace at a reciprocal linear dispersion of 7·3 Å/mm. A total of 52 single-headed and violet degraded bands have been recorded and are classified into a single system. Vibrational analysis has been carried out and it has been suggested that system arises from the ground state with the vibrational constant $\omega_e'' = 153{\cdot}0\,\text{cm}^{-1}$.

Keywords. Thermal emission spectra; spectra of YbI molecule; vibrational analysis.

PACS No. 33·20

1. Introduction

Electronic spectrum of ytterbium monoiodide was first studied by Kramer [1] in the spectral region $\lambda\lambda$ 4500–6000 Å. He classified the observed single headed and violet degraded bands into two subsystems viz. $A^2\Pi_{1/2}$ and $A^2\Pi_{3/2}$ and reported two values of vibrational frequencies for the ground state ($^2\Sigma$). Lee and Zare [2] identified the presence of a new system in red region of YbF and YbCl molecule. However because of the highly perturbed upper state in both the cases (YbF and YbCl molecules) they could not present any data and vibrational analysis. Since YbF, YbCl and YbI molecules are isovalent molecules, similar band system for the YbI molecule can be reasonably expected. Therefore we examine the spectrum of YbI molecule in red region.

In the present paper we report the first observation of the thermal emission spectrum of YbI molecule in the region $\lambda\lambda$ 6100–6400 Å.

2. Experimental

The complete experimental set-up is described elsewhere [3] but a brief description is given here. A small quantity of spec-pure ytterbium metal (Johnson Matthey, 99·9%) and iodine (Sarabhai, 99·9%) was kept inside the experimental tube of Saha's high temperature furnace [4]. After making necessary routine adjustment and evacuation of the furnace chamber, argon gas was filled at a pressure of about 50 cm of mercury to prevent rapid effusion of molecular vapours from the open ends of the experimental tube. The spectrum has been photographed at 2000°C using first order of 2 meter plane grating spectrograph with a reciprocal linear dispersion 7·3 Å/mm. An exposure time of about three minutes was found sufficient to record the spectra on ORWO/INDU 125 ASA black and white film. Iron d.c. arc spectrum was used for the comparison

standard. The measurements were performed using CZ Abbe Comparator with the least count of 0·0001 cm.

3. Results and discussion

Thermal emission spectrum, attributed to $A'-X$ system of YbI molecule has been photographed for the first time in the spectral region $\lambda\lambda$ 6100–6400 Å and is shown in figure 1. The spectrum is free from atomic lines. A total of 52 single-headed and violet degraded bands have been recorded and classified into a single system viz. $A'-X$. The (0,0) of the system lies at 6309·6 Å. The observed band head data, their estimated relative intensities and classifications are given in table 1.

The equation given below [5] represents the wave numbers for the various observed band heads:

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

with

$$T_e = 15836{\cdot}9 \quad \omega'_e = 168{\cdot}0, \quad \omega'_e x'_e = 1{\cdot}20\,\text{cm}^{-1}$$
$$\omega''_e = 153{\cdot}0, \quad \omega''_e x''_e = 0{\cdot}85\,\text{cm}^{-1}$$

where ν is the wave number of the band head for a given vibrational transition between two electronic states; T_e is the electronic term value or the difference in electronic energy between the emitting and ground or terminal states; ω_e is the vibrational frequency; $\omega_e x_e$ is the anharmonicity; and v is the vibrational quantum number. The single prime denotes the upper state and the double prime denotes the lower state.

The proposed analysis of $A'-X$ system has certain intensity anomalies. This is due to the fact that graphite tube emits strong continuous radiations in red region which is difficult to remove. This gives rise to a different estimate of intensity rather than the actual one.

The earlier work on the YbI molecule by Kramer [1] has established the ground state vibrational frequency for this molecule to be 152·1 cm^{-1}. The proposed analysis of the system $A'-X$ recognized in the thermal emission from YbI molecule reveals the vibrational frequency of the lower state as 153·0 cm^{-1}. Thus the emitter of the new bands can be identified to be diatomic YbI. In addition no bands of Yb_2 and I_2 molecules are known in thermal emission in this region. All these considerations, therefore, confirm that bands can be rightly attributed to the YbI molecule.

The vibrational constants for the ground state of YbI molecule by us and those by Kramer [1] are compared in the following:

Kramer		Present authors	
$\omega''_e = 157{\cdot}9 \pm 3{\cdot}6$,	$\omega''_e x''_e = 1{\cdot}36 \pm 1{\cdot}24$,	$\omega''_e = 153{\cdot}0$	$\omega''_e x''_e = 0{\cdot}85\,\text{cm}^{-1}$
$\omega''_e = 152{\cdot}1 \pm 0{\cdot}7$,	$\omega''_e x''_e = 0{\cdot}34 \pm 0{\cdot}04$.		

The difference in the molecular constants is because Kramer [1] has reported two values of vibrational frequencies for the ground state $^2\Sigma$ while a $^2\Sigma$ should have single vibrational frequency. The value obtained by us for $\omega''_e = 153{\cdot}0\,\text{cm}^{-1}$ is very near to one of the values of $\omega''_e = 152{\cdot}1\,\text{cm}^{-1}$ reported by Kramer [1].

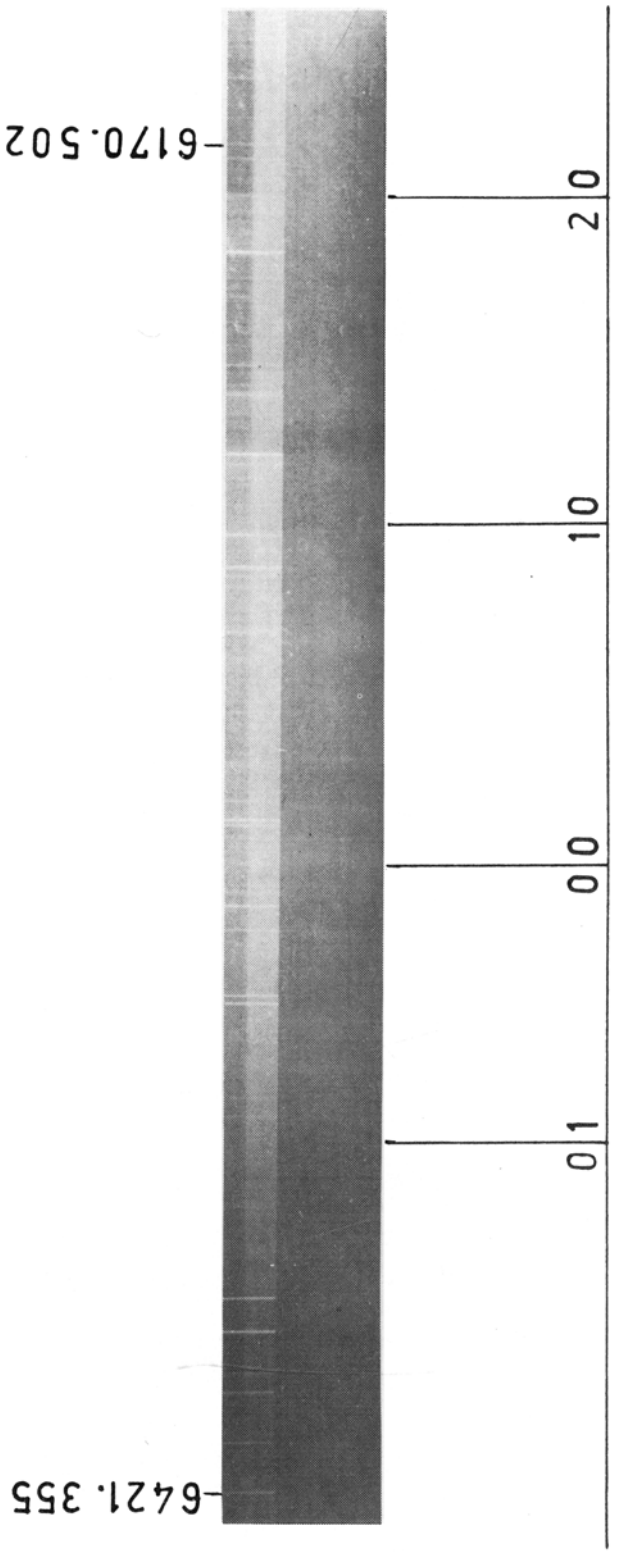

Figure 1. Thermal emission spectrum of YbI molecule at a reciprocal linear dispersion of 7·3 Å/mm.

Table 1. Band head data of YbI molecule: $A'-X$ system.

ν_{obs} (cm^{-1})	$\Delta\nu$ (cm^{-1})	Int	Analysis (v', v'')	ν_{obs} (cm^{-1})	$\Delta\nu$ (cm^{-1})	Int.	Analysis (v', v'')
15693·9	0·9	3	(0, 1)	15980·4	−0·4	2	(14, 14)
15710·5	1·5	3	(1, 2)	15984·7	−0·6	2	(15, 15)
15724·6	0·3	2	(2, 3)	16010·6	0·7	3	(1, 0)
15737·1	−1·1	2	(3, 4)	16021·7	−0·1	3	(2, 1)
15753·1	0·3	3	(4, 5)	16032·8	−0·2	3	(3, 2)
15765·0	−1·0	2	(5, 6)	16045·3	1·8	4	(4, 3)
15778·5	0	2	(6, 7)	16052·8	−0·5	2	(5, 4)
15790·0	−0·3	4	(7, 8)	16062·2	−0·2	5	(6, 5)
15802·7	1·3	4	(8, 9)	16069·9	−0·9	4	(7, 6)
15810·8	−1·1	4	(9, 10)	16077·8	−0·7	3	(8, 7)
15822·1	0·6	5	(10, 11)	16086·8	1·3	3	(9, 8)
15831·8	1·3	5	(11, 12)	16092·2	0·4	2	(10,9)
15844·3	0	6	(0, 0)	16096·5	−0·9	2	(11, 10)
15858·4	−0·2	4	(1, 1)	16101·7	−0·6	2	(12, 11)
15871·6	−0·6	4	(2, 2)	16105·3	−1·2	2	(13, 12)
15884·2	−0·9	4	(3, 3)	16109·8	−0·2	2	(14, 13)
15896·2	−1·1	4	(4, 4)	16113·9	1·1	2	(15, 14)
15909·3	0·5	3	(5, 5)	16174·4	1·3	2	(2, 0)
15918·9	−0·7	3	(6, 6)	16181·3	−1·3	2	(3, 1)
15928·9	−0·8	3	(7, 7)	16192·3	0·9	2	(4, 2)
15939·5	0·4	3	(8, 8)	16201·2	1·7	2	(5, 3)
15948·0	0·2	3	(9, 9)	16207·2	0·3	2	(6, 4)
15954·9	−0·9	3	(10, 10)	16213·3	−0·3	2	(7, 5)
15962·1	−1·0	3	(11, 11)	16218·1	−1·5	1	(8, 6)
15970·3	0·6	3	(12, 12)	16225·1	0·2	1	(9, 7)
15977·1	1·5	2	(13, 13)	16228·3	−1·2	1	(10,8)

$\Delta\nu = \nu_{obs} - \nu_{cal}$

The electronic configuration of ytterbium and iodine atoms are:

$$_{70}\text{Yb} = 1s^2, 2s^2 2p^6, 3s^2 3p^6 3d^{10}, 4s^2 4p^6 4d^{10} 4f^{14}, 5s^2 5p^6, 6s^2 — {}^1S$$

$$_{53}\text{I} = 1s^2, 2s^2 2p^6, 3s^2 3p^6 3d^{10}, 4s^2 4p^6 4d^{10}, 5s^2 5p^5 — {}^2P.$$

Consider the separated atom model, we have Yb with ^1S and chlorine with ^2P as their ground states. Combination of these two atomic states gives rise to $^2\Pi$ and $^2\Sigma$ electronic states. It is well established [2, 3] that ground state for YbF and YbCl molecule is to be $^2\Sigma$. Since YbF, YbCl and YbI molecules are isoelectronic molecule, we expect YbI to have the same ground state as YbF and YbCl molecules. If $^2\Sigma$ is the ground state of YbI molecule, the optically accessible transitions are $^2\Sigma$–$^2\Sigma$ and $^2\Pi$–$^2\Sigma$. Further the observed bands of the $A'-X$ system are single headed therefore this system involves $^2\Sigma$–$^2\Sigma$ transition.

Acknowledgement

One of the authors (KNU) is thankful to CSIR, New Delhi for the financial assistance.

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