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Estimation of Rotational Temperature of the 1-1 Band of $B^2\Sigma^+$ - $X^2\Sigma^+$ System of AlO Molecule

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ABSTRACT

The $B^2\Sigma^+$ - $X\ ^2\Sigma^+$ transition of AlO molecule was recorded on BOMEM DA8 Fourier Transform Spectrometer at a resolution of 0.05 cm^{-1}. The intensities of well-resolved rotational lines of R_1 and R_2 of (1-1) band of the $B\ ^2\Sigma^+$ - $X\ ^2\Sigma^+$ transition of AlO molecule were measured. The average rotational temperature estimated from these lines is 1925 K.

Keywords: Intensity measurement, Rotational temperature, AlO molecule.

I. INTRODUCTION

The vibrational and rotational temperature derived from the band spectra are of importance in spectroscopy, chemical physics, thermodynamics etc. Since AlO has astrophysical significance, spectroscopic temperature of AlO molecules is of interest [1-12]. Mentall & Nicholls [13] derived the vibrational temperature of AlO using laser produced plasma. Recently Dores, et al [14] also determined the vibrational temperature using laser ablation technique. They used the 266 nm radiation from a Nd: YAG laser and the alumina Al_2O_3 as a target. Chaudhari, et al [15] also determine rotational temperature using dc arc discharge. They use dc arc in air running between two aluminium electrodes of about 1 cm in diameter and tapered towards tips. The arc current was 3 A at 110 V. The $B^2\Sigma^+$ - $X^2\Sigma^+$ system of AlO was photographed in the first order of a 10.6 m concave grating spectrograph. Recently Behere and et al [16] and Londhe et al[17] determined rotational temperature of 0-1 and (1-0) band of the $B\ ^2\Sigma^+$ - $X\ ^2\Sigma^+$ transition of AlO molecule measured using microwave discharge method.

In present study the rotational temperature of AlO is estimated by exciting the molecule in the microwave.

II. EXPERIMENTAL

The AlO molecule was excited using a microwave discharge. A narrow quartz tube of 0.8 cm diameter was found optimum. Aluminium trichloride vapors along with oxygen and argon gases were allowed to flow in the tube. A small quartz boat containing $AlCl_3$ was sealed in a side tube. A moderate heating of $AlCl_3$ sample and flowing argon at a pressure of 10 torr gave a blue green glow when a microwave power (2450 MHz, 150 watt) power was applied to a discharge tube.

In order to stop the possibility of $AlCl_3$ vapors going to pump oil, a liquid nitrogen trap was connected between the discharge tube and the rotary pump. The gas pressures were so optimized as to give very intense characteristic glow of AlO [18]. A spherical lens was used to focus the emission signal into the interferometer. The spectra in the region 18000 – 22000 cm^{-1} were recorded with BOMEM DA8 Fourier transform spectrometer with an apodized resolution of 0.05 cm^{-1} using quartz UV beam splitter and silicon detector. The emission signal being strong no filter was required. Fifty scans (integration time ~75 min.) were co added to obtain an improved signal-to-noise ratio [17]. The prints of the traces of (1,1) bands are shown in Fig. 1. The areas of the profiles of the rotational lines were measured with the help of a digital plannimeter with an accuracy of 10^{-2} cm^2 and more. Intensity measurement of rotational lines of (1,1) band shown in table 1. To avoid the congregation of point's graph of R_1 and R_2 lines for each band is shown separately in Fig. 2 and Fig. 3 respectively. From the slope of each graph the rotational temperature is calculated. Average intensity of each line was employed to calculate the rotational temperature and results are summarized in table 2.

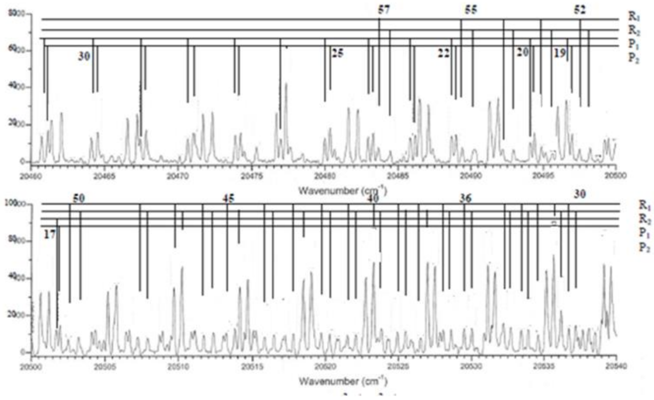

Fig. 1: Rotational fine structure of (1,1) band of $B^2\Sigma^+$-$X^2\Sigma^+$ transition of AlO molecule

Table 1: Intensity measurements of the rotational lines of (1,1) band of $B^2\Sigma^+$-$X^2\Sigma^+$ System of AlO molecule

	R_1 Branch					R_2 Branch			
K	K+1	I_{em}	ln [Iem/K+1]	Bv' (K+1)* (K+2)	K	K+1	I_{em}	ln [I_{em}/K+1]	Bv' (K+1)* (K+2)
61	62	0.5	-4.82028	2341.491	61	62	0.5	-4.82028	2341.491
60	61	0.4	-5.02716	2267.158	60	61	0.5	-4.80402	2267.158
59	60	0.4	-5.01064	2194.024	59	60	0.5	-4.78749	2194.024
58	59	0.5	-4.77068	2122.088	58	59	0.5	-4.77068	2122.088
57	58	0.5	-4.75359	2051.352	57	58	0.6	-4.57127	2051.352
56	57	0.5	-4.7362	1981.815	56	57	0.7	-4.39973	1981.815
55	56	0.5	-4.7185	1913.476	55	56	0.7	-4.38203	1913.476
54	55	0.5	-4.70048	1846.337	54	55	0.8	-4.23048	1846.337
53	54	0.5	-4.68213	1780.396	53	54	0.7	-4.34566	1780.396
52	53	0.7	-4.32697	1715.655	52	53	0.7	-4.32697	1715.655
51	52	0.6	-4.46207	1652.112	51	52	0.8	-4.17439	1652.112
50	51	0.7	-4.2885	1589.768	50	51	0.8	-4.15497	1589.768
49	50	0.8	-4.13517	1528.623	49	50	0.75	-4.19971	1528.623
48	49	0.8	-4.11496	1468.677	48	49	0.8	-4.11496	1468.677
47	48	0.8	-4.09434	1409.93	47	48	0.9	-3.97656	1409.93

46	47	0.9	-3.95551	1352.382	46	47	0.9	-3.95551	1352.382
45	46	0.8	-4.05178	1296.033	45	46	1	-3.82864	1296.033
44	45	0.9	-3.91202	1240.882	44	45	0.8	-4.02981	1240.882
43	44	1.1	-3.68888	1186.931	43	44	0.7	-4.14086	1186.931
42	43	1	-3.7612	1134.178	42	43	0.8	-3.98434	1134.178

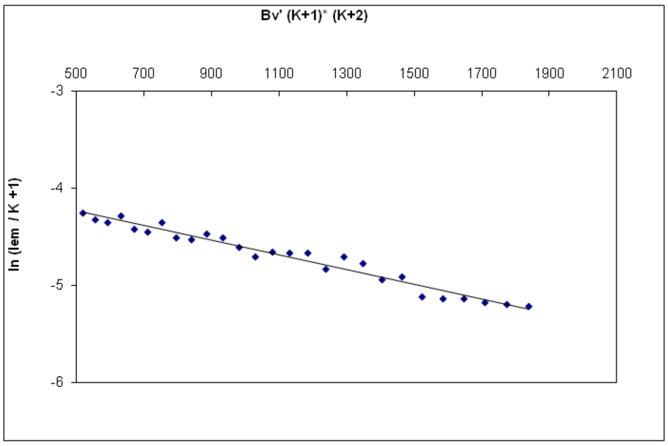

Fig. 2 Plot of R_1 branch $\ln(I_{em}/ K+1)$ vs $B_{v'}$ (K+1)*(K'+1) of (1,1) band of the $B^2\Sigma^+$-$X^2\Sigma^+$ system of AlO molecule

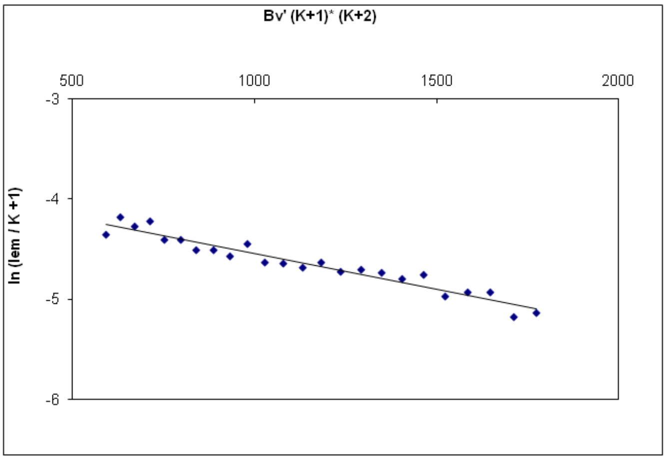

Fig. 3 Plot of R_2 branch $\ln(I_{em}/ K+1)$ vs $B_{v'}$ (K+1)*(K'+1) of (1,1) band of the $B^2\Sigma^+$-$X^2\Sigma^+$ system of AlO molecule

Table 2: The average rotational temperature of of (1,1) band of the $B^2\Sigma^+$-$X^2\Sigma^+$ system of AlO molecule

Band	B′v	Branch	Slope x10^{-4}	Rot. Temp.
(1,1) Band	0.59721	R1	7.97	1805
		R2	7.03	2045
			Mean	1925

III. CALCULATIONS OF ROTATIONAL TEMPERATURE

Assuming the Maxwell Boltzmann distribution valid, the intensity of the rotational line can be given by the expression,

$I_{J' J''} = C\, S_{J' J''} \exp\,[-F_{v'}(J') / k\, T_{rot}]$ … (1)

Where J' and J" are the rotational quantum numbers of the upper and lower energy states. C is a constant and $S_{J' J''}$ is a HÖnl London factor [19]. $F_{v'}(J')$ is the rotational energy in cm^{-1} for dimensionless factor of the exponential $F_{v'}(J')$ is to be multiplied by hc T_{rot} is the rotational temperature and k is Boltzmann constant. For $^2\Sigma$ - $^2\Sigma$ transition J is replaced by K. The slope of the graph between ln $I_{K' K''}/ S_{K' K''}$ against $F_{v'}$ (K') is – $B_{v'}hc / kT_{rot}$.

In present work the R branch lines are chosen for intensity measurements, especially those which are free from overlap. The B-X system is a $^2\Sigma$- $^2\Sigma$ transition and so two P branches and two R branches are expected. Due to higher resolution it was possible to resolve the R_1 and R_2 components. The HÖnl London factor for $^2\Sigma$ - $^2\Sigma$ transition is given by the equation,

$S_J^R = (J''+1+ \Lambda'') (J''+1- \Lambda'')/ J'' +1 = (J'+ \Lambda') (J'+ \Lambda')/J' = J'$ … (2)

For R branch lines J' = J+1 i.e. (K+1) and J"=J i.e. K

Thus a graph of ln($I_{J' J''}$/ J") vs $B_{v'}$ J'(J'+1) gives a slope –hc/ kT_{rot}. knowing all other quantities T_{rot} can be calculated.

Here, J' = K+1 and J" = K, then on ordinate axis ln (I_K/ K) is taken and on abscissa axis $B_{v'}$ (K+1)(K+2) is plotted. The expression for T_{rot} is T_{rot} = (hc / k)(1/slope) = 1.439/ slope … (3)

IV. RESULTS AND DISCUSSION

The vibrational temperature of AlO reported by Mentall and Nicholls [13] is 3600 ± 400 K where they have used Laser produced plasma as an excitation source. A Ruby laser having output power of 2.5 J with pulse duration of the order of 500 μ sec was employed. The spectrum was recorded on a Bausch & Lamb 1.5 m spectrograph having a reciprocal dispersion 15A^0mm^{-1}. A rotational temperature of AlO reported by Dors et al [14] is 3384 K. They used the laser ablation technique using a 266 nm lines from Nd: YAG laser. The spectrograph was 0.275 m Jarell Ash equipment fitted with Optical Multichannel Analyser (OMA). The rotational temperature of AlO using the arc source has yielded T_{rot} as 2880 ± 100 K, reported by Chaudhari et al which is lower, compared to that of Mentall and also of Dors et al. The rotational temperature of 0-1 band of the B $^2\Sigma^+$ - X $^2\Sigma^+$ system of AlO molecule measured using microwave discharge has shown still lower T_{rot}, which is 1925 K which is agreement with Behere et al [16]. and Londhe et al [17].

V. ACKNOWLEDGEMENT

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