Rotational Temperature of AlO Molecule from Fourier Transform Spectrum of the 0-1 band of B²Σ⁺ - X²Σ⁺ System

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Abstract: Rotational structure of (0-1) bands of the B²Σ⁺ - X²Σ⁺ system of AlO molecule was recorded on Fourier Transform Spectrometer. Intensity distribution among the well-resolved rotational lines of R1 and R2 for each band was recorded and average rotational temperature calculated from these lines which is 1813 K.

1. Introduction
The vibrational and rotational temperature derived from the band spectra are of importance in spectroscopy, chemical physics, thermodynamics etc. The blue–green system, B²Σ⁺ - X²Σ⁺ transition, of AlO has been known for over 100 years and extensively studied both experimentally and theoretically [1–12]. The astrophysical importance of AlO and its aeronomical significance is well known [13–17]. The existence of AlO molecule in cool stellar atmospheres has been shown through the identification of B–X system in spectrum of some normal Mira giants and Mira variables [13, 17]. In stars of lower temperature the absorption of the head of 0–0 band of the B–X system strengthens. The strengthening of AlO (λ = 4842Å) intensity, in these stars is quite variable from cycle to cycle. In normal Mira giants because of higher temperature the band is seen in emission. In Mira variables the AlO absorption is greater than in normal giants and the maximum intensities far exceed those obtained in the normal M giants. Spectroscopic temperature of AlO molecules is of interest. Mentall & Nicholls [18] derived the vibrational temperature of AlO using laser produced plasma. Dores, et al [19] determined the vibrational temperature using laser ablation technique. They used the 266 nm radiation from a Nd: YAG laser and the alumina Al₂O₃ as a target. Recently Chaudhari, et al [20] 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 B²Σ⁺ - X²Σ⁺ system of AlO was photographed in the first order of a 10.6 m concave spectrograph. In present study the rotational temperature of AlO is determined by exciting the molecule in the microwave discharge.
2. **Experimental**
The spectrum of AlO was excited in a microwave discharge (2450 MHz, 180 W) through a flowing mixture of AlCl$_3$ vapours, buffer gas argon and a small amount of oxygen. The AlCl$_3$ kept in a small quartz boat of side arm of a discharge tube was heated by an electrical furnace and vapours, along with argon and oxygen, were let in the discharge zone. 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 [21]. 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. The prints of the traces of (0,1) bands are shown in Figure 1. The areas of the profiles of the rotational lines were measured with the help of a digital planimeter with an accuracy of $10^{-2}$ cm$^2$ and more. Intensity measurement of rotational lines of (0,1) 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 Figure 2 and Figure 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.

![Figure 1. Rotational fine structure of (0,1) band of B$^2\Sigma^+$-X$^2\Sigma^+$ transition of AlO](image1)

![Figure 2. Plot of $R_1$ branch ln(I$_{em}$ / K+1) vs $B_v(K+1)^*(K'+1)$ of (0,1) band of the B$^2\Sigma^+$-X$^2\Sigma^+$ system of AlO molecule](image2)
Figure 3. Plot of $R_2$ branch $\ln(I_{em}/K+1)$ vs $B_{v'}(K+1)^*(K'+1)$ of (0,1) band of the $B^2\Sigma^+-X^2\Sigma^+$ system of AlO molecule.

Table 1: Intensity measurements of the rotational lines of (0,1) band of $B^2\Sigma^+-X^2\Sigma^+$ System of AlO molecule

| $K$ | $K+1$ | $I_{em}$ | $\ln[I_{em}/K+1]$ | $B_{v'}(K+1)^*(K+2)$ | $K$ | $K+1$ | $I_{em}$ | $\ln[I_{em}/K+1]$ | $B_{v'}(K+1)^*(K+2)$ |
|-----|-------|---------|-------------------|----------------------|-----|-------|---------|-------------------|----------------------|
| 54  | 55    | 0.3     | -5.21131          | 1839.407             | 55  | 56    | 0.3     | -5.22932          | 1906.294             |
| 53  | 54    | 0.3     | -5.19296          | 1773.714             | 55  | 55    | 0.9     | -4.11269          | 1839.407             |
| 52  | 53    | 0.3     | -5.17426          | 1709.215             | 54  | 54    | 0.2     | -5.59842          | 1773.714             |
| 51  | 52    | 0.1     | -6.25383          | 1645.911             | 52  | 53    | 0.3     | -5.17426          | 1709.215             |
| 50  | 51    | 0.3     | -5.1358           | 1583.801             | 51  | 52    | 0.4     | -4.86753          | 1645.911             |
| 49  | 50    | 0.3     | -5.116            | 1522.886             | 50  | 51    | 0.3     | -5.1358           | 1583.801             |
| 48  | 49    | 1.2     | -3.7095           | 1463.165             | 49  | 50    | 0.2     | -5.52146          | 1522.886             |
| 47  | 48    | 0.3     | -5.07517          | 1404.638             | 48  | 49    | 0.9     | -3.99718          | 1463.165             |
| 46  | 47    | 1.1     | -3.75484          | 1347.306             | 47  | 48    | 0.4     | -4.78749          | 1404.638             |
| 45  | 46    | 0.3     | -5.03261          | 1291.168             | 46  | 47    | 0.3     | -5.05412          | 1347.306             |
| 44  | 45    | 0.3     | -5.01064          | 1236.225             | 45  | 46    | 0.3     | -5.03261          | 1291.168             |
| 43  | 44    | 0.3     | -4.98816          | 1182.476             | 44  | 45    | 0.4     | -4.72295          | 1236.225             |
| 42  | 43    | 0.9     | -3.86656          | 1129.921             | 43  | 44    | 0.5     | -4.47734          | 1182.476             |
| 41  | 42    | 0.4     | -4.65396          | 1078.561             | 42  | 43    | 0.4     | -4.67749          | 1129.921             |
| 40  | 41    | 0.2     | -5.32301          | 1028.396             | 41  | 42    | 0.3     | -4.94164          | 1078.561             |
| 39  | 40    | 0.4     | -4.60517          | 979.4244             | 40  | 41    | 0.4     | -4.62986          | 1028.396             |
| 38  | 39    | 0.3     | -4.86753          | 931.6476             | 39  | 40    | 0.9     | -3.79424          | 979.4244             |
| 37  | 38    | 1.1     | -3.54228          | 885.0652             | 38  | 39    | 0.3     | -4.86753          | 931.6476             |
| 36  | 37    | 0.4     | -4.52721          | 839.6773             | 37  | 38    | 0.2     | -5.24702          | 885.0652             |
| 35  | 36    | 0.3     | -4.78749          | 795.4837             | 36  | 37    | 0.3     | -4.81489          | 839.6773             |
| 34  | 35    | 1       | -3.55535          | 752.4846             | 35  | 36    | 0.4     | -4.49981          | 795.4837             |
| 33  | 34    | 0.4     | -4.44265          | 710.6799             | 34  | 35    | 0.4     | -4.47164          | 752.4846             |
| 32  | 33    | 0.4     | -4.4128           | 670.0696             | 33  | 34    | 0.5     | -4.21951          | 710.6799             |
| 31  | 32    | 0.7     | -3.82241          | 630.6538             | 32  | 33    | 0.4     | -4.4128           | 670.0696             |
| 30  | 31    | 0.4     | -4.35028          | 592.4323             | 31  | 32    | 0.5     | -4.15888          | 630.6538             |
| 29  | 30    | 0.4     | -4.31749          | 555.4053             | 30  | 31    | 0.4     | -4.35028          | 592.4323             |
**Table 2: Rotational temperature of AlO molecule**

| Band      | B’v     | Branch | Slope x10^{-4} | Rot. Temp. |
|-----------|---------|--------|---------------|------------|
| (0,1) Band| 0.59946 | R1     | 7.91          | 1819       |
|           |         | R2     | 7.96          | 1807       |
| Mean      |         |        |               | 1813       |

3. **Calculations of rotational temperature**

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

\[ I_{J'} = C S_{J'} \exp \left\{ -F_{v'}(J') / k T_{\text{rot}} \right\} \]

Where \( J' \) and \( J'' \) are the rotational quantum numbers of the upper and lower energy states. \( C \) is a constant and \( S_{J'} \) is a HÖnl London factor [22]. \( F_{v'}(J') \) is the rotational energy in cm\(^{-1}\) for dimensionless factor of the exponential \( F_{v'}(J') \) is to be multiplied by \( \hbar c T_{\text{rot}} \) 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 \( \ln \left( I_{J'} / S_{J'} \right) \) against \( F_{v'}(K') \) is \(-\hbar c / kT_{\text{rot}}\).

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,

\[ S_{J}^R = (J''+1+ \Lambda'') (J''+1- \Lambda'') / J'' +1 = (J+ \Lambda) (J'+ \Lambda) / J' = J' \]

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

Thus a graph of \( \ln(I_{J'}) / J' \) vs \( B_{v'} J(J'+1) \) gives a slope \(-\hbar c / kT_{\text{rot}}\). knowing all other quantities \( T_{\text{rot}} \) 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 \( T_{\text{rot}} \) is

\[ T_{\text{rot}} = \left( \hbar c / k \right)(1/slope) = 1.439/ \text{slope} \]

4. **Results and discussion**

The vibrational temperature of AlO reported by Mentall and Nicholls [18] is 3600 ± 400 K where they have used Laser produced plasma as an excitation source. A Ruby laser having out put 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/mm\(^{-1}\). A rotational temperature of AlO reported by Dors et al [19] 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 \( T_{\text{rot}} \) 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 \( T_{\text{rot}} \), which is 1813 K which is agreement with Behere and et al [23].

5. **Conclusions**

Rotational Temperature of (0-1) band of the B \( ^2\Sigma^+ - X ^2\Sigma^+ \) system of AlO molecule has been calculated from well-resolved rotational lines of R\(_1\) and R\(_2\) and the average rotational temperature calculated from these lines which is 1813 K.
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