

Some vibrational bands of B-X system of AlO molecule in the sunspot spectra

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Abstract. Vibrational transition probabilities, namely Franck-Condon factors and \bar{r} -centroids, have been evaluated using an approximate analytical method for the B-X system of AlO molecule. RKR potential energy curves for $X^2\Sigma^+$ and $B^2\Sigma^+$ states of AlO have been constructed using the latest spectroscopic data. The value of \bar{r} -centroids for the band have been found to increase linearly with the corresponding wavelengths. The sequence differences $\Delta\bar{r}$ remain approximately constant for the \bar{r} -centroids.

Key words : AlO molecule—vibrational bands—sunspot spectra

1. Introduction

When one tries to estimate the physical conditions (*i.e.* temperature, pressure, density, and abundance) of the emitter from the relative intensities of the bands of a molecule, one must have a theoretical knowledge of the corresponding potential energy curves, \bar{r} -centroids, and the vibrational transition probabilities (FCFs) for the respective bandheads in a band system. The (0, 0), (0, 1) and (1, 0) bands of A-X system of the AlO have been found in the umbral spectrum (Bobcock 1945; Stenvinkel, Svensson & Olsson 1938) and in M-type stellar spectra, such as those of Betelgeuse, β Pegasi, R Leonis and O Ceti (Davis 1947). The Morse FCFs and \bar{r} -centroids of C-X system of the AlO have been evaluated by Singh (1972), and PRK, FCFs (for blue and UV transition) by Liszt & Smith (1972).

We analyse here vibrational FCFs, \bar{r} -centroids and RKR potential energy curves of $X^2\Sigma^+$ and $B^2\Sigma^+$ states of the AlO molecule using the experimental data available in literature (Jevons 1963).

2. Calculations

2.1. Franck-Condon factors

The relative intensities of the vibrational bands within a band system of a diatomic molecule are controlled mainly by the population distribution over the vibrational levels and by the Franck-Condon factor ($q_{v',v''}$) defined as

$$q_{v',v''} = \left| \int \psi_{v'} \psi_{v''} dr \right|^2,$$

where v' and v'' are the vibrational quantum numbers of the upper and lower electronic states respectively; $\psi_{v'}$ and $\psi_{v''}$ are the vibrational eigenfunctions; and r is the internuclear distance. The derived molecular constants α , K and ρ have been calculated by using molecular constants μ , T_e , w_e , $w_e x_e$, B_e , α_e and r_e of Huber & Herzberg (1979) and equations given by Fraser & Jarman (1953). These results are listed in table 3. FCFs have been calculated for a Morse (1929) model by using Fraser & Jarman (1953) method and experimental data of Jevons (1963) (table 4).

The applicability of the Morse potential for the states involved in the transition has been tested by computing the classical turning points for the various vibrational levels, using the expression given by RKR method as modified by Lakshman & Rao (1971) and comparing the levels with the values obtained from the Morse potential. These values are listed in tables 1 and 2 which show that the states $X^2\Sigma^+$ and $B^2\Sigma^+$ obey the Morse potential.

2.2. \bar{r} -centroids

The \bar{r} -centroids, $\bar{r}_{v',v''}$ representing the characteristic internuclear separation corresponding to (v' , v'') transition in a diatomic molecular band system have been defined by Nicholls & Jarman (1956) by the relation

$$\bar{r}_{v',v''} = \frac{\int \psi_{v'} r \psi_{v''} dr}{\int \psi_{v'} \psi_{v''} dr},$$

where r is the internuclear separation.

Table 1. Values of turning points, centres and half-widths in Å for the $B^2\Sigma^+$ state of AlO molecule

Vibrational quantum number v	Rydberg-Klein-Rees-Vanderstice				Morse			
	r_{\min}	r_{\max}	Centre	Halfwidth	r_{\min}	r_{\max}	Centre	Half-width
0	1.6082	1.7326	1.6704	0.0622	1.6076	1.7320	1.6698	0.0622
1	1.5687	1.7850	1.6769	0.1082	1.5673	1.7836	1.6755	0.1082
2	1.5433	1.8235	1.6834	0.1401	1.5410	1.8212	1.6811	0.1401
3	1.5237	1.8563	1.6900	0.1663	1.5205	1.8532	1.6869	0.1664
4	1.5074	1.8859	1.6967	0.1893	1.5034	1.8819	1.6927	0.1893
5	1.4933	1.9133	1.7033	0.2100	1.4885	1.9084	1.6985	0.2100
6	1.4810	1.9391	1.7101	0.2191	1.4753	1.9334	1.7044	0.2291
7	1.4699	1.9638	1.7169	0.2470	1.4633	1.9572	1.7103	0.2470
8	1.4518	2.0075	1.7297	0.2779	1.4524	1.9800	1.7162	0.2638
9	1.4507	2.0105	1.7306	0.2799	1.4423	2.0021	1.7222	0.2799
10	1.4422	2.0329	1.7376	0.2954	1.4330	2.0236	1.7283	0.2953

Table 2. Values of turning points, centres and half-widths in Å for the $X^2\Sigma^+$ state of AlO molecule

Vibrational quantum number v	Rydberg-Klein-Rees-Vanderstice				Morse			
	r_{\min}	r_{\max}	Centre	Halfwidth	r_{\min}	r_{\max}	Centre	Half-width
0	1.5628	1.6803	1.6216	0.0588	1.5627	1.6801	1.6214	0.0587
1	1.5263	1.7309	1.6286	0.1023	1.5262	1.7308	1.6285	0.1023
2	1.5028	1.7687	1.6358	0.1330	1.5028	1.7686	1.6357	0.1329
3	1.4848	1.8013	1.6431	0.1583	1.4847	1.8012	1.6430	0.1583
4	1.4698	1.8309	1.6504	0.1806	1.4698	1.8310	1.6504	0.1806
5	1.4569	1.8587	1.6578	0.2009	1.4570	1.8588	1.6579	0.2009
6	1.4456	1.8852	1.6654	0.2198	1.4458	1.8853	1.6656	0.2198
7	1.4353	1.9106	1.6730	0.2377	1.4357	1.9109	1.6733	0.2376
8	1.4261	1.9354	1.6808	0.2547	1.4265	1.9358	1.6812	0.2547
9	1.4175	1.9596	1.6886	0.2711	1.4182	1.9602	1.6892	0.2710
10	1.4097	1.9834	1.6966	0.2869	1.4105	1.9841	1.6973	0.2868

Table 3. Basic and derived molecular constants for $B-X$ system of the AlO molecule, $\mu=10.04195071$

State	From Huber & Herzberg (1979)				Derived molecular constant			
	T_e (cm^{-1})	w_e (cm^{-1})	$w_e x_e$ (cm^{-1})	B_e (cm^{-1})	r_e Å	α (Å^{-1})	K	ρ
$B^2\Sigma^+$	20688.95	870.05	3.52	0.60408	1.6670	1.44790	247.17330	1.0165948
$X^2\Sigma^+$	0	979.23	6.97	0.64136	1.6179	2.03744	140.49211	0.9839383

Table 4. Franck-Condon factors, \bar{r} -centroids, wavelengths and band origin for $B-X$ system of AlO molecule

Bands	Franck-Condon factors	\bar{r} -centroids (Å)	Wavelengths with visual estimates of intensity (Å)	Band origin (cm^{-1})
(0, 0)	0.7230	1.6465	4842.1 (10)	20635.252
(0, 1)	0.2892	1.7263	5079.3 (4)	19669.962
(0, 2)	0.0723	1.8123	5336.9 (1)	18718.612
(1, 0)	0.5784	1.5752	4648.2 (8)	21498.262
(1, 1)	0.6507	1.6578	4866.1 (9)	20532.972
(1, 2)	0.3615	1.7371	5102.1 (5)	19581.622
(1, 3)	0.1446	1.8239	5358.1 (2)	18644.212
(2, 0)	0.1446	1.5093	4470.5 (2)	22354.232
(2, 1)	0.5784	1.5832	4672.0 (8)	21388.942
(2, 2)	0.4338	1.6717	4888.4 (6)	20437.592
(2, 3)	0.3615	1.7483	5123.3 (5)	19500.182
(2, 4)	0.1446	1.8357	5377.4 (2)	18576.713
(3, 1)	0.2169	1.5172	4494.0 (3)	22237.872
(3, 2)	0.5061	1.5908	4694.6 (7)	21286.522
(3, 4)	0.2892	1.7598	5142.9 (4)	19425.642
(3, 5)	0.2169	1.8477	5394.8 (3)	18516.112
(4, 2)	0.2892	1.5247	4516.3 (4)	22128.412
(4, 3)	0.4338	1.5983	4715.5 (6)	21191.002
(4, 5)	0.2169	1.7720	5160.8 (3)	19358.002
(4, 6)	0.2169	1.8598	5410.5 (3)	18462.412
(5, 3)	0.2892	1.5318	4537.6 (4)	22025.852
(5, 4)	0.4338	1.6055	4735.5 (6)	21102.382
(5, 7)	0.1446	1.8721	5424.3 (2)	18415.612
(6, 3)	0.0723	1.4677	4373.7 (1)	22853.662
(6, 4)	0.2169	1.5385	4557.5 (3)	21930.193
(7, 4)	0.0723	1.4750	4393.8 (1)	22750.962

Table 5. Values for (0, 0) sequence for B-X system of the AlO molecule

Band (v' , v'')	$\bar{r}_{v',v''}$ (Å)	$\bar{r} = (\bar{r}_{v'+1,v''+1}) - (\bar{r}_{v',v''})$ (Å)
(0, 0)	1.6465	—
(1, 1)	1.6578	0.0113
(2, 2)	1.6717	0.0139
(3, 3)	—	—
(4, 4)	—	—

The \bar{r} -centroids have been computed by the quadratic equation method of Nicholls & Jarman (1956).

2.3. Potential energy curves

The quantities r_{\min} and r_{\max} are computed by solving the Morse function and by solving the modified RKR potential function (Lakshman & Rao 1971). Tables 1 and 2 list the various quantities.

3. Discussion

Since $\bar{r}_{0,0}$ is slightly greater than $(r_{e1} + r_{e2})/2$, the potentials are not very anharmonic. Further we note that the internuclear separation for the transition is very small, so the primary Condon locus is quite narrow and $q_{0,0}$ has the largest value.

In the present case $\bar{r}_{v'+1,v''+1} - \bar{r}_{v',v''}$ for a sequence is greater than 0.01 Å showing that the two potentials involved in the transition are wide. It may be remarked that the values of \bar{r} -centroids for any band is found to increase linearly with the corresponding wavelength (figure 1).

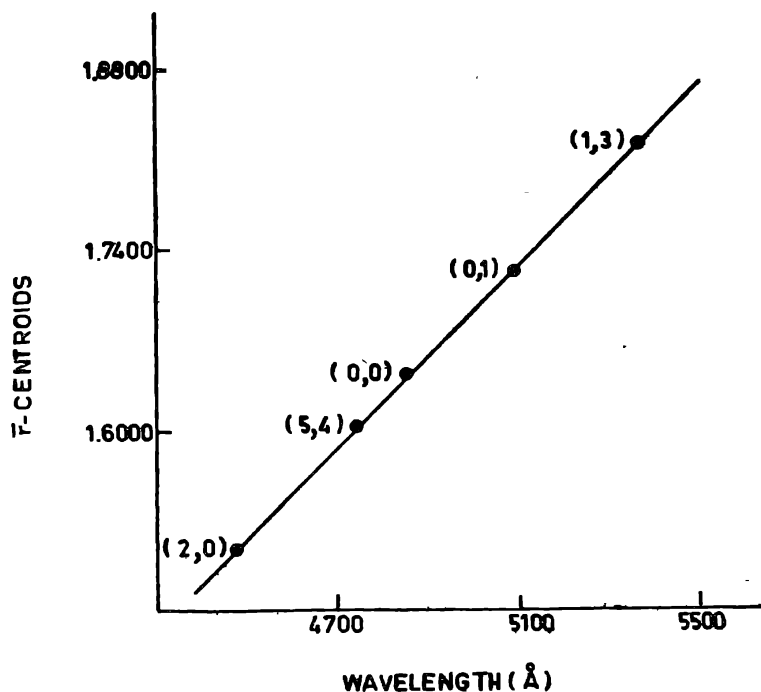


Figure 1. Variation of \bar{r} -centroids with corresponding wavelengths.

Now table 4 shows that the laboratory band heads of $B-X$ system at wavelengths, 4648.2Å, 4672.0Å, 4694.6Å, 4715.5Å, 4735.5Å, 4842.1Å, 4866.1Å, 4888.4Å, 5102.1Å and 5123.3Å could also be present, since the corresponding transition probabilities are appreciable.

References

- Babcock, H. D. (1945) *Ap. J.* **102**, 154.
Davis D. N. (1947) *Ap. J.* **106**, 28.
Fraser, P. A. & Jarmain, W. R. (1953) *Proc. Phys. Soc.* **66A**, 1145.
Huber, K. P. & Herzberg, G. (1979) *Molecular Spectra and Molecular Structure 4*, Van Nostrand.
Jevons, W. (1963) *The Identification of Molecular Spectra* (eds : R. W. B. Pearse & A. G. Gaydon) Chapman & Hall, p. 63.
Lakshman, S. V. J. & Rao, T. V. R. (1971) *J. Phys.* **B4**, 269.
Liszt, H. S. & Smith, W. H. (1972) *J. Q. S. R. T.* **12**, 947.
Morse, P. (1929) *Phys. Rev.* **34**, 57.
Nicholls, R. W. & Jarmain, W. R. (1956) *Proc. Phys. Soc.* **69A**, 253.
Singh, G. C. (1972) *J. Q. S. R. T.* **12**, 1343.
Stenvinkel, G., Svensson, E. & Olsson, E. (1938) *Ark. Mat. Astr. Fys.* **26A**, No. 10.