ON THE INFRARED BANDS OF AlO RELATED TO MIRA PHENOMENA

(*Letter to the Editor*)

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Abstract. The calculated band positions and intensity factors for the bands of the infrared *A–X* transition of AlO, suggest that an investigation for the infrared bands in the 1 to 5 μm region of the spectra of Mira stars and M supergiants, along with the 'blue-green' (*B–X*) bands, could provide clues to the Mira phenomena. The need for additional laboratory investigation of the infrared electronic transition is emphasized.

Aluminum oxide is an important constituent of the cool stars, as it has been observed primarily in normal M giants of spectral type later than M3 and in Mira variables. Keenan *et al.* (1969) have noted in the Mira stars near maximum light that the (0, 0) band of the 'blue-green' system ($B^2\Sigma^+ - X^2\Sigma^+$) is highly variable in strength and at times appears in emission. The strength of the band does not correlate with the spectral type.

It is of interest to consider some of the spectroscopic properties of the lowest lying electronic states of AlO in order to gain a better understanding of the Mira phenomena.

It is known that the electronic ground state of the AlO molecule is $X^2\Sigma^+$, with the $A^2\Pi_i$ and $B^2\Sigma^+$ states as the lowest lying excited states respectively. The $A^2\Pi_i$ state, located at 5406 cm^{-1} above the ground state, has been discovered by McDonald and Innes (1969), as the common lower state of the ultraviolet *D–A* and *E–A* transitions. Bands due to the $A^2\Pi_i - X^2\Sigma^+$ transition are expected to occur in the infrared region and are yet to be studied in detail in the laboratory. For these bands to be used in the cool star spectra, laboratory measurements of their position, structure and transition probabilities are needed. However, as the molecular constants for both the $X^2\Sigma^+$ and $A^2\Pi_i$ states are known, it will be possible to predict the expected intense band positions based upon the calculated Franck–Condon (FC) intensity factors.

Molecular constants for the $X^2\Sigma^+$ and $A^2\Pi_i$ states are given in Table I. Using these constants, FC-factors as well as *r*-centroids, which are useful for a study of the variation of electronic transition moment with internuclear separation, are calculated and these values for bands up to $v' = v'' = 0$ to 5 are given in Table II.

Using the molecular constants given in Table I, wavelengths (μm) are calculated for the expected intense bands of the system. These calculated wavelengths and intensities of the bands are given in Table III, along with the band head assignments.

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TABLE I

Molecular constants of the X and A states of AlO*

State	T_e (cm^{-1})	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	B_e (cm^{-1})	r_e (Å)
$X^2\Sigma^+$	0	979.2	6.9	0.6413	1.618
$A^2\Pi_i$	5406	728.12	4.203	0.5373	1.768

* Molecular constants for the $X^2\Sigma^+$ state are as compiled by Rosen (1970), and for the $A^2\Pi_i$ state are as assessed by Murty (1978). The symbols are conventional (Herzberg, 1950).

It is seen from Table III that most of the intense bands of the A–X transition are expected to lie in the region between 1 and 5 μm, with the (0, 0) band at 1.8931 μm.

Based on the estimated molecular column densities (Goon and Auman, 1970) above optical depth $\tau_\lambda = 0.3$ for a set of model atmospheres for K and M stars, Luck and Lambert (1974), have concluded that the lines of detectable intensity are produced for $NL \gtrsim 10^{16.2}$ in the (1, 0) band and that the A–X system could be detectable in cool stars. Their search for the (1, 0) band, using high resolution spectra of Mira-type stars (o Ceti, R Leonis and W Hydrae) and M supergiants (W Orionis, α Herculis and α Scorpii) is unfortunately negative.

TABLE II

Franck–Condon factors and r-centroids (Å) for the A–X transition of AlO*

v'	v'' = 0	1	2	3	4	5
0	0.057	0.182	0.268	0.242	0.151	0.068
	1.691	1.722	1.754	1.787	1.821	1.857
1	0.142	0.194	0.052	0.010	0.128	0.200
	1.669	1.699	1.730	1.762	1.795	1.829
2	0.193	0.071	0.019	0.127	0.057	0.005
	1.648	1.677	1.707	1.738	1.770	1.803
3	0.191	0.002	0.101	0.042	0.024	0.110
	1.628	1.654	1.685	1.715	1.746	1.778
4	0.154	0.023	0.087	0.005	0.092	0.011
	1.609	1.636	1.664	1.693	1.723	1.754
5	0.108	0.073	0.024	0.062	0.031	0.035
	1.590	1.617	1.644	1.672	1.701	1.731

* The constants of Table I are used in the calculations. The upper member of each entry is the Franck–Condon factor (calculated by the method of Fraser and Jarmain, 1953) and the lower member is the r-centroid (Å) (calculated by the method of Nicholls and Jarmain, 1956).

TABLE III

Predicted intense bands of the A–X transition of AlO

Band v'	Band v''	Wavenumber ν (cm^{-1})	Wavelength (μm)	Intensity*
1	5	1312	7.6199	0.005
0	4	1502	6.6560	0.005
1	4	2222	4.4992	0.014
0	3	2426	4.1209	0.035
3	5	2726	3.6674	0.022
2	4	2933	3.4085	0.014
0	2	3364	2.9718	0.102
3	4	3636	2.7345	0.012
2	3	3857	2.5290	0.073
1	2	4084	2.4479	0.035
5	5	4107	2.4342	0.024
0	1	4316	2.3163	0.146
4	4	4331	2.3083	0.075
3	3	4560	2.1924	0.040
2	2	4795	2.0849	0.021
5	4	5017	1.9927	0.039
1	1	5035	1.9856	0.248
0	0	5281	1.8931	0.084
3	2	5498	1.8184	0.168
2	1	5747	1.7396	0.135
5	3	5941	1.6828	0.130
1	0	6001	1.6659	0.307
4	2	6193	1.6143	0.207
2	0	6712	1.4895	0.584
5	2	6879	1.4533	0.078
4	1	7144	1.3994	0.084
3	0	7415	1.3483	0.779
5	1	7830	1.2768	0.350
4	0	8110	1.2327	0.821
5	0	8796	1.1366	0.735

* Intensity is $(\nu^3 q)_{v'v''} \times 10^{-11}$. This is a *partial relative* intensity indicating which band originating from a particular v' level will be stronger.

The present study throws some light on the above situation. From the magnitude of the intensity factors (Table II) it is seen that (1) the A–X system would mainly consist of two long progressions (as expected for a transition with $\Delta r_e = 0.15$ Å and $\Delta\omega_e = 251$ cm^{-1}); and (2) the (0, 2) and (0, 3) bands are the strongest bands of the system, the (0, 0) band being relatively weak in intensity.

The (0, 2) and (0, 3) bands are expected to occur at 2.9718 and 4.1209 μm, respectively. Thus a search for these bands in the region beyond 2 μm of the spectra of cool stars, appears to be interesting and a successful detection of the bands of the A–X

system, along with the bands of the B–X system, should provide clues to the unusual behavior of the blue–green system in the Mira stars.

In connection with the laboratory investigations of the A–X system, it is to be noted that the study is far from complete. Knight and Weltner (1971) reported the observation of weak absorption from the ground state to low vibrational levels of the A state of AlO molecules trapped in a frozen neon matrix. Recently, Rosenwaks *et al.* (1975) reported the emission spectrum during their chemiluminescence study of the AlO molecule. However, these studies on the infrared transition are limited to the v'-progression ($v'' = 0$) only, below 1 μm region. An extension of this study to further infrared up to 5 μm would be most welcome and valuable, in view of the astrophysical significance of the infrared transition.

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