

## Research Article

# Evaluation of the Effective Temperature of Sunspots Using Molecular Parameters of AlF

K. Balachandrakumar,<sup>1</sup> V. Raja,<sup>2</sup> B. Karthikeyan,<sup>1</sup> S. P. Bagare,<sup>3</sup> and N. Rajamanickam<sup>4</sup>

<sup>1</sup>Department of Physics, Kamaraj College of Engineering and Technology, Virudhunagar 626 001, India

<sup>2</sup>Department of Physics, RD Government Arts College, Sivagangai 630 560, India

<sup>3</sup>Indian Institute of Astrophysics, Bangalore 560 034, India

<sup>4</sup>Physics Research Centre, V.H.N.S.N College, Virudhunagar 626 001, India

Correspondence should be addressed to K. Balachandrakumar; [dkbaldr@gmail.com](mailto:dkbaldr@gmail.com)

Received 9 September 2014; Revised 4 December 2014; Accepted 15 December 2014

Academic Editor: Dean Hines

Copyright © 2015 K. Balachandrakumar et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

The physical conditions of celestial objects can be analyzed using the spectrum of atoms or molecules present in the object. The present work focuses on the spectroscopic analysis of astrophysically significant molecule AlF. The evaluation of Franck-Condon (FC) factors and  $r$ -centroids is done by a numerical integration procedure using the suitable potential energy curves for  $C^1\Sigma^+ - A^1\Sigma^+$ ,  $b^3\Sigma^+ - a^3\Pi_r$ ,  $c^3\Sigma - a^3\Pi_r$ , and  $f^3\Pi - a^3\Pi_r$  band systems of AlF molecule. The intensity of various bands is discussed with the help of derived FC factors. The band degradation and the nature of potential energy curves are studied using  $r$ -centroid values. The vibrational temperature of sunspot is estimated to be around  $1220 \pm 130$  K which falls in the reported temperature range of cold sunspots.

## 1. Introduction

The existence of AlF molecule in various astrophysical sources has been confirmed by various researchers. For instance, Cernicharo [1] and Turner [2] identified the presence of AlF molecule in the envelope of brightest C-rich evolved object IRC + 10216. The AlF molecular species was also found in the gas or dust envelopes of asymptotic giant branch (AGB) stars [3]. With reference to HF spectroscopy of the red giant stars, the presence of AlF in IRC + 10216 indicated that large quantities of fluorine were present in the inner stellar envelope and the element was produced in helium shell flashes and not in explosive nucleosynthesis [4]. Turner [2] has predicted that the AlF molecule must have a significant presence in the region of thermochemical equilibrium occurring in the dense, hot, and innermost envelope of the stellar atmosphere. Sauval and Tatum [5] have reported that the AlF molecule may be present in the stellar and cometary spectra.

According to Joshi et al. [6], the AlF molecule is likely to be present in the sunspots umbral atmosphere. Wöhl [7]

examined sunspots spectra towards the identification of various diatomic molecules and found 100 lines of AlF molecule. Bagare et al. [8] made an extensive search for AlF molecular lines in the spectra of sunspots and confirmed their presence. With the help of vibronic transition probability parameters such as Franck-Condon (FC) factors,  $r$ -centroids, relative intensities, oscillator strength, and vibrational temperature of diatomic molecular species, the spectroscopic technique could be very useful in the identification of molecular lines and in the estimation of relative abundance of the species in astrophysical sources. A number of workers have therefore undertaken theoretical studies to provide those parameters for diatomic molecules which are of importance not only in astrophysics, but also in the fields of gas kinetics, combustion process, and so forth [9–11].

The literature on the reports of Franck-Condon factors and  $r$ -centroids for the  $b^3\Sigma^+ - a^3\Pi_r$ ,  $c^3\Sigma - a^3\Pi_r$ , and  $f^3\Pi - a^3\Pi_r$  band systems of AlF molecule is not made. Murty [12] reported on a partial array of FC factors and  $r$ -centroids for  $C^1\Sigma^+ - A^1\Sigma^+$  band system. The present study focuses on

TABLE 1: Molecular constants taken from the compilation of Huber and Herzberg [13] for the electronic states of AlF molecule.

State	$\omega_e$ (cm <sup>-1</sup> )	$\omega_e x_e$ (cm <sup>-1</sup> )	$\omega_e y_e$ (cm <sup>-1</sup> )	$\alpha_e$	$\beta_e$	$r_e$ (Å)
C	938.22	5.09	-0.017	0.00480	0.58992	1.6010
A	803.94	5.99	-0.050	0.00534	0.55640	1.6485
f	938.90	5.90	—	0.00480	0.59355	1.5961
c	933.66	4.81	—	0.00457	0.58861	1.6028
b	786.37	7.64	-0.009	0.00650	0.56280	1.6391
a	827.80	3.90	—	0.00453	0.55703	1.6476

TABLE 2: Turning points for the molecular vibration in the C-state of AlF.

$\nu$	$G(\nu)$ in cm <sup>-1</sup>	Morse		RKR	
		$r_{\max}$ in Å	$r_{\min}$ in Å	$r_{\max}$ in Å	$r_{\min}$ in Å
0	467.83	1.661	1.547	1.661	1.547
1	1395.82	1.709	1.511	1.709	1.512
2	2313.47	1.744	1.488	1.745	1.489
3	3220.69	1.775	1.469	1.777	1.471
4	4117.37	1.802	1.454	1.805	1.457
5	5003.41	1.828	1.441	1.830	1.444

the complete array of the FC factors and  $r$ -centroids using experimental vibrational levels and vibrational temperature of the source using relative intensity of the bands.

## 2. Theory and Computational Procedure

**2.1. Franck-Condon Factors and  $r$ -Centroids.** The intensity of a vibrational band within a band system of a diatomic molecule is controlled mainly by the population on the vibrational level from which the transition takes place and by the FC factor ( $q_{\nu'\nu''}$ ) which is defined as the square modulus of the vibrational overlap integral that is [10]

$$q_{\nu'\nu''} = \left| \int \psi_{\nu'} \psi_{\nu''} dr \right|^2 = |\langle \psi_{\nu'} | \psi_{\nu''} \rangle|^2, \quad (1)$$

where  $\nu'$  and  $\nu''$  are the vibrational quantum numbers and  $\psi_{\nu'}$  and  $\psi_{\nu''}$  are the vibrational wave functions for the upper and lower states, respectively.

The  $r$ -centroids  $\bar{r}_{\nu'\nu''}$  are seen to be the weighted average with respect to  $\psi_{\nu'} \psi_{\nu''}$  of the range of  $r$  values experienced by the molecule in both states of the  $\nu' - \nu''$  transition. The form of  $\bar{r}_{\nu'\nu''}$  can be expressed as [10]

$$\bar{r}_{\nu'\nu''} = \frac{\langle \psi_{\nu'} | r | \psi_{\nu''} \rangle}{\langle \psi_{\nu'} | \psi_{\nu''} \rangle}. \quad (2)$$

Using the molecular constants [13] mentioned in Table 1, the potential energy curves for the electronic states  $A$ ,  $C$ ,  $a$ ,  $b$ ,  $c$  and  $f$  of AlF molecule have been constructed first using Morse [14] and Rydberg-Klein Rees (RKR) [15] functions. The turning points of the potential energy curves are finally presented in the Tables 2–7, where the potential energy curves derived from Morse function coincide well with the RKR curves. The Morse potential can yield reliable FC factors and

TABLE 3: Turning points for the molecular vibration in the A-state of AlF.

$\nu$	$G(\nu)$ in cm <sup>-1</sup>	Morse		RKR	
		$r_{\max}$ in Å	$r_{\min}$ in Å	$r_{\max}$ in Å	$r_{\min}$ in Å
0	400.47	1.714	1.591	1.714	1.591
1	1192.26	1.767	1.553	1.768	1.553
2	1971.63	1.807	1.528	1.807	1.529
3	2738.27	1.841	1.510	1.842	1.510
4	3491.88	1.873	1.494	1.874	1.494
5	4232.15	1.902	1.481	1.903	1.481
6	4958.80	1.930	1.469	1.932	1.469
7	5671.52	1.957	1.459	1.959	1.458
8	6370.00	1.983	1.449	1.983	1.448

TABLE 4: Turning points for the molecular vibration in the  $b$ -state of AlF.

$\nu$	$G(\nu)$ in cm <sup>-1</sup>	Morse		RKR	
		$r_{\max}$ in Å	$r_{\min}$ in Å	$r_{\max}$ in Å	$r_{\min}$ in Å
0	391.27	1.706	1.581	1.706	1.581
1	1162.33	1.761	1.543	1.761	1.544
2	1981.03	1.803	1.520	1.803	1.520
3	2658.31	1.839	1.501	1.839	1.502
4	3383.13	1.873	1.487	1.873	1.487
5	4092.42	1.905	1.473	1.905	1.474
6	4786.14	1.935	1.463	1.935	1.462
7	5464.22	1.965	1.453	1.965	1.452
8	6126.62	1.995	1.444	1.994	1.443

$r$ -centroids for the bands in an electronic transition involving low vibrational quantum numbers [16].

The computation of FC factor is made using the Bates' method of numerical integration [16] and Ureña et al.'s detailed procedure [17]. The Morse wave functions are calculated at the intervals of 0.01 Å for  $r$  ranging from 1.42 Å to 2.01 Å, from 1.42 Å to 2.01 Å, from 1.44 Å to 1.88 Å, and from 1.49 Å to 1.82 Å, for every observed vibrational level of each state of  $C - A$ ,  $b - a$ ,  $c - a$ , and  $f - a$  of the AlF molecule. The FC factors ( $q_{\nu'\nu''}$ ) and  $r$ -centroids ( $\bar{r}_{\nu'\nu''}$ ) are computed numerically by integrating the integrals in (1) and (2) for the bands of  $C - A$ ,  $b - a$ ,  $c - a$ , and  $f - a$  of the AlF molecule and the results are given in the Tables 8–11 with the available wavelengths ( $\lambda_{\nu'\nu''}$ ) [18–20] for all the band systems.

TABLE 5: Turning points for the molecular vibration in the  $c$ -state of AIF.

$\nu$	$G(\nu)$ in $\text{cm}^{-1}$	Morse		RKR	
		$r_{\max}$ in $\text{\AA}$	$r_{\min}$ in $\text{\AA}$	$r_{\max}$ in $\text{\AA}$	$r_{\min}$ in $\text{\AA}$
0	465.63	1.663	1.549	1.663	1.549
1	1389.67	1.711	1.512	1.711	1.513
2	2304.09	1.746	1.489	1.747	1.490
3	3208.89	1.776	1.470	1.777	1.472
4	4104.07	1.804	1.455	1.806	1.457

TABLE 6: Turning points for the molecular vibration in the  $f$ -state of AIF.

$\nu$	$G(\nu)$ in $\text{cm}^{-1}$	Morse		RKR	
		$r_{\max}$ in $\text{\AA}$	$r_{\min}$ in $\text{\AA}$	$r_{\max}$ in $\text{\AA}$	$r_{\min}$ in $\text{\AA}$
0	467.98	1.656	1.542	1.656	1.543
1	1395.08	1.705	1.507	1.705	1.507

TABLE 7: Turning points for the molecular vibration in the  $a$ -state of AIF.

$\nu$	$G(\nu)$ in $\text{cm}^{-1}$	Morse		RKR	
		$r_{\max}$ in $\text{\AA}$	$r_{\min}$ in $\text{\AA}$	$r_{\max}$ in $\text{\AA}$	$r_{\min}$ in $\text{\AA}$
0	412.93	1.711	1.590	1.712	1.590
1	1232.93	1.762	1.551	1.763	1.552
2	2045.13	1.798	1.526	1.801	1.528
3	2849.53	1.831	1.506	1.833	1.509
4	3646.13	1.859	1.490	1.863	1.493
5	4434.93	1.886	1.476	1.890	1.480
6	5215.93	1.911	1.463	1.916	1.469
7	5989.13	1.935	1.452	1.941	1.458
8	6754.53	1.958	1.442	1.964	1.448

2.2. *Variation of Electronic Transition Moment and Band Strength.* With the help of FC factors and  $r$ -centroids, one can determine the band strength of the vibrational bands using the relation

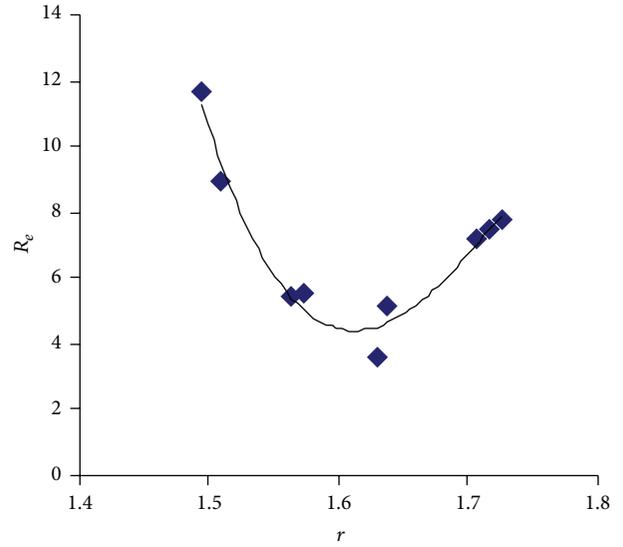
$$p_{\nu'\nu''} = R_e^2(\bar{r}_{\nu'\nu''}) q_{\nu'\nu''}, \quad (3)$$

where  $R_e^2(\bar{r}_{\nu'\nu''})$  is the variation of electronic transition moment. Mathematically the intensity ( $I_{\nu'\nu''}$ ) of a molecular band for an electronic transition in emission ( $\nu' - \nu''$ ) is written as [9]

$$I_{\nu'\nu''} = DN_{\nu'} E_{\nu'\nu''}^4 p_{\nu'\nu''}, \quad (4)$$

where  $D$  is a constant partly depending on the geometry of the apparatus and  $N_{\nu'}$  is the population of the level  $\nu'$  and  $E_{\nu'\nu''}$  the energy quantum.

In the present study, the intensities ( $I_{\nu'\nu''}$ ) of (0, 0), (0, 1), (0, 2), (1, 0), (1, 1), (1, 2), (1, 3), (2, 1), and (3, 2) bands as reported by Naudé and Hugo [21] are used to evaluate the electronic transition moment variation with internuclear distance for the band system  $C - A$  of AIF. A plot of  $(IE^{-4}/q)_{\nu'\nu''}^{1/2}$  versus  $\bar{r}_{\nu'\nu''}$  yields the variation of  $R_e$  with  $\bar{r}_{\nu'\nu''}$  over a progression. To place all progression on the same

FIGURE 1: The variation of  $R_e$  with  $r$  for AIF ( $C - A$ ) band system.

ordinate, the rescaling procedure of Turner and Nicholls [22] was adopted. A plot of rescaled values of  $R_e = (IE^{-4}/q)_{\nu'\nu''}^{1/2}$  versus  $\bar{r}_{\nu'\nu''}$  is shown in Figure 1 for the  $C - A$  band system of AIF. A least square fit yields

$$R_e(r) = \text{const.} \times (1 - 1.73r + 0.10r^2 - 0.19r^3) \quad (5)$$

$$1.49 \text{ \AA} \leq r \leq 1.73 \text{ \AA}$$

with standard deviation 0.63. The form of  $R_e(r)$  represented by (5) is adopted in conjunction with (3) to calculate the band strengths using the computed  $q_{\nu'\nu''}$  values. The band strengths have been relatively scaled by assuming the value of most intense band (0, 0) as one. The relative band strengths are evaluated using the relation  $S_{\nu'\nu''} = p_{\nu'\nu''}/p_{00}$ .

2.3. *Effective Vibrational Temperature.* The vibrational quanta  $G(\nu')$  are calculated from

$$G(\nu') = \omega'_e \left[ \nu' + \frac{1}{2} \right] - \omega'_e x'_e \left[ \nu' + \frac{1}{2} \right]^2. \quad (6)$$

Using the relative band strengths  $S_{\nu'\nu''} = p_{\nu'\nu''}/p_{00}$ , (4) becomes

$$\sum (IE^{-4})_{\nu'\nu''} = DN_{\nu'} p_{00} S_{\nu'\nu''}. \quad (7)$$

Since  $N_{\nu'} = N_0 \exp[(-hc/kT)G(\nu')]$ , (7) becomes [23]

$$\ln \left[ \frac{\sum_{\nu''} (IE^{-4})_{\nu'\nu''}}{\sum_{\nu''} S_{\nu'\nu''}} \right] = \text{const.} \times \left[ \left( -\frac{hc}{kT} \right) G(\nu') \right], \quad (8)$$

where  $h$  is the Planck constant,  $c$  is the velocity of light,  $k$  is the Boltzmann's constant, and  $T$  is the effective vibrational temperature of the source.

A plot of  $\ln[\sum_{\nu''} (IE^{-4})_{\nu'\nu''} / \sum_{\nu''} S_{\nu'\nu''}]$  versus  $G(\nu')$  in Figure 2 shows a linear dependence. By least square fitting, the slope is determined and vibrational temperature  $T$  is evaluated and discussed in the following section.

TABLE 8: Franck-Condon factors and  $r$ -centroids of  $C^1\Sigma^+ - A^1\Sigma^+$  band system of AlF molecule.

		$\nu'' = 0$	$\nu'' = 1$	$\nu'' = 2$	$\nu'' = 3$	$\nu'' = 4$	$\nu'' = 5$	$\nu'' = 6$	$\nu'' = 7$	$\nu'' = 8$	
$\nu' = 0$	(a)	(i)	0.714	0.236	0.044	0.006	0.001	*	*	*	*
		(ii)	0.717	0.234	0.043	—	0.001	—	—	—	—
	(b)	(i)	1.629	1.562	1.494	1.423	1.349	1.271	—	—	—
		(ii)	1.628	1.560	1.483	—	1.346	1.282	—	—	—
	(c)		7245.9	7686.2	8175.4	—	—	2040.0	—	—	—
	$\nu' = 1$	(a)	(i)	0.243	0.303	0.322	0.107	0.022	0.004	0.001	*
(ii)			0.241	0.312	0.320	0.102	0.020	—	—	—	—
(b)		(i)	1.706	1.638	1.574	1.508	1.439	1.368	1.293	—	—
		(ii)	1.705	1.640	1.573	1.499	1.394	—	—	—	—
(c)			6789.9	7174.9	7599.2	8068.8	8590.8	8461.7	—	—	—
$\nu' = 2$		(a)	(i)	0.039	0.346	0.084	0.306	0.166	0.048	0.010	0.001
	(ii)		0.038	0.343	0.096	0.310	0.159	0.043	—	—	—
	(b)	(i)	1.778	1.716	1.645	1.586	1.522	1.455	1.386	1.404	1.334
		(ii)	1.780	1.715	1.651	1.586	1.515	1.425	—	—	—
	(c)		6392.3	6732.1	7104.2	7512.8	7963.3	8461.7	8334.5	—	—
	$\nu' = 3$	(a)	(i)	0.004	0.101	0.345	0.004	0.232	0.206	0.081	0.022
(ii)			0.004	0.096	0.350	—	0.247	0.199	—	—	—
(b)		(i)	1.847	1.787	1.725	1.634	1.597	1.535	1.471	1.404	1.334
		(ii)	1.857	1.789	1.725	—	1.599	1.531	—	—	—
(c)			6036.9	6345.3	6674.5	—	7426.9	7858.7	8334.5	—	—
$\nu' = 4$		(a)	(i)	*	0.015	0.166	0.282	0.013	0.142	0.216	0.116
	(ii)		*	—	0.157	0.299	—	0.166	—	—	—
	(b)	(i)	1.915	1.855	1.796	1.735	1.690	1.608	1.549	1.486	1.422
		(ii)	1.938	—	1.799	1.735	—	1.611	—	—	—
	(c)		—	—	6298.1	6616.8	—	7341.5	7755.2	8211.1	—
	$\nu' = 5$	(a)	(i)	*	0.002	0.035	0.220	0.191	0.064	0.062	0.196
(ii)			*	—	—	0.210	0.222	—	—	—	—
(b)		(i)	1.981	1.922	1.863	1.805	1.744	1.692	1.618	1.562	1.502
		(ii)	2.025	—	—	1.808	1.745	—	—	—	—
(c)			—	—	—	6251.4	6559.5	—	—	—	8093.6

(a)  $q_{\nu',\nu''}$ : (i) present study; (ii) Murty (1977) [12], (b)  $\bar{r}_{\nu',\nu''}$  (Å), (c)  $\lambda_{\nu',\nu''}$  (Å), and \*:  $q_{\nu',\nu''} = 0$ .

### 3. Results and Discussion

In the case of  $C - A$  band system the FC factors manifest that (0, 0), (0, 1), (1, 0), (1, 1), (1, 2), (2, 1), (2, 3), (2, 4), (3, 2), (3, 4), (3, 5), (4, 2), (4, 3), (4, 5), (4, 6), (5, 3), (5, 4), (5, 7), and (5, 8) bands are intense. In the case of the  $b - a$  band systems of the AlF molecule, the FC factors indicate that the  $\Delta\nu = 0$  sequence bands are more intense and all other bands are relatively weak. The FC factors of  $c - a$  and  $f - a$  band systems indicate that the  $\Delta\nu = 0$  sequence bands are significantly intense followed by the  $\Delta\nu = \pm 1$  sequence bands.

The  $r$ -centroid value increases for the  $C - A$ ,  $c - a$  and  $f - a$  band systems of AlF, since  $r'_e < r''_e$  with the decrease in wavelength which is expected in the violet degraded band system. For the  $b - a$  band system, the  $r$ -centroids value increases with the increase in wavelength which is expected in the red degraded band system.

The sequence differences are found to be constant nearly  $0.01 \text{ \AA}$  for all the four band systems of AlF molecule. For  $C - A$  band system, the sequence difference is varying from  $0.002 \text{ \AA}$  to  $0.056 \text{ \AA}$ . This suggests that the potentials are not so wide. The  $r$ -centroid value for the (0, 0) transition is slightly greater than  $(r'_e + r''_e)/2$  for all the band systems of AlF molecule which implies that the potentials are not very anharmonic.

The vibrational temperature of the source of  $C - A$  band system is estimated as  $1220 \pm 130 \text{ K}$  and is found in the temperature range of cold sunspots. To confirm the presence of AlF molecule in sunspots spectrum, a careful study of sunspot umbral spectra in the wavelength region of  $4400 - 9000 \text{ \AA}$  was carried out to search for the presence of AlF molecular lines of different band systems [8]. The presence of several transitions of AlF molecule in sunspot spectra was confirmed with a total of 602 rotational lines. The rotational temperature for the  $D - A$  band system was  $1240 \pm 120 \text{ K}$ .

TABLE 9: Franck-Condon factors and  $r$ -centroids of  $b^3\Sigma^+ - a^3\Pi_r$  band system of AlF molecule.

		$\nu'' = 0$	$\nu'' = 1$	$\nu'' = 2$	$\nu'' = 3$	$\nu'' = 4$	$\nu'' = 5$	$\nu'' = 6$	$\nu'' = 7$	$\nu'' = 8$
$\nu' = 0$	(a)	0.995	0.005	*	*	*	*	*	*	*
	(b)	1.649	1.028							
	(c)	5681.0	—							
$\nu' = 1$	(a)	0.005	0.990	*	0.003	*	*	*	*	*
	(b)	2.242	1.660		1.521					
	(c)	—	5697.1		—					
$\nu' = 2$	(a)	*	0.004	0.990	*	0.005	*	*	*	*
	(b)		2.579	1.671		1.585				
	(c)		—	5715.1		—				
$\nu' = 3$	(a)	*	0.003	*	0.989	*	0.009	*	*	*
	(b)		1.698		1.683		1.655			
	(c)		—		5735.3		—			
$\nu' = 4$	(a)	*	*	0.005	*	0.974	*	0.014	*	*
	(b)			1.767		1.693		1.725		
	(c)			—		5758.4		—		
$\nu' = 5$	(a)	*	*	*	0.008	*	0.938	0.021	0.023	*
	(b)				1.841		1.703	2.540	1.790	
	(c)				—		5782.9	—	—	
$\nu' = 6$	(a)	*	*	*	*	0.011	0.036	0.871	0.046	0.034
	(b)					1.930	1.234	1.711	2.334	1.847
	(c)					—	—	5809.3	—	—
$\nu' = 7$	(a)	*	*	*	*	*	0.010	0.083	0.768	0.078
	(b)						2.056	1.401	1.716	2.225
	(c)						—	—	5837.9	—
$\nu' = 8$	(a)	*	*	*	*	*	0.002	0.007	0.155	0.625
	(b)						1.620	2.286	1.504	1.717
	(c)						—	—		5869.0

(a)  $q_{\nu'\nu''}$ , (b)  $\bar{r}_{\nu'\nu''}$  (Å), (c)  $\lambda_{\nu'\nu''}$  (Å), and \*:  $q_{\nu'\nu''} = 0$ .TABLE 10: Franck-Condon factors and  $r$ -centroids of  $c^3\Sigma^+ - a^3\Pi_r$  band system of AlF molecule.

		$\nu'' = 0$	$\nu'' = 1$	$\nu'' = 2$	$\nu'' = 3$	$\nu'' = 4$
$\nu' = 0$	(a)	0.751	0.215	0.032	0.003	*
	(b)	1.628	1.556	1.476	1.376	
	(c)	3608.2	3702.4	—	—	
$\nu' = 1$	(a)	0.216	0.380	0.314	0.079	0.011
	(b)	1.713	1.636	1.566	1.488	1.393
	(c)	3492.2	3592.1	3702.4	—	—
$\nu' = 2$	(a)	0.031	0.317	0.161	0.335	0.129
	(b)	1.785	1.723	1.642	1.574	1.499
	(c)	—	3480.8	—	3687.1	—
$\nu' = 3$	(a)	0.003	0.078	0.343	0.048	0.308
	(b)	1.864	1.795	1.734	1.642	1.584
	(c)		—	3469.6	—	3672.2
$\nu' = 4$	(a)	*	0.009	0.128	0.320	0.004
	(b)		1.874	1.805	1.744	1.597
	(c)		—	—	3458.6	—

(a)  $q_{\nu'\nu''}$ , (b)  $\bar{r}_{\nu'\nu''}$  (Å), (c)  $\lambda_{\nu'\nu''}$  (Å), and \*:  $q_{\nu'\nu''} = 0$ .

TABLE 11: Franck-Condon factors and  $r$ -centroids of  $f^3\Pi - a^3\Pi_r$  band system of AlF molecule.

		$v'' = 0$	$v'' = 1$	$v'' = 2$
$v' = 0$	(a)	0.686	0.251	0.053
	(b)	1.626	1.562	1.501
	(c)	2592.2	2648.6	—
$v' = 1$	(a)	0.268	0.271	0.312
	(b)	1.698	1.636	1.570
	(c)	2531.0	2584.5	2639.6

(a)  $q_{v',v''}$ , (b)  $\bar{r}_{v',v''}$  (Å), and (c)  $\lambda_{v',v''}$  (Å).

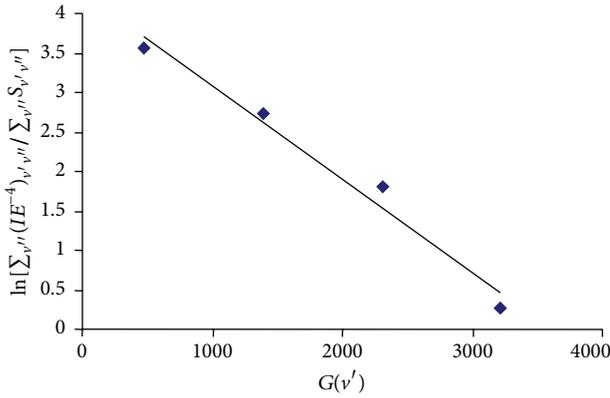


FIGURE 2: Plot of  $\ln[\sum_{v''} (IE^{-4})_{v',v''} / \sum_{v''} S_{v',v''}]$  with  $G(v')$  for AlF (C-A) band system.

Thus it clears that the vibrational temperature evaluated in the present study coincides with the reported rotational temperature.

#### 4. Conclusions

The present work evaluates the transition probability parameters FC factors and  $r$ -centroids which are mainly influencing the intensity of vibrational bands. Using the derived transition probability parameters and reported wavelength of the bands, the vibrational temperature of a band system of AlF molecule is determined. Since the vibrational temperature of the AlF molecule is found to coincide well with the reported sunspot temperature, the present work acts as the additional support for the confirmation of AlF molecule in sunspots.

#### Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

#### Acknowledgments

The authors thank the reviewer for the valuable suggestions and constructive remarks. The authors (K. Balachandrakumar and B. Karthikeyan) would also like to thank the management of Kamaraj College of Engineering and Technology for their support and encouragement in pursuing research.

#### References

- [1] J. Cernicharo, "Molecules in AGB stars observed with ISO," *Astrophysics and Space Science*, vol. 255, no. 1-2, pp. 303-313, 1997.
- [2] B. E. Turner, "Gaseous refractory-element molecules in IRC10216," *Astrophysics and Space Science*, vol. 224, no. 1-2, pp. 297-303, 1995.
- [3] H. Olofsson, "Molecules in envelopes around AGB-stars," *Astrophysics and Space Science*, vol. 251, no. 1-2, pp. 31-39, 1997.
- [4] L. M. Ziurys, A. J. Apponi, and T. G. Phillips, "Exotic fluoride molecules in IRC +10216: confirmation of AlF and searches for MgF and CaF," *The Astrophysical Journal*, vol. 433, no. 2, pp. 729-732, 1994.
- [5] A. J. Sauval and J. B. Tatum, "A set of partition functions and equilibrium constants for 300 diatomic molecules of astrophysical interest," *The Astrophysical Journal Supplement*, vol. 56, pp. 193-209, 1984.
- [6] G. C. Joshi, U. C. Joshi, L. M. Punetha, and M. C. Pande, "Franck-Condor factor for some abundant umbral molecules," *Bulletin of the American Astronomical Society*, vol. 10, p. 159, 1982.
- [7] H. Wöhl, "On molecules in sunspots," *Solar Physics*, vol. 16, no. 2, pp. 362-372, 1971.
- [8] S. P. Bagare, K. B. Kumar, and N. Rajamanickam, "Identification of AlF molecular lines in sunspot umbral spectra," *Solar Physics*, vol. 234, no. 1, pp. 1-20, 2006.
- [9] N. Rajamanickam, "Intensity distribution in the bands of the  $D^1\Pi \rightarrow X^1\Sigma^+$  system of SnO," *Pramana*, vol. 25, no. 2, pp. 179-186, 1985.
- [10] N. Rajamanickam, *Intensity distribution in band spectra and the dissociation energies of diatomic molecules [Ph.D. thesis]*, University of Mysore, Mysore, India, 1987.
- [11] B. Karthikeyan, K. Balachandrakumar, V. Raja, and N. Rajamanickam, "Spectral dataset for an astrophysically significant BaF molecule," *Journal of Applied Spectroscopy*, vol. 80, no. 5, pp. 790-797, 2013.
- [12] P. S. Murty, "On AlF lines in sunspots," *Solar Physics*, vol. 54, no. 2, pp. 377-378, 1977.
- [13] K. P. Huber and G. Herzberg, *Molecular Spectra and Molecular Structure*, vol. 4 of *Constants of Diatomic Molecules*, Van Nostrand Reinhold, New York, NY, USA, 1979.
- [14] P. M. Morse, "Diatomic molecules according to the wave mechanics. II. Vibrational levels," *Physical Review*, vol. 34, no. 1, pp. 57-64, 1929.
- [15] J. T. Vanderslice, E. A. Mason, W. G. Maisch, and E. R. Lippincott, "Errata—ground state of hydrogen by the Rydberg-Klein-Rees method," *Journal of Molecular Spectroscopy*, vol. 5, pp. 83-88, 1961.
- [16] R. W. Nicholls, "Franck-Condon factor formulae for astrophysical and other molecules," *The Astrophysical Journal Supplement*, vol. 47, pp. 279-290, 1981.
- [17] F. P. Ureña, M. F. Gómez, J. J. L. González, and N. Rajamanickam, "Astrophysical molecules AlD and CaH: transition probabilities and dissociation energy," *Astrophysics and Space Science*, vol. 272, no. 4, pp. 345-352, 2000.
- [18] R. F. Barrow, I. Kopp, and C. Malmberg, "The electronic spectrum of gaseous AlF," *Physica Scripta*, vol. 10, no. 1-2, pp. 86-102, 1974.
- [19] R. F. Rowlinson and H. C. Barrow, "The band spectrum of aluminium monofluoride," *Proceedings of the Physical Society*, vol. 66, pp. 437-446, 1952.

- [20] P. G. Dodsworth and R. F. Barrow, "The triplet band systems of aluminium monofluoride," *Proceedings of the Physical Society A*, vol. 68, no. 9, pp. 824–828, 1955.
- [21] S. M. Naudé and T. J. Hugo, "The emission spectrum of aluminium monofluoride I," *Canadian Journal of Physics*, vol. 31, no. 7, pp. 1106–1114, 1953.
- [22] R. G. Turner and R. W. Nicholls, "An experimental study of band intensities in the first positive system of  $N_2$ : I. Vibrational transition probabilities," *Canadian Journal of Physics*, vol. 32, pp. 468–474, 1954.
- [23] A. P. Thorne, *Spectrophysics*, Chapman & Hall, London, UK, 1974.



**Hindawi**

Submit your manuscripts at  
<http://www.hindawi.com>

