Journal of Physical Science, Vol. 29(1), 133–140, 2018

Investigation of A−X Band System of Astrophysically Significant Molecule BS

Karthikeyan Balasubramanian,[1*] Shanmugapriya Ganesan[2] and
Rajamanickam Narayanan[3]

[1]Department of Physics, Mepco Schlenk Engineering College, Sivakasi 626005, India
[2]Department of Physics, V.V.Vanniaperumal College for Women,
Virudhunagar 626001, India
[3]Physics Research Centre, VHNSN College, Virudhunagar 626001, India

[*]Corresponding author: karthi.madhubalan@gmail.com

To cite this article: Karthikeyan, B., Shanmugapriya, G. & Rajamanickam, N. (2018). Investigation of A−X band system of astrophysically significant molecule BS. *J. Phys. Sci.*, 29(1), 133–140, https://doi.org/10.21315/jps2018.29.1.9

To link to this article: https://doi.org/10.21315/jps2018.29.1.9

ABSTRACT: *It is widely known that molecular signatures in celestial object play a vital role in deriving the physical conditions of the object using spectroscopic technique. The present study therefore focuses on the evaluation of Franck-Condon factors (FCFs) and r-centroids for the A−X band system of Boron mono-sulphide (BS) molecule by a numerical integration method using the suitable potential. With the help of FCFs and r-centroids, the vibrational temperature of the source is estimated and is found to be about 6893 K. The vibrational temperature estimated in the present study reveals that the rotational temperature of the molecule has to be considered for the identification of the chosen band system in the astrophysical spectra. The vibration rotation interaction (VRI) effect for the chosen band system is discussed. It is found that the VRI effect may influence the effective temperature of the source and hence the effect of VRI has to be considered at the time of identifying the BS molecular lines in the spectra of sunspot or any celestial object.*

Keywords: BS molecule, Franck-Condon factors, r-centroids, vibrational temperature, sunspot

1. INTRODUCTION

The knowledge of potential energy curves, Franck-Condon factors (FCFs) and r-centroids is essential for the interpretation of spectral intensities in terms of source conditions. A number of researchers have therefore undertaken theoretical studies to provide the above-said parameters for the diatomic molecules which are of important in astrophysics gas kinetics, molecular spectroscopy and combustion process.[1] Accurate values of FCFs and r-centroids are essential to arrive at the variation of electronic transition moment, band strength and vibrational temperature of the source.[2,3]

The researchers pay attention to the theoretical work on the diatomic molecule BS for many years. Recently, the potential energy of the electronic states X, C and G of BS radical were calculated by the Davidson-modified high resolution internal-contraction multiple-reference configuration interaction method.[4] It is also worthy to mention here the astrophysical significance of BS molecule, that according to the calculation of the weighted column densities for 248 molecules, Jhonson and Sauval reported that BS may be possibly present in an Oxygen rich (O-rich) stars under the effective temperature T_{eff} =2500 K.[5] It was also observed that the BS emission lines from the cirrus dark cloud centred on the BO star HD1 located in the Numbbum Association.[6] Karthikeyan et al. reported the FC factors and r-centroids for the C−X, E−X and B−A band systems of BS molecule and predicted the existence of BS molecule in sunspot with the help of derived FCFs and r-centroids.[7] An extensive search of rotational lines of the A−X and B−A band systems in the sunspot spectral atlas was performed by Karthikeyan et al. and it was concluded that the chance to find the existence BS molecule in sunspot was considerably high.[8]

The aims of the present work are: to provide the transition probability parameters for the A–X band system of BS molecule; to evaluate the vibrational temperature of the source; and to study the vibration rotation interaction effect for the $A^2\Pi_i$–$X^2\Sigma^+$ system of BS molecule, in view of the astrophysical application, using the numerical integration method described in the following section.

2. COMPUTATIONAL PROCEDURE

2.1 Franck-Condon Factor and r-centroid

The square of the overlap integral is termed as Franck-Condon factor ($q_{v'v''}$) and it is given by:[3]

$$q_{v'v''} = |< \Psi_{v'}|< \Psi_{v''} >|^2 \quad (1)$$

where $\psi_{v'}$ and $\psi_{v''}$ are the upper and lower vibrational level wave function.

The r-centroid ($\tilde{r}_{v'v''}$) for the v′–v″ transition is defined by:[3]

$$r_{v'v''} = \frac{< \Psi_{v'}|\, r\, |\Psi_{v''} >}{< \Psi_{v'}|\Psi_{v''} >} \quad (2)$$

From the above equation it is seen to be the weighted average with respect to $\Psi_{v'v''}$ of the range of *r* values experienced by the molecule in both states of the v′–v″ transition.

The computation of the FCFs is made using the Bates' method, with numerical integration according to the detailed procedure provided by Partal Urena.[9,10] Having the Morse potential energy curves, Morse wave functions are calculated at intervals of 0.01 Å for the range of r values from 1.42 to 2.32 Å for every observed vibrational levels of the states A and X involved in the A–X band system of BS molecule.[11] Once the wave functions are obtained, the FCFs can be calculated by integrating Equation 1. The definition of r-centroid offers a method of computing r-centroids directly.[12] The results ($q_{v'v''}$ and $\tilde{r}_{v'v''}$) along with available wavelengths are entered in Table 1. The molecular constants necessary for the present study are collected from compilation by Huber and Herzberg.[13]

Table 1: FCFs and r-centroids for the A–X band system of BS molecule.

v′/v″		0	1	2	3	4	5	6	7	8	9	10
0	a)	0.007	0.037	0.099	0.168	0.206	0.192	0.141	0.084	0.042	0.017	0.006
	b)	1.705	1.730	1.756	1.783	1.809	1.836	1.864	1.892	1.921	1.951	1.982
1	a)	0.038	0.105	0.153	0.106	0.021	0.007	0.074	0.141	0.151	0.112	0.062
	b)	1.688	1.714	1.739	1.765	1.789	1.824	1.847	1.874	1.902	1.931	1.961
2	a)	0.068	0.141	0.083	0.002	0.043	0.099	0.057	0.001	0.033	0.108	0.141
	b)	1.672	1.697	1.722	1.740	1.776	1.801	1.826	1.838	1.886	1.913	1.941
3	a)	0.109	0.114	0.007	0.041	0.083	0.017	0.016	0.080	0.062	0.004	0.025
	b)	1.656	1.681	1.704	1.733	1.757	1.780	1.814	1.837	1.862	1.880	1.926
4	a)	0.139	0.054	0.013	0.080	0.017	0.022	0.072	0.018	0.013	0.074	0.055
	b)	1.640	1.665	1.692	1.716	1.739	1.769	1.793	1.815	1.851	1.874	1.899
5	a)	0.147	0.009	0.059	0.041	0.009	0.065	0.012	0.024	0.064	0.010	0.020
	b)	1.625	1.650	1.676	1.610	1.729	1.751	1.772	1.805	1.828	1.848	1.887
6	a)	0.137	0.002	0.075	0.002	0.053	0.024	0.016	0.056	0.003	0.035	0.053
	b)	1.610	1.636	1.660	1.680	1.710	1.733	1.763	1.785	1.800	1.840	1.863
7	a)	0.114	0.026	0.050	0.014	0.051	0.001	0.053	0.007	0.031	0.041	0.000
	b)	1.595	1.620	1.645	1.671	1.694	1.729	1.744	1.764	1.797	1.819	1.885
8	a)	0.087	0.058	0.015	0.048	0.014	0.033	0.026	0.014	0.044	0.000	0.045
	b)	1.581	1.606	1.631	1.656	1.679	1.705	1.727	1.757	1.778	1.916	1.830
9	a)	0.062	0.081	0.000	0.057	0.001	0.048	0.000	0.045	0.004	0.034	0.022
	b)	1.566	1.591	1.628	1.641	1.670	1.690	1.887	1.739	1.755	1.789	1.810
10	a)	0.041	0.087	0.010	0.037	0.022	0.024	0.021	0.025	0.013	0.034	0.003
	b)	1.552	1.577	1.601	1.627	1.652	1.675	1.701	1.722	1.751	1.771	1.809

Notes: $q_{v'v''}$, $\tilde{r}_{v'v'}$ *(in Å)*, * $q_{v'v''} \cong 0$

2.2 Vibrational Temperature

If the intensities of a sufficient number of bands can be measured, a determination of vibrational temperature can be obtained if the overlap integrals are calculated for the measured bands, using the following equation.[14,15]

$$\ln\left(IE^{-4}/q\right)_{v'v''} = \text{Const.} - \left\{\frac{hc}{kT}G(v')\right\} \tag{3}$$

where *I* is the intensity of the band, *E* is the energy quantum, $q_{v'v''}$ is the value of FCF, *h* is Planck's constant, *c* is the velocity of the light, *k* is Boltzmann constant, and *T* is the effective vibrational temperature of the source. Here, G(v′) is the vibrational quantum energy of the molecule in the level v′ and it is given by Equation 4.

$$G(v') = \omega_e'\left(v' + \frac{1}{2}\right) - \omega_e'x_e'\left(v' + \frac{1}{2}\right)^2 \tag{4}$$

By plotting $\ln\left(IE^{-4}/q\right)_{v'v''}$ against G(v′), a straight line is obtained whose slope is *hc/kT* from which *T* can be calculated. Here, the effective vibrational temperature of the source for BS A–X system is determined, and the data required for the evaluation are given in Table 2.

Table 2: Various parameters involved in the calculation of vibrational temperature.

Band	$\lambda_{v'v''}$(Å)	I	$q_{v'v''}$	G(v′) (in cm^{-1})	$\ln\left(IE^{-4}/q\right)_{v'v''}$
1,0	5969.3	2	0.038	1119.907	99.446
2,0	5721.0	6	0.068	1854.837	98.760
3,0	5492.0	4	0.109	2580.427	99.474
4,0	5283.0	9	0.139	3296.677	98.751
5,0	5092.8	9	0.147	4003.587	98.660
6,0	4917.0	7	0.137	4701.157	98.700
7,0	4753.5	8	0.114	5389.387	98.248
8,0	4611.0	5	0.087	6068.277	98.326
9,0	4472.0	2	0.062	6737.827	98.781
10,0	4342.8	4	0.041	7398.037	97.557

2.3 Effect of Vibration Rotation Interaction

It is widely known that the intensity of a spectral line of a diatomic molecule is influenced by vibration rotation interaction (VRI) effect.[16] According to Gowda, it was found that larger the change in $|\Delta r_0 - \Delta r_e|$ value, the greater will be the influence of VRI on FCFs.[17]

The minimum of effective potential is given by:

$$r_0 = r_e\left[1 + 4B_e^2 J(J+1)/\omega_e^2\right] \tag{5}$$

where r_e, B_e and ω_e are molecular constants, and J is the rotational quantum number. The effect of VRI on FCFs is negligible in case of few diatomic molecules for relatively lower values of J. However, for higher values of J there may be an appreciable influence of VRI on FCFs. Hence, it is necessary to ensure this effect for the diatomic molecules of astrophysical interest. Hence, a study on the effect of VRI on FCFs for certain band systems of BS molecule has been carried out using the molecular constants reported by Huber and Herzberg, and the results of this effect are discussed in the following section.[13]

3. RESULTS AND DISCUSSION

Table 1 provides the set of FCFs and r-centroids for the A–X band system for BS molecule. The FCFs of A–X system of BS evaluated in the present study indicates that the (3,0), (4,0), (5,0), (6,0), (7,0), (2,1) and (3,1) bands are intense compared to others. It is worth mentioning that the r-centroid values are found to increase linearly with the corresponding wavelength following $r_{e'} > r_{e''}$ and hence the band system is expected as red degraded. Singh and Tewari also observed that the bands of the A–X system were red degraded and the band origin was located at 16,002.2 cm^{-1}.[12]

As mentioned in the previous section, the vibrational temperature of the source is calculated by choosing only the bands whose experimental band intensities are available in the literature. The parameters used for the evaluation of vibrational temperature are given in Table 2.

A graphical plot of $\ln\,(IE^{-4}/q)_{v'v''}$ versus $G(v')$ for A–X band system for BS molecule is shown in Figure 1 and a straight line is fitted for the plot by least-squares method. From the slope, the effective vibrational temperature of 6893 K is obtained by assuming that the electronic transition moment is constant over the range of study. The slope of the straight line shown in Figure 1 has a very small standard deviation of 5.75×10^{-5}. The effective vibrational temperature obtained for the source of BS, A–X band system is not in the range of temperature of sunspots available in the literature. Hence, it is clear from the vibration band analysis that the possibility for the presence of BS molecule in the sunspot is very less.

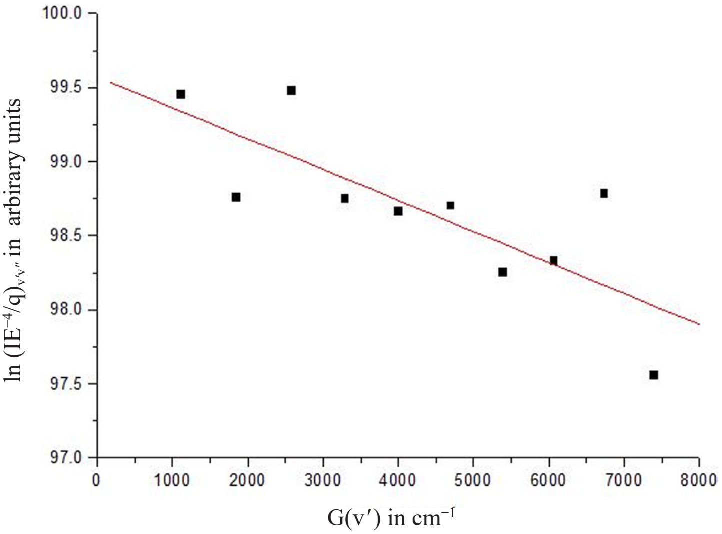

Figure 1: Plot of ln (IE^{-4}/q)$_{v'v''}$ versus G(v′) for A–X band system.

However, it was already reported in the literature that the rotational temperatures of various bands of A–X and B–A systems of BS molecule lie in the value around 1500 K.[8] This contradiction in the effective temperature of the source can be explained by considering the VRI effect as follows.

It is well known that the value of $|\Delta r_0 - \Delta r_e|$ may serve as an indicator to represent the effect of VRI on FCFs. Table 3 gives the values of $|\Delta r_0 - \Delta r_e|$ for the A–X band system of BS molecule.

Table 3: Effect of VRI on FCFS.

		When J = 50		When J = 100		When J = 200	
System	Δr_e (Å)	Δr_0 (Å)	$\|\Delta r_0 - \Delta r_e\|$ (Å)	Δr_0 (Å)	$\|\Delta r_0 - \Delta r_e\|$ (Å)	Δr_0 (Å)	$\|\Delta r_0 - \Delta r_e\|$ (Å)
A–X	0.2090	0.2141	0.0051	0.2293	0.02037	0.2900	0.2849

It is apparent from the results contained in Table 3 that the FCFs are affected significantly with increase in *J* for the A–X band system of BS molecule, since $|\Delta r_0 - \Delta r_e|$ increases with increasing *J* values. Thus, it is not advisable in neglecting the VRI effect at the time of identification of BS molecule in celestial object. This may be reason for obtaining very high vibrational temperature for BS molecule in the present study because of neglecting the rotational lines and by considering only the vibrational bands. Hence, the identification of BS molecule in the sunspot or in any celestial object can be done only with the help of rotational lines as performed by Karthikeyan et al.[8]

4. CONCLUSION

The FCFs and r-centroids have been derived and their physical significance is discussed. The vibrational temperature of the source has been evaluated using the standard procedure and it is observed that the discrepancy in the observed temperature of the sunspot might be due to the VRI effect on FCFs. The results of the present study reveal the valuable information that the identification of a diatomic molecule in interstellar medium or nebula or in any celestial object can be done only by performing the line identification technique and by deriving the rotational temperature.[8]

5. ACKNOWLEDGEMENTS

Authors B. Karthikeyan and G. Shanmugapriya thank the management of Mepco Schlenk Engineering College and VVV College for Women, India for their support towards the research.

6. REFERENCES

1. Singh, M (1988). Spectral studies of molecules of astrophysical interest *Astrophys. Space Sci.*, 141(1), 75–101, https://doi.org/10.1007/BF00641917.
2. Rajamanickam, N. (1985). Intensity distribution in the bands of the $D^1\Pi \rightarrow X^1\Sigma^+$ system of SnO. *Pramana. J. Phys.*, 25(2), 179–186, https://doi.org/10.1007/BF02847657.
3. Rajamanickam, N. (1987). Intensity distribution in band spectra and dissociation energies of diatomic molecules. PhD diss., Mysore University, India.
4. Hui, L. & Yue-Feng, Q. (2012). Spectroscopic properties of $X^2\ \Sigma^+$, $C^2\ \Pi$ and $G^2\ \Sigma^+$ electronic states of BS radical. *J. Xinyang Normal Uni. Nat. Sci. Ed.*, 25(109), 35 – 40.
5. Johnson, H. R. & Sauval, A. J. (1982). Molecules in red-giant stars: Column densities in models for K and M stars. *A A Suppl. Ser.*, 49, 77–87.
6. Charfman, J. J. (1980). Detection of interstellar BS in the cirrus dark cloud of the Numbbum association: I. An intuitive model and its subsequent observation. *Symp. Int. Astron. Un.*, 645–648. https://doi.org/10.1017/S0074180900073447.
7. Karthikeyan, B., Rajamanickam, N. & Bagare, S. P. (2007). Some useful data for the astrophysical molecules AlSand BS. *Astropart. Phys.*, 27(5), 82–385, https://doi.org/10.1016/j.astropartphys.2006.12.006.

8. Karthikeyan, B. et al. (2009). On the search of for BF, BH and BS molecular lines in sunspot spectra. *Astropart. Phys.*, 31(1), 6–12. https://doi.org/10.1016/j.astropartphys.2008.10.009.
9. Bates, D. R. (1949). The intensity distribution in the nitrogen band systems emitted from the earth’s upper atmosphere. *Proc. Roy. Soc.*, A196(1045), 217–250, https://doi.org/ 10.1098/rspa.1949.0025.
10. Partal Urena, F. et al. (2000). Astrophysical molecules AID and CaH: Transition probabilities and dissociation energy. *Astrophys. Space Sci.*, 272(4), 345–352, https://doi.org/10.1023/A:1002661027470.
11. Morse, P. M. (1929). Diatomic molecules according to the wave mechanics: II. Vibrational levels. *Phys. Rev.*, 34, 57–64, http://dx.doi.org/10.1103/PhysRev.34.57.
12. Singh, J., Tewari, D. P. &Mohan, H. (1971). Thermally excited emission spectrum of gaseous boron monosulphide. *Ind. J. Pure Appl. Phys.*, 9, 269.
13. Huber, K. P. & Herzberg, G. (1979). *Molecular spectra molecular structure: IV. Constants of diatomic molecules*. New York: Van Nostrand Reinhold.
14. Herzberg, G. (1950). *Molecular spectra and molecular structure: I. Spectra of diatomic molecules*, 2nd ed. New York: Van Nostrand Reinhold.
15. Thorne, A. P. (1974). *Spectrophysics*. London: Chapman and Hall.
16. Kemble, E. C. (1925). The application of the correspondence principle to degenerate systems and the relative intensities of band lines. *Phys. Rev.*, 25, 1–22, https://doi.org/10.1103/PhysRev.25.1.
17. Siddarame Gowda, L. & Sreedhara Murthy, N. (1976). An index of the influence of vibration rotation interaction on intensities in electronic spectra of diatomic molecules. *Ind. J. Pure Appl. Phys.*, 4, 238–239.