ESTIMATION OF VIBRATIONAL TEMPERATURE AND TRANSITION PROBABILITY PARAMETERS OF ^{121}SbO MOLECULE

PONSAMY SRIRAMACHANDRAN, RAMACHANDRAN SHANMUGAVEL,
NARAYANAN RAJAMANICKAM

Physics Research Centre, VHNSN College
Virudhunagar – 626 001, India
E-mail: `sri_ramnivash@rediffmail.com`

Abstract. Franck-Condon (FC) factors and *r*-centroids for the $a_1^4\Pi_{3/2} - X_1^2\Pi_{1/2}$, $a_2^4\Pi_{1/2} - X_1^2\Pi_{1/2}$, $a_4^4\Pi_{-1/2} - X_1^2\Pi_{1/2}$ and $b_1^4\Sigma^- - X_1^2\Pi_{1/2}$ band systems of the antimony monoxide molecule have been estimated by a numerical integration method, by using a suitable potential. The measured intensity of the experimentally known bands and the estimated FC factors were used to estimate the effective vibrational temperature for the $a_1^4\Pi_{3/2} - X_1^2\Pi_{1/2}$, $a_2^4\Pi_{1/2} - X_1^2\Pi_{1/2}$ and $a_4^4\Pi_{-1/2} - X_1^2\Pi_{1/2}$ band systems of ^{121}SbO molecule. It is concluded that ^{121}SbO is likely to be present in the atmosphere of K type stars and interstellar space.

Key words: astrophysics – FC factors – *r*-centroids – effective vibrational temperature – SbO molecule.

1. INTRODUCTION

Molecular bands of many diatomic molecules are found in the spectra of stellar radiation. Intensities of these bands could be used to estimate the effective vibrational temperature, which is important for the astrophysicists in studying the conditions of stellar atmospheres. The band spectroscopic method for the determination of effective temperatures of interstellar molecules is a key tool in astrophysics to determine the chemical composition of stars and interstellar space.

Franck-Condon (FC) factors are essential parameters for every molecular band system, since they enter into the calculation of the relative band intensity, which is significant source of information in quantitative physics, astrophysics, gas kinetics and combustion physics. The knowledge of *r*-centroids has been found very useful in the discussion of the variation of the electronic transition moment with the internuclear

separation and the band strengths. Variation of *r*-centroids with band wavelengths provides useful connection between experimental measurements, which are often expressed as a function of wavelength, and theoretical estimation, which are often made in terms of internuclear separation. Accurate values of FC factors and *r*-centroids are essential to arrive at the variation of electronic transition moment, band strength, radiative lifetime and effective vibrational temperature of the source (Rajamanickam 1985, 1987).

Spectra of the radiation coming from astronomical sources point out many bands that are attributed to diatomic molecules. A number of lighter (as well as heavier) diatomic molecules have been detected in stellar spectra, in the Earth's atmosphere, in planets and in interstellar sources.

We must emphasize the fact that, dealing with 300 diatomic molecules of known (or of possible) astrophysical interest, Sauval and Tatum (1984) have also reported polynomial expressions of the partition functions and equilibrium constants of the SbH, SbO, SbF and SbP molecules.

Based on estimates of the abundances of Sb, the oxide of antimony is expected to be present in stars. Estimates of the relative abundances of these metallic species are of importance for the understanding of the evolutionary phases of the observed stars, and are also essential inputs in the modeling of the stellar atmospheres of late type stars. Their relative abundances in the interstellar medium give estimates of stellar activity, such as supernovae, in the observed region. Suresh Kumar et al. (2003) have reported that the SbO molecule is likely to be present in the atmosphere of K-type stars and in the interstellar space.

The FC factors and *r*-centroids for $A^2\Pi_{3/2} - X^2\Pi_{3/2}$ and $B^1\Pi - X^1\Sigma^+$ band systems of ^{123}SbO, $C^2\Sigma - X^2\Pi_{3/2}$ and $D^2\Pi - X^2\Pi$ band systems of ^{121}SbO molecules have been reported by Sriramachandran et al (2008). In the present paper, the reliable values of the FC factors and *r*-centroids for the $a_1^4\Pi_{3/2} - X_1^2\Pi_{1/2}$, $a_2^4\Pi_{1/2} - X_1^2\Pi_{1/2}$, $a_4^4\Pi_{-1/2} - X_1^2\Pi_{1/2}$ and $b_1^4\Sigma^- - X_1^2\Pi_{1/2}$ band systems of the ^{121}SbO molecule have been computed by resorting to a numerical integration procedure, which uses the RKR (Rydberg-Klein-Rees) potential. The effective vibrational temperatures for the $a_1^4\Pi_{3/2} - X_1^2\Pi_{1/2}$, $a_2^4\Pi_{1/2} - X_1^2\Pi_{1/2}$ and $a_4^4\Pi_{-1/2} - X_1^2\Pi_{1/2}$ band systems of the ^{121}SbO molecule have been reported. Knowledge of the FC factors and *r*-centroids of these bands will undoubtedly aid the spectroscopists in the search for and the interpretation of the intensity distribution among the observed bands.

The procedure for computing the FC factors, *r*-centroids, electronic transition moment, band strength and effective vibrational temperature of the source using ^{121}SbO molecule is described in the following section.

2. THEORY AND COMPUTATIONAL PROCEDURE

2.1. FRANCK-CONDON FACTORS AND *r*-CENTROIDS

In an electronic transition between the vibrational levels ν' and ν'' of a diatomic molecule, the square of the overlap integral is termed as the FC factor (Bates 1952):

$$q_{\nu'\nu''} = \left| \left\langle \psi_{\nu'} \mid \psi_{\nu''} \right\rangle \right|^2, \tag{1}$$

where $\psi_{\nu'}$ and $\psi_{\nu''}$ are the vibrational wave functions for the upper and lower electronic states, respectively, between which the transition takes place.

The *r*-centroids $\bar{r}_{\nu'\nu''}$ represent the unique value of average internuclear separation of a transition in a diatomic molecular band system and are defined by

$$\bar{r}_{\nu'\nu''} = \frac{\left\langle \psi_{\nu'} \mid r \mid \psi_{\nu''} \right\rangle}{\left\langle \psi_{\nu'} \mid \psi_{\nu''} \right\rangle}. \tag{2}$$

The computation of FC factors is made by Bates' (1949) method of numerical integration according to the detailed procedure provided by Partel Urena et al. (2000). The accuracy of the FC factors depends on the potential energy used. The best results are obtained using the RKR potential, but in many cases a Morse curve fits very well to the numerical RKR potential derived from the spectroscopic data, particularly for low quantum levels. In this manner, the RKR potential function yields reliable FC factor and *r*-centroid values especially for a band in an electronic transition involving low vibrational quantum numbers. The required molecular constants for the present study have been taken from Alekseyev et al. (1995) and Shestakov and Fink (1995) and are listed in Table 1.

Table 1

Molecular constants for ^{121}SbO molecule

Molecule	States	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	r_e (Å)	B_e*	α_e*
SbO	$X_1^2\Pi_{1/2}$	817.8	4.13	1.826	0.358	0.00225
	$a_1^4\Pi_{3/2}$	558.0	2.95	2.067	0.279	0.00189
	$a_2^4\Pi_{1/2}$	559.4	3.09	2.067	0.279	0.00195
	$a_4^4\Pi_{-1/2}$	558.3	2.93	2.065	0.280	0.00188
	$b_1^4\Sigma^-$	609.6	7.70	1.958	0.311	0.00379
	$\mu = 14.1261081$ a.m.u					

* from Gallas et al. (1979) formula

Many authors have employed the RKR potential method and have constructed the potential energy curves (Reddy et al. 1999; Kuzmanović et al. 2005). Therefore the potential energy curves have been here constructed resorting to the method of the RKR potential by utilizing the molecular constants in Table 1 and the results are presented in Table 2.

Table 2

Potential Energy Curves for the Electronic State of ^{121}SbO Molecule

$X_1^2\Pi_{1/2}$ -State			
v	$G(v)$	r_{max} (Å)	r_{min}(Å)
0	408	1.88	1.77
1	1217	1.93	1.74
2	2019	1.96	1.72

$a_1^4\Pi_{3/2}$ -State			
v	$G(v)$	r_{max} (Å)	r_{min}(Å)
0	278	2.14	2.00
1	830	2.19	1.96
2	1377	2.23	1.94
3	1917	2.27	1.92
4	2451	2.30	1.90
5	2980	2.33	1.88
6	3502	2.35	1.87
7	4019	2.38	1.86
8	4530	2.41	1.85

$a_2^4\Pi_{1/2}$ -State			
v	$G(v)$	r_{max} (Å)	r_{min}(Å)
0	279	2.14	2.01
1	832	2.19	1.96
2	1379	2.23	1.94
3	1920	2.27	1.92
4	2455	2.30	1.90
5	2983	2.33	1.88
6	3506	2.36	1.87
7	4022	2.38	1.86
8	4532	2.41	1.85
9	5035	2.43	1.84
10	5533	2.46	1.83
11	6024	2.48	1.82
12	6510	2.51	1.81
13	6989	2.53	1.80

$a_4^4\Pi_{-1/2}$ -State			
v	$G(v)$	r_{max} (Å)	r_{min}(Å)
0	278	2.13	2.00
1	831	2.19	1.96
2	1377	2.23	1.93
3	1918	2.27	1.91
4	2453	2.30	1.90
5	2982	2.33	1.88
6	3505	2.35	1.87
7	4022	2.38	1.86

$b_1^4\Sigma^-$ -State			
v	$G(v)$	r_{max} (Å)	r_{min}(Å)
0	303	2.03	1.90
1	897	2.08	1.86
2	1476	2.13	1.84
3	2039	2.17	1.82
4	2587	2.20	1.81

The vibrational wave functions have been calculated at intervals of 0.01Å for the range of r, respectively from 1.72 Å to 2.43 Å, from 1.70 Å to 2.55 Å, from 1.75 Å to 2.37 Å and from 1.70 Å to 2.22 Å for the observed vibrational band systems $a_1^4\Pi_{3/2} - X_1^2\Pi_{1/2}$, $a_2^4\Pi_{1/2} - X_1^2\Pi_{1/2}$, $a_4^4\Pi_{-1/2} - X_1^2\Pi_{1/2}$ and $b_1^4\Sigma^- - X_1^2\Pi_{1/2}$ of

[121]SbO molecule. Integrals in (1) and (2) for the FC factors ($q_{v'v''}$) and r-centroids ($\bar{r}_{v'v''}$) have been computed numerically, and the results are tabulated in Tables 3–6 for the respective band systems of the [121]SbO molecule.

Table 3

FC factors, r-centroids, wavelengths, intensities and band strengths

for the $a_1^4\Pi_{3/2} - X_1^2\Pi_{1/2}$ band system

v',v''	$q_{v'v''}$	$\bar{r}_{v',v''}$ (Å)	$\lambda_{v'v''}$ (Å)	$I_{v'v''}$	$P_{v'v''}$
1, 0	0.002	1.928	5784.24	3	0.000003
1, 1	0.015	1.945	6068.39		0.000011
2, 0	0.006	1.916	5606.95	8	0.000011
3, 0	0.015	1.905	5441.95	9	0.000034
4, 0	0.029	1.894	5288.18	9	0.000081
4, 1	0.089	1.910	5524.69		0.000180
5, 0	0.046	1.883	5144.37	10	0.000157
6, 0	0.064	1.873	5009.70	8	0.000258
7, 0	0.080	1.863	4883.04	9	0.000375
8, 0	0.091	1.853	4765.13	9	0.000492

Table 4

FC factors, r-centroids, wavelengths, intensities and band strengths

for the $a_2^4\Pi_{1/2} - X_1^2\Pi_{1/2}$ band system

v',v''	$q_{v'v''}$	$\bar{r}_{v',v''}$ (Å)	$\lambda_{v'v''}$ (Å)	$I_{v'v''}$	$P_{v'v''}$
1, 0	0.002	1.929	5688.53	3	0.000013
1, 1	0.014	1.946	5963.35		0.000113
1, 2	0.049	1.964	6262.73		0.000488
2, 0	0.006	1.917	5516.82	7	0.000032
2, 1	0.036	1.934	5774.92		0.000248
2, 2	0.089	1.951	6055.20		0.000762
3, 0	0.014	1.906	5357.47	4	0.000064
4, 0	0.027	1.895	5208.15	9	0.000101
4, 1	0.086	1.911	5437.46		0.000423
5, 0	0.043	1.884	5068.39	2	0.000130
6, 0	0.061	1.874	4937.65	7	0.000149
6, 1	0.084	1.889	5143.17		0.000281
7, 0	0.076	1.864	4814.80	10	0.000146
8, 0	0.087	1.855	4699.44	9	0.000131
10, 0	0.093	1.836	4488.24	1	0.000074
11, 0	0.088	1.827	4391.48	1	0.000047
12, 0	0.08	1.819	4300.00		0.000028
13, 0	0.07	1.810	4213.38		0.000013

Table 5

FC factors, *r*-centroids, wavelengths, intensities and band strengths

for the $a_4^4\Pi_{-1/2} - X_1^2\Pi_{1/2}$ band system

v',v''	$q_{v'v''}$	$\bar{r}_{v',v''}$ (Å)	$\lambda_{v'v''}$ (Å)	$I_{v'v''}$	$P_{v'v''}$
1, 0	0.002	1.927	–		0.000049
2, 0	0.007	1.915	5356.52	4	0.000155
3, 0	0.016	1.904	5205.82	4	0.000324
4, 0	0.031	1.893	5064.82	6	0.000572
5, 0	0.049	1.882	4932.41	10	0.000818
6, 0	0.067	1.872	4808.54	7	0.001017
7, 0	0.082	1.861	4691.72		0.001115

Table 6

FC factors, *r*-centroids and wavelengths

for the $b_1^4\Sigma^- - X_1^2\Pi_{1/2}$ band system

v',v''	$q_{v'v''}$	$\bar{r}_{v',v''}$ (Å)	$\lambda_{v'v''}$ (Å)
0, 0	0.067	1.893	4146.28
0, 1	0.200	1.921	4290.37
0, 2	0.275	1.950	4443.04
1, 0	0.147	1.872	4046.53
1, 1	0.187	1.898	–
1, 2	0.063	1.924	–
2, 0	0.185	1.853	3953.94
2, 1	0.063	1.875	–
2, 2	0.023	1.912	–
3, 0	0.176	1.835	3867.72
3, 1	0.002	1.832	–
3, 2	0.098	1.888	–
4, 0	0.141	1.818	3787.44
4, 1	0.017	1.851	–
4, 2	0.087	1.867	–

2.2. ELECTRONIC TRANSITION MOMENT

The integrated intensity in emission of a vibrational band $v'-v''$ can be written as

$$I_{v'v''} = \frac{64\,\pi^4}{3} N_{v'} \lambda_{v'v''}^{-4} R_e^2 (\bar{r}_{v'v''}) q_{v'v''}, \tag{3}$$

where $\lambda_{v'v''}$ is the wavelength of the transition $v'-v''$, R_e is the electronic transition

moment expressed as a function of *r*-centroid, and $N_{v'}$ is the population in the excited state. The band strength for the transition $v'-v''$ may be expressed as

$$P_{v'v''} = R_{\mathrm{e}}^2 (\bar{r}_{v'v''}) q_{v'v''} . \tag{4}$$

Fraser (1954) has suggested that observed intensities can be used to determine the functional form of electronic transition moment by means of "the *r*-centroid method". From (3), the variation of R_{e} as a function of $\bar{r}_{v'v''}$ can be written as

$$R_{\mathrm{e}} (\bar{r}_{v'v''}) \propto N_{v'}^{-1} \left(\frac{I\lambda^4}{q} \right)_{v'v''}^{1/2} . \tag{5}$$

Thus a plot of $(I\lambda^4/q)_{v'v''}^{1/2}$ versus $\bar{r}_{v'v''}$ for each progression illustrates the dependence of $R_{\mathrm{e}}(\bar{r}_{v'v''})$ on r-centroid for bands of a progression. The family of curves obtained for each progression may be rescaled to eliminate the population factor and hence in result got a single smooth curve showing the variation of R_{e} as a function of $\bar{r}_{v'v''}$ for the band system. The electronic transition moment and band strength values are tabulated in the respective tables.

2.3. RADIATIVE LIFETIME

The radiative lifetime ($\tau_{v'}$) of a vibrational level depends on the sum of the transition probabilities to all lower vibrational levels in all lower electronic states. If rotational effects are neglected, the lifetime can be written as

$$\tau_{v'} = \left(\sum_{v'} A_{v'v''} \right)^{-1} , \tag{6}$$

where $A_{v'v''}$ is the probability of spontaneous emission per second from the level (v') to the level (v'') and the sum is taken over all levels of the ground state for which the transition is allowed. Therefore

$$A_{v'v''} = 2.026 \times 10^{-6} \, g \bar{v}_{v'v''}^3 \left| R_e (\bar{r}_{v'v''}) \right|^2 , \tag{7}$$

where $\bar{v}_{v'v''}^3$ is the transition energy in cm^{-1} between the levels (v') and (v''), whereas g is a statistical weighting factor, equal to two for $\Sigma \to \Pi$ transitions and unity for all other transitions.

2.4. EFFECTIVE VIBRATIONAL TEMPERATURE OF THE SOURCE

In case, the intensity of a sufficient number of bands cannot be measured and the band system has only the intensity of diagonal elements, a determination of the effective vibrational temperature can still be obtained if the overlap integrals are calculated for the measured bands (Herzberg 1950) using the following equation (Thorne 1974):

$$\log\left(\frac{I\lambda^4}{q}\right)_{v'v''} = \text{const.} - \left\{\frac{hc}{KT}G(v')\right\} \tag{8}$$

where $\lambda_{v'v''}$ is the wavelength of the band, h is the Planck's constant, c is the speed of light, K is the Boltzmann's constant, T is the effective vibrational temperature of the source radiating the band system and $G(v')$ is the vibrational quantum of energy of the molecule in the level v'. The vibrational quanta $G(v')$ have been calculated from the expression

$$G(v') = \omega_e'(v'+1/2) - \omega_e'x_e'(v'+1/2)^2 . \tag{9}$$

Therefore by plotting $\log\left(\frac{I\lambda^4}{q}\right)_{v'v''}$ against $G(v')$, a straight line can be obtained by the method of least-square fit, and its slope will yield a value of the effective vibrational temperature of the source.

The wavelengths $(\lambda_{v'v''})$ data and the relative intensities of the respective band systems $R_{k1}^{\text{obs}}(I_{v'v''})$ used in the present study have been collected from the paper by Shestakov and Fink (1995).

3. RESULTS AND DISCUSSION

The computed FC factor values for the bands of four systems of SbO molecule are listed in Tables 3–6, together with r-centroids, experimentally known wavelengths and the visually estimated band intensities. As can be seen, the FC factor values of 0, 0 band for the transition from the $X_1^2\Pi_{1/2}$ ground state to three spin-orbit components of the $a^4\Pi$ states are zero. The wavelength values for the said bands reported by Shestakov and Fink (1995) are just calculated ones, not experimentally observed in the Laser-Induced Fluorescence (LIF) excitation spectra. The distribution of the values of FC factors in the v', v'' scheme indicates that all the band systems have weak transitions. It can be seen that the vibrational sum rule is not satisfied for the experimentally known

progression of all the systems of the [121]SbO molecule. Therefore, it is suggested that if more experimental work is done on the band spectrum of this molecule; it may yield more new bands of high intensity.

The computed *r*-centroid values of each band of the systems are notably connected with the experimentally observed wavelengths of the corresponding bands. The presented data of each band system shows that in Fig. 1, the *r*-centroid $(\bar{r}_{v'v''})$ is an increasing function of wavelength $(\lambda_{v'v''})$ in each progression, which is to be expected in a red-degraded band system. It is also noted that the sequence differences $\Delta \bar{r}_{v'v''} = \bar{r}_{v'+1,v''+1} - \bar{r}_{v'v''}$ was not found to be constant for a given sequence, and it can be interpreted that the potential curves are wide.
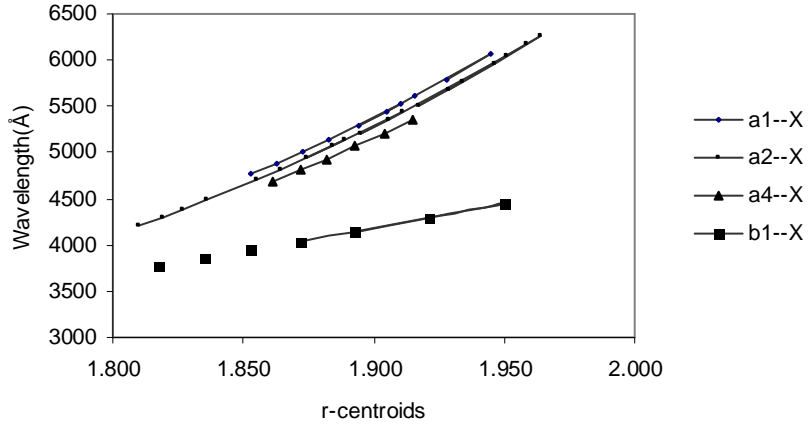

Fig. 1 – Plot of the *r*-centroid versus wavelength.

The relative band intensities have been estimated by visually scaling with the most intense band as 10 units for the $a_1^4\Pi_{3/2} - X_1^2\Pi_{1/2}$, $a_2^4\Pi_{1/2} - X_1^2\Pi_{1/2}$ and $a_4^4\Pi_{-1/2} - X_1^2\Pi_{1/2}$ systems of the [121]SbO molecule except the $b_1^4\Sigma^- - X_1^2\Pi_{1/2}$ system. The estimated FC factors, *r*-centroids and estimated intensities were used to obtain the relations between the electronic transition moment and the internuclear separation for the [121]SbO molecule as

[121]SbO: $a_1^4\Pi_{3/2} - X_1^2\Pi_{1/2}$: $R_e(\bar{r}_{v'v''}) = const.(1 - 0.50r)$; $1.72 \le r \le 2.43$ Å;

$a_2^4\Pi_{1/2} - X_1^2\Pi_{1/2}$: $R_e(\bar{r}_{v'v''}) = const.(1 - 0.56r)$; $1.70 \le r \le 2.45$ Å;

$a_4^4\Pi_{-1/2} - X_1^2\Pi_{1/2}$: $R_e(\bar{r}_{v'v''}) = const.(1 - 0.60r)$; $1.75 \le r \le 2.37$ Å.

Since the intensities are the estimated values, these relations are expected to be not very far from the actual ones. The *r*-centroid method ascribes all discrepancies between the calculated and observed intensities to the variation of R_e as a function of $\bar{r}_{v'v''}$, it should be emphasized that the results can only be valid if both the experimental intensity and the calculated FC factors are highly accurate.

The radiative lifetime for the $a_1^4\Pi_{3/2} - X_1^2\Pi_{1/2}$, $a_2^4\Pi_{1/2} - X_1^2\Pi_{1/2}$ and $a_4^4\Pi_{-1/2} - X_1^2\Pi_{1/2}$ band systems of ^{121}SbO molecule were estimated to be 206.79 µs, 189.82 µs and 135.71 µs, respectively. (Shestakov and Fink 1995) obtained the experimental radiative lifetime of 190 ± 10 µs for the $a_2^4\Pi_{1/2} - X_1^2\Pi_{1/2}$ system of ^{121}SbO molecule. This excellent agreement between the experimental and estimated radiative lifetime value of the $a_2^4\Pi_{1/2} - X_1^2\Pi_{1/2}$ band system is also evident that the experimental intensity, estimated FC factors and *r*-centroids are reliably accurate.
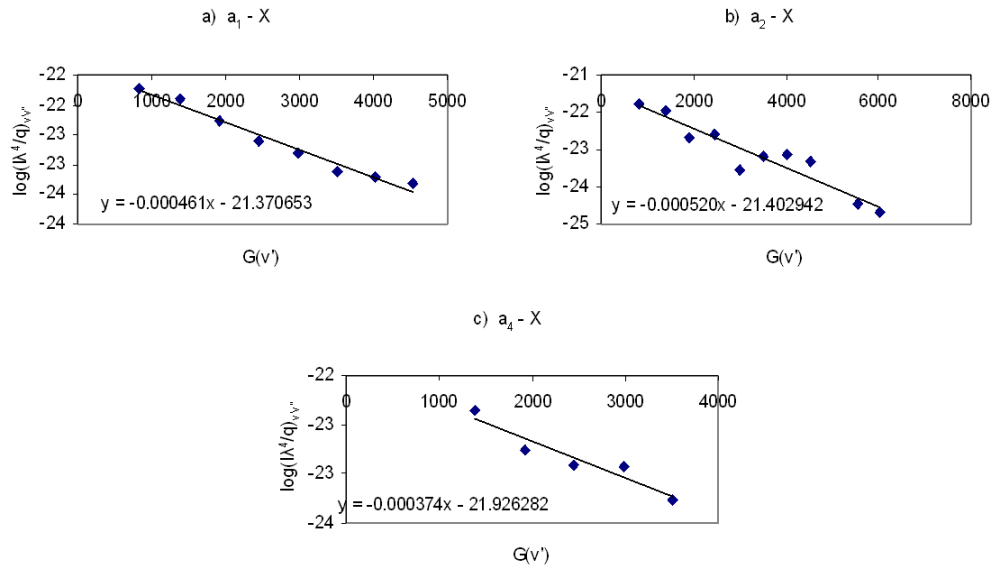

Fig. 2 – Plot of $\log(I\lambda^4/q)_{v'v''}$ versus $G(v')$.

The relative intensities of (v', 0) bands could be known only for $a_1^4\Pi_{3/2} - X_1^2\Pi_{1/2}$, $a_2^4\Pi_{1/2} - X_1^2\Pi_{1/2}$ and $a_4^4\Pi_{-1/2} - X_1^2\Pi_{1/2}$ band systems. Therefore the effective vibrational temperatures of the source using these ^{121}SbO molecular systems have determined from (3). A similar way of calculation was made for PbO (B – X) system by Rajamanickam (1988). A graphical plot of $\log(I\lambda^4/q)_{v'v''}$

versus $G(v')$ for the $a_1^4\Pi_{3/2} - X_1^2\Pi_{1/2}$, $a_2^4\Pi_{1/2} - X_1^2\Pi_{1/2}$ and $a_4^4\Pi_{-1/2} - X_1^2\Pi_{1/2}$ systems of ^{121}SbO molecule is shown in Fig. 2 and the straight lines have obtained by using the method of least square fit.

From slopes, the effective vibrational temperatures of 1507 ± 93 K, 1336 ± 159 K and 1858 ± 349 K were estimated assuming the electronic transition moment as constant over the range of study for the respective systems. The effective rotational temperature estimated earlier (Sureshkumar et al. 2003) for the main band system B – X of the ^{121}Sb^{16}O molecule is to be 4730 ± 111 K. L-type brown dwarfs have surface temperatures of about 1300–2000 K (Andersson et al. 2003). Therefore, the estimated data provide further evidence to ascertain the possible presence of SbO molecule in near star forming regions and in circumstellar envelopes of late-type stars.

REFERENCES

Aleksyev, A. B., Liebermann, H.-P., Buenker, R. J., Hirsch, G.: 1995, *J. Chem. Phys.*, **102**, 2539.

Andersson, N., Balfour, W. J., Bernath, P. F., Lindgren, B., Ram, R. S.: 2003, *J. Chem. Phys.*, **118**, 3543.

Bates, D. R.: 1949, *Proc. Roy. Soc. A*, **196**, 217.

Bates, D. R.: 1952, *Mon. Not. Roy. Astron. Soc.*, **112**, 614.

Fraser, P. A.: 1954, *Can. J. Phys.*, **32**, 516.

Gallas, J. A. C., Francke, R. E., Grieneisen, H. P., Chakraborty, B. P.: 1979, *Astrophys. J.*, **229**, 851.

Herzberg, G.: 1950, *Molecular Spectra and Molecular Structures*, D. Van Nostrand, New York.

Kuzmanović, M., Antić-Jovanović, A., Pešić, D., Bojović, V.: 2005, *J. Serb. Chem. Soc.*, **70**, 727.

Partel Urena, F., Fernandez Gomez, M., Lopez Gonzalez, J. J., Rajamanickam, N.: 2000, *Astrophys. Space Sci.*, **272**, 345.

Rajamanickam, N.: 1985, *Pramana – J. Phys.*, **25**, 179.

Rajamanickam, N.: 1987, *J. Quant. Spectrosc. Radiat. Transfer*, **37**, 207.

Rajamanickam, N.: 1988, *Pramana – J. Phys.*, **30**, 51.

Reddy, R. R., Nazeer Ahammed, Y., Rama Gopal, K., Abdul Azeem, P., Anjaneyulu, S.: 1999, *Astrophys. Space Sci.*, **262**, 223.

Sauval, A. J., Tatum, J. B.: 1984, *Astrophys. J. Suppl. Ser.*, **56**, 193.

Shestakov, O., Fink, E. H.: 1995, *J. Mol. Spectrosc.*, **172**, 215.

Sriramachandran, P., Raja, V., Rajamanickam, N.: 2008, *J. Serb. Chem. Soc.*, **73**, 65.

Sureshkumar, M. B., Shah, N. R., Ashish, J.: 2003, *Pramana*, **60**, 95.

Thorne, A. P.: 1974, *Spectrophysics*, Chapman and Hall, London.