EVALUATION OF ASTROPHYSICALLY USEFUL PARAMETERS FOR LaO MOLECULE

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Abstract. Vibrational transition probabilities namely Franck-Condon (FC) factors and r-centroids for the band $C^2\Pi_{3/2}$–$A'\,^2\Delta_{5/2}$, $C^2\Pi_{1/2}$–$A'\,^2\Delta_{3/2}$, $C^2\Pi_{3/2}$–$X^2\Sigma^+$, and $C^2\Pi_{1/2}$–$X^2\Sigma^+$, systems of Lanthanum Oxide (LaO) molecule have been calculated. They are very closely related to transition probabilities, which have been evaluated by the more reliable numerical integration using a suitable potential. In each electronic state, wave functions are computed for all observed vibrational levels by numerical solution of the radial Schrödinger equation in which the potential energy function is calculated at equally spaced intervals of 0.01 Å in the range of nuclear separation range. The effect of high rotational quantum numbers on FC factors has been studied. The vibration-rotation interaction (VRI) on the FC factors of molecular band systems is negligible for relatively low rotational quantum numbers (J). Values of FC factors and r-centroids are given for all allowed bands of each system, and the available band wavelengths are also entered in the respective tables.

Key words: LaO, Franck-Condon factors, r-centroids.

1. INTRODUCTION

The molecular band spectroscopic methods for the determination of temperature of sources and for the study of physical processes occurring in various relative sources require an accurate theoretical knowledge of the corresponding potential energy curves and vibrational transition probabilities for the respective band heads in a band system. To a good approximation, the FC factors are proportional to these vibrational transition probabilities. The FC factor of a molecular band plays a controlling role in the determination of the relative band intensity. The theoretical prediction of intensity distribution in the spectra of many diatomic molecules, which are of interest in astrophysics, is necessary for an understanding of the physical-chemical conditions of the emitting sources. The knowledge of r-centroids is also useful in the discussion of the variation of the electronic transition moment with internuclear separation for each

Rom. Astron. J., Vol. **18**, No. 1, p. 21–28, Bucharest, 2008

vibrational band and for the study of other molecular properties. Consequently the transition probability parameters are required for diagnostic applications in astronomy, astrophysics and allied subjects.

The prominent bands of LaO were detected in the absorption spectrum of S-type stars by Keenan (1948) and Bidelman (1953). The presence of bands due to metal oxide LaO was reported in cool stars (an abundant molecule in O Ceti and X Cyg type stars) by Wöhl (1971). Metal oxide molecules were possibly detectable in sunspots on the basis of dissociation energies and metal abundances (Dirscherl et al., 1978). The estimates of relative abundances of these metallic species are important for understanding the evolutionary phases of the stars observed and are also the essential inputs in modeling the stellar atmospheres of the late type stars. Their relative abundances in interstellar medium give estimates of stellar activity like supernovae in the region observed. Similarly their abundance variations in cometary spectra can be used to study the interaction of solar wind with cometary material. Further, the relative abundances of these metallic species are useful in studying the cosmic recipe in these pristine objects.

As there is no report on the FC factor and r-centroid values for the band systems $C^2\Pi_{3/2} - A'^2\Delta_{5/2}$ and $C^2\Pi_{1/2} - A'^2\Delta_{3/2}$ of astrophysical molecule LaO in the literature, we have taken up the evaluation of reliable FC factor and *r*-centroid values for these systems. In the case of $C^2\Pi_{3/2} - X^2\Sigma^+$ and $C^2\Pi_{1/2} - X^2\Sigma^+$ systems of LaO molecule, Prahllad et al. (1985) reported a partial array of FC factors. Hence we have evaluated the FC factors and *r*-centroids for the experimentally observed vibrational levels using the molecular constants from the compilation of Huber and Herzberg (1979). FC factors are not only useful for calculating of individual values, and their band-by-band application, but are also useful in studies of radiative transfer in stellar and other astrophysical atmospheres which contain molecular species. As the molecule is of astrophysical interest, we have taken the present work to evaluate the values of FC factors and *r*-centroids for these band systems of the LaO molecule by the numerical integration method adopting a suitable potential.

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

One of the parameters which control the intensity distribution in the emission of molecular bands is the FC factor, which is the square of the overlap integral between the upper state wave function and the lower state wave function:

$$q_{v'v''} = \left|\langle \psi_{v'} \mid \psi_{v''} \rangle\right|^2 . \qquad (1)$$

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

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

$$\bar{r}_{v'v''} = \langle \psi_{v'} | r | \psi_{v''} \rangle / \langle \psi_{v'} | \psi_{v''} \rangle . \qquad (2)$$

For a proper understanding of the intensity distribution in the band systems of the molecules, it is necessary to choose a suitable potential. In this manner, Morse's (1929) potential function yields reliable FC factor and r-centroid values especially for a band in an electronic transition involving low vibrational quantum numbers (Sriramachandran et al., 2006). The computation of FC factor is made by Bates' (1949) method of numerical integration according to the detailed procedure provided by Rajamanickam et al (2001). Morse wave functions have been calculated at intervals of 0.01Å for the range of r respectively from 1.63 Å to 2.11 Å, from 1.62 Å to 2.12 Å, from 1.59 Å to 2.16 Å and from 1.57 Å to 2.17 Å of observed vibrational band $C^2\Pi_{3/2} - A'^2\Delta_{5/2}$, $C^2\Pi_{1/2} - A'^2\Delta_{3/2}$, $C^2\Pi_{3/2} - X^2\Sigma^+$ and $C^2\Pi_{1/2} - X^2\Sigma^+$ systems of LaO molecule. Integrals in the equations (1) and (2) for the FC factors $(q_{v'v''})$ and r-centroids $(\bar{r}_{v'v''})$ are computed numerically and the results are tabulated in Tables 1 to 4 for the respective band systems of LaO molecule. The available wavelengths $(\lambda_{v'v''})$ data (Green 1971) are also included in the respective tables. The necessary molecular constants have been collected from the compilation of Huber and Herzberg (1979) and Carette (1990).

3. EFFECT OF ROTATIONAL QUANTUM NUMBERS ON FRANCK-CONDON FACTORS

The effect of vibration-rotation interaction (VRI) on the FC factors and band strengths of molecular band system is negligible for relatively low rotational quantum numbers (J). Shumaker (1969) obtained the expression for the minimum r_0 of an effective potential in the case of a vibrating rotator:

$$r_0 = r_e\left[1 + 4J(J+1)B_e^2 / \omega_e^2\right], \qquad (3)$$

where r_e, B_e, and ω_e are the usual spectroscopic constants. This is evident that the main effect of vibration-rotation interaction is the displacement of the minimum of the potential to larger r_0 values with increasing J. The FC factor, neglecting rotation, depends on the value of Δr_e, the difference of the minima of the two potentials for the two participating electronic states. For the vibrating rotator, the change in r_0 with J affects the FC factor and gives an idea of the effect of VRI on FC factor. Consequently, the value of $|\Delta r_0 - \Delta r_e|$ may serve as an indicator to represent the effect of VRI on FC factors. Therefore, the value of $|\Delta r_0 - \Delta r_e|$ is

$$|\Delta r_0 - \Delta r_e| = 4J(J+1)\left\{\left|\frac{B_e'^2 r_e'^2}{\omega_e'^2} - \frac{B_e''^2 r_e''^2}{\omega_e''^2}\right|\right\}. \tag{4}$$

Murthy and Gowda (1977) have revealed that, the larger the value of $|\Delta r_0 - \Delta r_e|$ is, the greater the effect of VRI on FC factors will be.

4. RESULTS AND DISCUSSION

In the case of $C^2\Pi_{3/2} - X^2\Sigma^+$ and $C^2\Pi_{1/2} - X^2\Sigma^+$ band systems, the difference in the internuclear separation is very small (0.004 Å). It is seen from Tables 3 and 4 that the $\Delta v = 0$ sequence bands are most intense. Since only $\Delta v = 0$ sequence bands are experimentally observed, also the theoretical evaluation of these systems for the $\Delta v = \pm 1$, $\Delta v = 0 \pm 2$, etc. sequence band are not desirable, as indicated by the FC factors. Prahllad et al. (1985) reported the partial array of FC factors for these systems. Hence we have evaluated numerically FC factors and r-centroids for the experimentally observed vibrational levels.

The difference in internuclear separation for $C^2\Pi_{3/2} - A'^2\Delta_{5/2}$ and $C^2\Pi_{1/2} - A'^2\Delta_{3/2}$ transitions are small (0.019 Å). The magnitude of the $(q_{v'v''})$ values, as seen from Tables 1 and 2, indicate that the $\Delta v = 0$ sequence bands are most intense. These band systems should therefore be readily observable in sunspots and other astrophysical sources where the molecule is expected to be present under favorable physical conditions of temperature and abundance. The effective rotational temperature of $C^2\Pi_{1/2} - A'^2\Delta_{3/2}$ (0,0) of LaO molecule reported so far is 1897 K under suitable conditions (Sriramachandran et al., 2008). This report also discuss about the favorable conditions for the formation of LaO molecule in cool region of the umbral sunspots.

For a given r_e' and r_e'', the r-centroid values depend only on the difference between v' and v'', but not on their values taken individually. The sequence difference $\Delta\bar{r}_{v'v''}$ $(= \bar{r}_{v'+1,v''+1} - \bar{r}_{v'v''})$ was found to be approximately constant (≈ 0.01 Å) for a given sequence, indicating that the potential curves are not wide (Kuzmanović et al., 2005). For the band systems $C^2\Pi_{3/2} - A'^2\Delta_{5/2}$, $C^2\Pi_{1/2} - A'^2\Delta_{3/2}$, $C^2\Pi_{3/2} - X^2\Sigma^+$, and $C^2\Pi_{1/2} - X^2\Sigma^+$ of LaO molecule, the sequence difference of r-centroid is found to be nearly a constant and is about 0.01 Å, which suggests that the potentials are not wide.

In the case of $C^2\Pi_{3/2} - X^2\Sigma^+$ and $C^2\Pi_{1/2} - X^2\Sigma^+$ band systems, since $r_e' > r_e''$, the presented data show that the r-centroid value has an increasing function of wavelength in each observed progression, which suggests that these bands are degraded to longer wavelength. For the $C^2\Pi_{3/2} - A'^2\Delta_{5/2}$ and $C^2\Pi_{1/2} - A'^2\Delta_{3/2}$ band systems, since $r_e' < r_e''$, the shallower part of the excited state potential is probed, resulting in a sharper intensity distribution and hence the r-centroid value increases with decrease in wavelength, which is to be expected in violet-degraded band systems. These variations are of the expected nature, and the decrease or increase is found to be linear.

Generosa and Harris (1970) reported that the larger value of $|\Delta r_0 - \Delta r_e|$ is 27.60 mÅ ($J = 100$) for the NO $B^2\Pi_r - X^2\Pi_r$ band system, and indicated an appreciable effect of high rotational quantum number on FC factors. Chakraborty et al. (1971) also reported that the relatively low value of $|\Delta r_0 - \Delta r_e|$ is 7.83 mÅ ($J = 100$) for the N_2 $B^3\Pi_g - A^3\Sigma_u^+$ band system and shows a negligible effect on VRI. In the present study, from Table 5, the band systems $C^2\Pi_{3/2} - A'^2\Delta_{5/2}$, $C^2\Pi_{1/2} - A'^2\Delta_{3/2}$, $C^2\Pi_{3/2} - X^2\Sigma^+$, and $C^2\Pi_{1/2} - X^2\Sigma^+$ ($J = 100$) of LaO have relatively low values of $|\Delta r_0 - \Delta r_e|$, and hence the effect of VRI here in the calculated FC factor values is negligible.

Table 1

FC factors, r-centroids for $C^2\Pi_{1/2} - A'^2\Delta_{3/2}$ of LaO molecule

		$v'' = 0$	$v'' = 1$	$v'' = 2$	$v'' = 3$	$v'' = 4$
$v' = 0$	a)	0.945	0.050	0.005	0.001	*
	b)	1.843	1.669	1.650	1.604	
	c)	6607.76	–	–	–	
$v' = 1$	a)	0.055	0.844	0.085	0.014	0.002
	b)	2.007	1.851	1.665	1.650	1.604
	c)	–	6597.05	–	–	–
$v' = 2$	a)	*	0.111	0.727	0.146	0.014
	b)		2.009	1.857	1.699	1.573
	c)		–	6586.35	–	–
$v' = 3$	a)	*	*	0.155	0.677	0.125
	b)			2.013	1.871	1.655
	c)			–	6575.71	–
$v' = 4$	a)	*	*	*	0.199	0.608
	b)				2.017	1.883
	c)				–	6565.52
$v' = 5$	a)	*	*	*	*	0.241
	b)					2.020
	c)					–
$v' = 6$	a)	*	*	*	0.001	*
	b)				1.983	
	c)				–	
$v' = 7$	a)	*	*	*	*	0.001
	b)					1.996
	c)					–

Table 2

FC factors, *r*-centroids for $C^2\Pi_{3/2} - A'^2\Delta_{5/2}$ of LaO molecule

		$v''=0$	$v''=1$	$v''=2$	$v''=3$	$v''=4$
$v'=0$	a)	0.942	0.056	*	*	*
	b)	1.842	1.688			
	c)	6821.54	–			
$v'=1$	a)	0.058	0.831	0.104	*	*
	b)	2.002	1.850	1.694		
	c)	–	6808.87	–		
$v'=2$	a)	*	0.111	0.729	0.145	*
	b)		2.009	1.858	1.700	
	c)		–	6796.29	–	
$v'=3$	a)	*	*	0.159	0.637	0.178
	b)			2.016	1.866	1.707
	c)			–	6783.71	–
$v'=4$	a)	*	*	*	0.202	0.553
	b)				2.023	1.874
	c)				–	6771.16
$v'=5$	a)	*	*	*	0.010	0.241
	b)				2.227	2.030
	c)				–	–
$v'=6$	a)	*	*	*	*	0.014
	b)					2.235
	c)					–

Table 3

FC factors, *r*-centroids for $C^2\Pi_{3/2} - X^2\Sigma^+$ of LaO molecule

v', v''	$q_{v'v''}$ This work	$q_{v'v''}$ (Prahllad)	$\bar{r}_{v'v''}$ This work	$\bar{r}_{v'v''}$ (Prahllad)	$\lambda_{v'v''}$
0, 0	0.998	0.9975	1.831	1.8306	4371.87
1, 1	0.991	0.9923	1.838	1.8366	4375.71
2, 2	0.983	0.9869	1.845	1.8427	4379.61
3, 3	0.975	0.9813	1.852	1.8487	4383.53
4, 4	0.965	0.9755	1.860	1.8548	4387.49
5, 5	0.953	0.9695	1.867	1.8609	4391.47
6, 6	0.941	0.9633	1.875	1.8670	4395.69
7, 7	0.927		1.882		4400.05
8, 8	0.911		1.889		4404.78
9, 9	0.893		1.897		4409.64
10, 10	0.872		1.904		4414.65

Table 4

FC factors, *r*-centroids for $C^2\Pi_{1/2} - X^2\Sigma^+$ of LaO molecule

v', v''	$q_{v'v''}$ This work	$q_{v'v''}$ (Prahllad)	$\bar{r}_{v'v''}$ This work	$\bar{r}_{v'v''}$ (Prahllad)	$\lambda_{v'v''}$
0, 0	0.998	0.9982	1.830	1.8306	4418.13
1, 1	0.992	0.9924	1.838	1.8366	4423.06
2, 2	0.986	0.9865	1.845	1.8427	4427.99
3, 3	0.981	0.9803	1.852	1.8487	4432.95
4, 4	0.975	0.9738	1.859	1.8548	4437.89
5, 5	0.968	0.9661	1.866	1.8608	4442.88
6, 6	0.962	0.9592	1.873	1.8669	4447.92
7, 7	0.956		1.880		4453.06
8, 8	0.950		1.888		4458.36
9, 9	0.943		1.895		4464.06
10, 10	0.936		1.902		4471.20

In all the above tables the notation is: $q_{v'v''}$: FC factor; $\bar{r}_{v'v''}$: *r*-centroid (Å); $\lambda_{v'v''}$: wavelength (Å); *: $q_{v'v''} = 0$.

Table 5

Values of Δr_e and $|\Delta r_0 - \Delta r_e|$
for various band systems of LaO molecule

Band System	Δr_e(Å)	$\lvert\Delta r_0 - \Delta r_e\rvert$ (10^{-3} Å)	
	$J = 0$	$J = 50$	$J = 100$
$C^2\Pi_{3/2} - A'^2\Delta_{5/2}$	0.019	0.1394	0.5520
$C^2\Pi_{1/2} - A'^2\Delta_{3/2}$	0.019	0.5453	2.1599
$C^2\Pi_{3/2} - X^2\Sigma^+$	0.004	0.1181	0.4676
$C^2\Pi_{1/2} - X^2\Sigma^+$	0.004	0.8579	3.3980

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Received on 7 July 2008