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TRANSITION PROBABILITY PARAMETERS FOR CERTAIN BAND SYSTEMS OF THE ASTROPHYSICAL MOLECULE PO

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Abstract. The transition probability parameters, Franck-Condon factors and r-centroids have been evaluated by a new more reliable numerical integration procedure for the bands of the PO molecule in the ultraviolet region (1800–2900 Å). These molecules are likely to be present in the atmospheres of cool stars and comets.

Key words: molecular data: Frank-Condon factors, PO molecule, stars: late-type

1. INTRODUCTION

The theoretical prediction of the intensity distribution in molecular band systems requires the knowledge of vibrational transition probability parameters, which are, to a good approximation, proportional to the Franck-Condon factors. The Frank-Condon (FC) factors and r-centroids are required for diagnostic applications in astronomy, astrophysics and allied subjects. These transition probability parameters are essential to understand and to calculate many

important aspects of the molecules such as the radiative life time, vibrational temperature of the source and relative band strengths. The FC factors are useful in studies of radiative transfer in the atmospheres of stellar and other astronomical objects which contain molecular species (Nicholls 1981).

Johnson and Sauval (1982) discussed in detail the importance of the PO molecule in astrophysics due to its possible presence in cool stars. Sauval and Tatum (1984) noted that the PO molecule may be present in the stellar and cometary spectra. Turner (1995) predicted the possible presence of PO molecule in stellar atmospheres. The estimates of the relative abundance of these molecules are important for understanding the evolutionary phases of the stars observed and are also essential inputs in modeling the stellar atmospheres of late-type stars. Their relative abundances in interstellar medium may 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. Also, the relative abundances of these molecules are useful in studying the cosmic recipe in these pristine objects.

The evaluation of molecular parameters for PO are therefore useful for many astrophysical studies. To our knowledge, there has been no report on the FC factors and r-centroids for the band systems $C'^2\triangle$, $D^2\Pi_r$, $E^2\triangle$, $G^2\Sigma^+$ and $I\Sigma^+ - X^2\Pi_r$ of PO molecule whose transitions are in the ultraviolet region (1800–2900 Å). Therefore we computed the reliable values of FC factors and r-centroids for these band systems of the astrophysical molecule PO by the more accurate numerical integration procedure using a suitable potential.

2. FRANK-CONDON FACTORS AND r-CENTROIDS

Mathematically, one can write for the intensity $I_{\nu'\nu''}$ of a molecular band for a $\nu' - \nu''$ electronic transition in emission as

$$I_{\nu'\nu''} = DN_{\nu'}E^4_{\nu'\nu''}R^2_e(\overline{r}_{\nu'\nu''})\, q_{\nu'\nu''}, \qquad (1)$$

where D is a constant partly depending on the geometry of the equipment, $N_{\nu'}$ is the population of the level ν', $E_{\nu'\nu''}$ is the energy quantum, $q_{\nu'\nu''}$ is the Franck-Condon factor, $\overline{r}_{\nu'\nu''}$ is the r-centroid and R_e is the electronic transition moment. The square of the overlap integral is termed as the FC factor

$$q_{\nu'\nu''} = |<\Psi_{\nu'}|\Psi_{\nu''}>|^2, \qquad (2)$$

where $\Psi_{\nu'}$ and $\Psi_{\nu''}$ are the vibrational wave functions for the upper and lower states, respectively. The r-centroid is a unique value of internuclear separation which may be associated with a $\nu' - \nu''$ band and is defined as

$$\overline{r}_{\nu'\nu''} = \frac{< \Psi_{\nu'} | r | \Psi_{\nu''} >}{< \Psi_{\nu'} | \Psi_{\nu''} >}. \tag{3}$$

The Morse (1929) potential yields accurate FC factors especially for vibrational transition involving low quantum numbers (Partal et al. 2000). The computation of the FC factor was made by the Bates (1949) method of numerical integration according to the detailed procedure provided by Rajamanickam et al. (2001). As the Morse curve represents the electronic state in question, the wave functions are evaluated at suitable intervals of r. The range of r values is fixed appropriate to the pair of electronic states depending on the equilibrium internuclear distance. The wave function is normalized according to orthonormality condition, i.e.,

$$\int_{-\infty}^{+\infty} |\Psi_\nu|^2 dr = 1. \tag{4}$$

Once the Morse wave functions are obtained, the FC factors and r-centroids were computed using the integrals in Equations (2) and (3).

A Fortran-77 program, written by us, was used to calculate Morse wave functions at intervals of 0.01 Å for the r values ranging respectively from 1.26 Å to 1.89 Å, from 1.32 Å to 1.63 Å, from 1.34 Å to 1.63 Å, from 1.30 Å to 1.63 Å and from 1.31 Å to 1.59 Å for every observed vibrational level of each state of the band C′–X, D–X, E–X, G–X and I–X systems of PO molecule. The calculated FC factors and r-centroids for these band systems are presented in Tables 1–5, respectively. The available data for wavelengths ($\lambda_{\nu'\nu''}$) (Santaram and Tiruvenganna Rao 1962, Prudhomme and Coquart 1974) for C′–X and E–X systems are also included in the appropriate Tables. The molecular constants used in the present study are collected from the compilation of Huber and Herzberg (1979).

3. RESULTS AND DISCUSSION

In the case of C′–X system of PO molecule, the FC factors indicate that the following bands (0,0), (0,1), (0,2), (0,3), (1,0), (1,3),

(1,4), (1,5), (2,0), (2,2), (2,5), (2,6), (2,7), (3,0), (3,1), (3,4), (3,7), (3,8), (3,9), (4,1), (4,3), (4,9), (4,10), (4,11), (5,1), (5,11), (5,12) and (6,2) are more intense and all other bands are comparatively weak. For the D–X and E–X band system, $\Delta\nu = 0$ sequence bands are most intense followed by $\Delta\nu = \pm 1$ sequence bands. For the G–X band system, the FC factors reveal that the (0,0), (0,1), (1,0), (1,1), (1,2), (2,1) and (3,2) bands are intense and all other bands are weak. In the case of the I–X band system, (0,0), (0,1), (1,0), (1,1) and (2,1) bands are more intense.

For the C′–X system, since $r'_e > r''_e$, the r-centroid values increase with the increase of wavelength which is expected in the red-degraded band system. The r-centroid values for the violet-degraded E–X system increase with the decrease of wavelength, since $r'_e < r''_e$.

The sequence difference for all these systems are found to be a constant and is about 0.01 Å which suggests that the potentials are not so wide. It is of interest to note that the r-centroid value for (0,0) transition is slightly greater than $(r'_e + r''_e)/2$ for all these band systems (except C′ – X) which imply that the potentials are not very anharmonic.

The demand for spectroscopic data for various molecular species in the ultraviolet region has markedly increased due to the fact that observation of astrophysical objects is now possible using space-borne telescopes.

The significant values of the FC factors (transition probabilities) for the studied five systems of PO favour an examination of stellar and cometary spectra for the presence of this molecule. These parameters are useful in studying physical conditions in the atmospheres of the cool stars.

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Table 1. Franck-Condon factors and r-centroids of the C′–X band system. (a) $q_{\nu'\nu''}$, (b) $\overline{r}_{\nu'\nu''}$ (Å), (c) $\lambda_{\nu'\nu''}$ (Å), * $q_{\nu'\nu''} = 0$.

		ν''=0	ν''=1	ν''=2	ν''=3	ν''=4	ν''=5
	(a)	0.173	0.300	0.266	0.158	0.070	0.025
ν'=0	(b)	1.525	1.561	1.595	1.628	1.659	1.691
	(c)	2290.8	2356.7	2425.7	2498.0	2573.8	2653.5
	(a)	0.289	0.099	0.006	0.128	0.199	0.155
ν'=1	(b)	1.501	1.540	1.567	1.605	1.637	1.669
	(c)	2248.9	2323.8	–	2448.3	2521.1	2597.5
	(a)	0.256	0.004	0.146	0.067	0.004	0.102
ν'=2	(b)	1.477	1.495	1.550	1.585	1.613	1.647
	(c)	–	–	2334.5	2401.5	–	–
	(a)	0.159	0.106	0.070	0.024	0.119	0.036
ν'=3	(b)	1.452	1.487	1.531	1.558	1.595	1.627
	(c)	–	–	–	–	–	–
	(a)	0.077	0.175	*	0.111	0.012	0.054
ν'=4	(b)	1.426	1.464		1.540	1.578	1.605
	(c)	–	–	–	–	–	–
	(a)	0.032	0.152	0.067	0.046	0.043	0.073
ν'=5	(b)	1.398	1.439	1.473	1.524	1.550	1.585
	(c)	–	–	–	–	–	–
	(a)	0.011	0.093	0.135	*	0.090	*
ν'=6	(b)	1.369	1.414	1.452		1.532	
	(c)	–	–	–	–	–	–

Table 1 (continued)

		ν''=6	ν''=7	ν''=8	ν''=9	ν''=10	ν''=11	ν''=12
	(a)	0.007	0.002	*	*	*	*	*
ν'=0	(b)	1.722	1.753					
	(c)	–	–					
	(a)	0.081	0.032	0.010	0.002	*	*	*
ν'=1	(b)	1.700	1.731	1.762	1.793			
	(c)	2677.8	–	–	–			
	(a)	0.170	0.138	0.074	0.029	0.009	0.002	*
ν'=2	(b)	1.679	1.709	1.740	1.771	1.802	1.833	
	(c)	2636.2	2702.7	2789.3	–	–	–	
	(a)	0.011	0.106	0.156	0.120	0.062	0.024	0.007
ν'=3	(b)	1.658	1.689	1.719	1.749	1.780	1.811	1.842
	(c)	2569.0	2645.2	2728.0	2814.0	–	–	–
	(a)	0.095	0.012	0.028	0.118	0.144	0.101	0.049
ν'=4	(b)	1.637	1.667	1.699	1.729	1.759	1.789	1.820
	(c)	–	–	2671.9	2754.1	2840.8	2931.1	–
	(a)	*	0.080	0.063	*	0.053	0.129	0.130
ν'=5	(b)		1.647	1.677		1.739	1.769	1.798
	(c)		–	–		–	2867.4	2958.9
	(a)	0.077	0.025	0.023	0.087	0.030	0.006	0.081
ν'=6	(b)	1.596	1.628	1.658	1.688	1.717	1.751	1.778
	(c)	–	–	–	–	–	–	2894.8

Table 2. Franck-Condon factors and r-centroids of the D–X band system. (a) $q_{\nu'\nu''}$, (b) $\overline{r}_{\nu'\nu''}$ (Å), * $q_{\nu'\nu''} = 0$.

		ν''=0	ν''=1	ν''=2
ν'=0	(a)	0.915	0.083	0.004
	(b)	1.469	1.357	1.209
ν'=1	(a)	0.082	0.754	0.154
	(b)	1.592	1.476	1.367
ν'=2	(a)	0.004	0.151	0.608
	(b)	1.673	1.601	1.483
ν'=3	(a)	*	0.012	0.203
	(b)		1.682	1.609

Table 3. Franck-Condon factors and r-centroids of the E–X band system. (a) $q_{\nu'\nu''}$, (b) $\overline{r}_{\nu'\nu''}$ (Å), (c) $\lambda_{\nu'\nu''}$ (Å).

		$\nu''=0$	$\nu''=1$	$\nu''=2$
	(a)	0.898	0.100	0.004
$\nu'=0$	(b)	1.468	1.370	1.204
	(c)	1879.3	1921.7	–
	(a)	0.097	0.732	0.163
$\nu'=1$	(b)	1.582	1.476	1.375
	(c)	–	1871.3	1912.9
	(a)	0.007	0.153	0.619
$\nu'=2$	(b)	1.633	1.602	1.485
	(c)	–	1824.4	–

Table 4. Franck-Condon factors and r-centroids of the G–X band system. (a) $q_{\nu'\nu''}$, (b) $\overline{r}_{\nu'\nu''}$ (Å).

		$\nu''=0$	$\nu''=1$	$\nu''=2$
$\nu'=0$	(a)	0.680	0.252	0.058
	(b)	1.457	1.403	1.356
$\nu'=1$	(a)	0.279	0.272	0.300
	(b)	1.518	1.468	1.409
$\nu'=2$	(a)	0.040	0.381	0.093
	(b)	1.587	1.528	1.484
$\nu'=3$	(a)	0.002	0.090	0.399
	(b)	1.699	1.599	1.538

Table 5. Franck-Condon factors and r-centroids of the I–X band system. (a) $q_{\nu'\nu''}$, (b) $\overline{r}_{\nu'\nu''}$ (Å).

		$\nu''=0$	$\nu''=1$
$\nu'=0$	(a)	0.664	0.263
	(b)	1.457	1.405
$\nu'=1$	(a)	0.279	0.225
	(b)	1.514	1.464
$\nu'=2$	(a)	0.051	0.360
	(b)	1.574	1.520