Presence of C₂ molecular Lines in Sunspot Umbral Spectra

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Abstract

The C₂ molecule is well known for its astrophysical importance. The radiative transition parameters that include Franck-Condon (FC) factor, r-centroid, electronic transition moment, Einstein coefficient, absorption band oscillator strength, effective temperatures and radiative life time have been estimated for the Swan band ($d^3\Pi_g - a^3\Pi_u$) system of C₂ molecule for experimentally observed vibrational levels using RKR (Rydberg-Klein-Rees) potential energy curve. The lifetime for the $d^3\Pi_g$ state of C₂ molecule was found to be 82.36 ns for the $v'=0$ level. A reliable numerical integration method has been used to solve the radial Schrödinger equation for the vibrational wave functions of upper and lower electronic states based on the latest available spectroscopic data and known wavelengths. The estimated radiative transition parameters are tabulated. The effective vibrational temperature of Swan band system of C₂ molecule is found agreed with the effective rotational temperature from photosphere spectrum. Hence, the radiative transition parameters and effective temperatures help us to ascertain the presence of C₂ molecule in the interstellar medium, photosphere and sunspots.

Keywords Molecular data • Electronic transition moment • Sunspot umbrae • Rotational temperature • C₂ molecule

1. Introduction

The spectra of the C₂, CO, CO⁺, and CN molecules have a particular place in the history of astrophysically useful spectroscopic studies of diatomic molecules. Diatomic carbon and the CN free radical are prominent constituents of many extra-terrestrial sources and thus are molecules of great astrophysical significance. However the spectroscopic studies of the carbon monoxide positive ion were initiated at the beginning of the 20th century, it still remains one of the most extensively studied diatomic molecules. After the detection of SiC in stellar atmosphere (Cernicharo et al., 1989) a number of other diatomic carbides are expected to be observed in space as the detection provides unquestionable proof that intractable elements combined with carbon present in stellar gas. Another aspect for studying the carbides is to understand homogeneous and heterogeneous catalysis (Crabtree, 1985), particularly in investigating the interaction between carbon containing gases and metal surfaces. In the interstellar medium, the dicarbon molecules have been detected in diffuse and translucent clouds, in the circumstellar shell of carbon stars and in comets as well and they play an important role in the formation of hydrogen-deficient carbon molecules and the formation of cyclic molecules (Kaiser, 2002).

Molecular bands of many diatomic molecules are found in the spectra of stellar radiation and sunspot umbrae. 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 (Sriramachandran and Shanmugavel, 2013). Spectra of the radiation coming from astronomical sources point out many bands that are attributed to diatomic molecules. Molecules are sensitive to their astrophysical environs and they serve as diagnostics for model atmospheres. 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. The occurrence of the molecules C_2 and TiO both in the quiet sun and sunspots seems mutually exclusive. Based on estimates of the abundances of carbon, the sun being an oxygen rich star, the formation of C_2 molecules is adversely affected by slight changes in the temperature structure of a model atmosphere. C_2 molecule is also to be present in stars and sunspots. Estimates of the relative abundances of these species are of importance for the understanding of the evolutionary phases of the observed stars, and are also essential inputs in the modelling of the stellar atmospheres of late type stars. The lines of C_2 Swan band have been identified in the spectra of sunspot by Richardson (1931) and Laborde (1961). Richardson has noted that sunspots provide the only instance of the simultaneous appearance of bands of C_2 and TiO molecule in stellar spectra. Molecular equilibrium calculations carried out for sub-giant and giant stars (Schadee, 1968) indicate that in stars of later spectral type than in G5, the concentration of C_2 decreases with decreasing temperature due to increased association of carbon in the CO molecule. Therefore a lowering of model temperatures increases CO formation and reduces C_2 abundance. Wöhl (1972) has reported that swan band lines are present in umbrae spectra, indeed the reports show that the lines are strengthened relative to the photosphere. Harvey (1972) has also pointed out that C_2 photospheric line was noticeably weakened or absent in umbrae spectrum.

The Einstein coefficients for the strong transitions, radiative lifetimes for the electronic states, and the data of absorption-band oscillator strengths are essential for determining the extent to which this molecule is an opacity source in stellar atmospheres. While Einstein coefficients can be obtained indirectly by measurements of radiative lifetimes, experimental measurements of absolute line intensities require specific experimental conditions, which are difficult to obtain for many high-temperature molecular species. The rapid increase in computing power and the recent developments in quantum chemistry today have made it possible to compute these data, in addition to making experimental measurements. Using semi-empirical methods that combine the best available experimental and theoretical data can provide the desired information for important molecular species. Therefore, accurate values of the Franck-Condon (FC) factors and related parameters are required to obtain the radiative lifetime and effective temperature for the astrophysical sources of the spectra. We report the radiative transition parameters such as the FC factor, r-centroids, Einstein coefficients, absorption band strengths, radiative lifetime for the transition, vibrational temperature of the source, the detection of $d^3\Pi_g - a^3\Pi_u$ transition rotational lines of C_2 molecule in the spectrum of photosphere, sunspot umbra and thereby evaluate the rotational temperatures of the source in the following sections.

2. Molecular data and Umbral spectra

The Swan system was observed up to $v'=10$ for the upper and $v'=9$ for lower electronic state in emission by Tanabashi et al. (2007). The sequence of bands is located in the 15,149 to 22,869 cm^{-1} region. In the sequence $\Delta v = 0$ is located in the 19,350 to 19,950 cm^{-1} region. The (0, 0) band is the strongest band in the spectrum and (1, 1) band is weaker than the (0, 0) band. The other succeeding bands especially up to (4, 4) the intensities are found rapidly diminished. Also after the bands (5, 5; 6, 6; 7, 7) are absent in the spectrum. The $\Delta v = +1$ sequence bands are located in 20,800 to 21,700 cm^{-1} region, with the first member of this sequence (1, 0) band head is at 21,104 cm^{-1} followed by the (2, 1; 3, 2; 4, 3; 5, 4; 6, 5; 7, 6; 8, 7; 9, 8; 10, 9) bands. The $\Delta v = +1$ sequence band is the most extensive one in the Swan system. The $\Delta v = -1$ sequence bands (0, 1; 1, 2; 2, 3; 3, 4; 4, 5; 5, 6) lie in the 17,740 to 18,600 cm^{-1} region. These bands are degraded to blue region and have single head in the P branch. The $\Delta v = -2$ sequence bands are located in the region between 16,150 and 17,100 cm^{-1} . Only the (0, 2; 3, 5; 4, 6; 5, 7; 6, 8; 7, 9) bands have been observed and not others. The $\Delta v = +2$ sequence has been observed in the range from 22,600 to 23,100 cm^{-1} . Strong lines of the A- X system of CH also appear in this region. Consequently the spectrum was rotationally analysed, only the (2, 0; 3, 1; 8, 6) bands have been observed. Bornhauser (2010) have been reported the perturbations occurring between vibronic levels of the $d^3\Pi_g$, $v'=4$ and $b^3\Sigma_g^-$, $v=16$ states of C_2 . Unambiguous assignments of perturbed transitions are achieved by intermediate level in the $a^3\Pi_u$ state of the Swan system and results in the reassignment of several line positions found by performing of the potential of four-wave mixing spectroscopy in combination with explored a discharge slit-jet source. Also the wavenumbers of 46 perturbed transitions in the (6,5) and (6,4) bands of the $d^3\Pi_g - a^3\Pi_u$ electronic Swan system have been observed by Bornhauser et al. (2011) and assigned unambiguously by intermediate level in the (4,5) and (3,4) bands. It is important to notice that several rotational levels of the $d^3\Pi_g$, $v'=4$ state used for labelling are affected by perturbations owing to the $b^3\Sigma_g^-$, $v=16$ state as well. Furthermore, most of the characterized energy levels in the upper electronic state $d^3\Pi_g$, $v'=6$ are accessed from different rotational levels in the lower $a^3\Pi_u$, $v=5$ or $v=4$ states. The bands from (4, 2) to (7, 5) are difficult to analyse because they are weak in intensity and the lines are heavily overlapped due to the formation of head of heads. Also two band heads have been identified at 22,902 and 22,904 cm^{-1} for the (4, 2; 5, 3) bands. In this sequence (8, 6) band is a headless one with a band origin located at 22,744 cm^{-1} and Phillips (1948) has previously identified the band (8, 6) of swan band system of C_2 molecule located at 4395 Å (22,753 cm^{-1}). The FC factors obtained from perturbed Morse oscillator model with rotational term for Swan band system of C_2 molecule have been reported by Dwivedi et al. (1978). Nichollas (1965) has computed Franck-Condon factor arrays numerically to highest known vibrational quantum numbers for the C_2 swan band system. The RKR model has been adopted here for molecular potentials in the computer program for all needed vibrational wave functions and their overlap integral squares. The input data used in the calculations have been referred from the literature (Tanabashi et al., 2007) and the molecular constants are summarized in the Table 1. These molecular constants of upper and lower electronic states have been derived from the effect of Born-Oppenheimer approximation such as the second – order contribution to the rotational energy from the electron-rotation interaction.

A sunspot umbra spectrum of a large sunspot on 24 March 1981 was obtained by Wallace et al. (1998 and 2000) with the Fourier Transform Spectrometer of the McMath–Pierce telescope of the

National Solar Observatory at Kitt Peak. This spectrum which was corrected for stray light, covers the wavenumber region corresponding to 8900 to 15050 cm^{-1} and 15000 to 25500 cm^{-1} . It has a high signal-to-noise (S/N) ratio and includes most of the bands of interest here. The spectra of sunspots contain a rich collection of molecular and atomic lines. Wallace *et al.* (1998) have reported three unidentified branches consisting of a total of 33 lines in the relatively uncluttered spectral region between 13173 cm^{-1} and 13580 cm^{-1} . This region is bounded at short wavenumbers by the strong (0, 1) head of the TiO γ bands (Ram *et al.*, 1999) and at long wavenumbers by the increasing strength of lines of the red-degraded bands of the $\Delta v = -1$ sequence of the CaH (A-X) bands and the $\Delta v = 0$ sequence of the TiO γ bands. Recently, AlO (Sriramachandran *et al.*, 2013) molecular lines have been identified in red and infrared regions of the solar sunspot spectrum published by Wallace *et al.* (1998) and by Wallace, Hinkle, and Livingston (2000). Further, the CN and C₂ Swan have been claimed to be uncertain (Wallace *et al.*, 2000), due to various reasons such as blending by stronger lines, or due to lack of accurate spectroscopic data. Many times, a small number of line coincidences, or presence of very weak features, makes the identification difficult. The significant values of computed transition probabilities and the suspected presence suggested by the observation of Wallace *et al.* (2000), called for a fresh search for the presence of C₂ Swan band lines in solar spectrum using accurate spectroscopic data reported by Tanabashi *et al.* (2007). The spectrum is available in electronic form at the NSO web site (<ftp://nsokp.nso.edu/pub/atlas>). The digital spectra downloaded through ftp from the NSO website were also plotted and compared with the atlas spectra. Since the resolutions of the two formats are identical, magnified prints of the atlas spectra were used here to identify the lines.

3. Results and Discussion

We computed FC factor and r-centroid using RKR (Rydberg-Klein-Rees) potential energy function for experimentally known electronic transition with the method of numerical integration according to the detailed procedure provided by Sriramachandran *et al.* (2004). The estimated FC factors of this band system of C₂ molecule were arranged in a form similar to that of Deslandre's table, the most intense bands in the array were then joined up to obtain a parabolic curve (Condon parabola) whose axis is its principal diagonal. It is seen from Table 2 that the $\Delta v = 0$ sequence bands except (0, 0) and (1, 1) bands are weak intense. In $\Delta v = 0$ sequence, the (5, 5), (6, 6) and (7, 7) bands have not been observed experimentally and its estimated FC factor value is found zero. These bands are expected to lie in the 4370 to 5800 Å region, with the most intense (0, 0) band at 5166 Å. Similarly, the array of intensity distribution of experimentally observed $\Delta v = \pm 1, \pm 2$ sequence bands mentioned in section 2 is replicated in the computation of FC factor values in Table 2. Nearly all of the intense bands are expected to be lying in the 4370 to 5800 Å wavelength region. The bands (2, 0), (3, 1) and (3, 3) have been experimentally observed but its FC factor value is less intense than the other observed bands. For 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 $\Delta \bar{r}_{v',v''} (= \bar{r}_{v'+1,v''+1} - \bar{r}_{v',v''})$ is found to be less than 0.2 Å and $\bar{r}_{00}$ is slightly greater than $(r'_e + r''_e)/2$, and these factors indicate that the potential curves are very wide for the $d^3\Pi_g - a^3\Pi_u$ system. Since $r'_e < r''_e$; the r-centroids increase with decreasing wavelength; hence the bands are expected to be degraded towards blue region. These variations are of the expected nature and the decrease or increase is found to be linear. This is in excellent agreement with the experimental wave number distribution of the bands (see Tanabashi *et al.*, 2007). The calculation of $P_{v',v''}$ in the r-centroid ($\bar{r}_{v',v''}$) approximation therefore depends on the FC factor, and on the electronic transition moment $R_e(\bar{r}_{v',v''})$, which can be obtained from the

procedure illustrated by Murthy and Murthy (1977). The relations between the electronic transition moment and the internuclear separation for Swan band system of the C_2 molecule as

$$R_e(\bar{r}_{v',v''}) = \text{const.} (1 - 0.55 \bar{r}_{v',v''}) ; 1.169 \leq \bar{r} \leq 1.498 \text{ a.u} \quad (1)$$

Hence the electronic transition moment $R_e(\bar{r}_{v',v''})$ is relatively large in magnitude and slowly decreases with increasing r-centroid values (see Figure 1). This variation is linear except the band (3, 3). Tanabashi et al. (2007) have reported that the (3, 3) band is much weaker intense and the computed FC factor value of this band is 0.055. Therefore the small deviation may be occurred by the masking of other bands or by the influence of other molecular bands. The determination of the carbon abundance from the C_2 lines is strongly dependent upon the dissociation energy of the molecule. Grevesse and Sauval (1973) have indicated the value of dissociation energy is 6.15 eV while other evidences have yielded a considerably higher value 7.75 eV by Gaydon (1968). The primary indication that the $v'=6$ levels might be pre-dissociated is that the $(6, v'')$ bands but no other swan bands are observed in discharge tubes containing CO at relatively high pressure, which suggests that dissociated CO molecules from new C_2 molecules via inverse pre-dissociation through the $v'=6$ level. Since direct measurement of radiative lifetimes is the most sensitive probe of pre-dissociation effects, the radiative life time of a vibrational level depends on the sum of the transition probabilities ($A_{v',v''}$) to all lower vibrational levels in lower electronic states, which can be obtained from the procedure illustrated by Sriramachandran et al. (2013). The radiative lifetime can be written as

$$\tau_{v'} = \left(\sum_{v''} A_{v',v''} \right)^{-1} \quad (2)$$

The computed lifetimes are tabulated in Table 4 with previous literature values. For the $d^3\Pi_g$ state, the lifetime values are found in a range between $\tau(v'=0) = 82.358 \text{ ns}$ and $\tau(v'=6) = 188.493 \text{ ns}$. The experimental radiative lifetime observed from laser induced fluorescence method by Stark and Davis (1985) for $v'=0$ is $92 \pm 5 \text{ ns}$ and Naulin et al. (1988) for $v'=1$ is $96.7 \pm 5 \text{ ns}$. The computed lifetime should slowly increase with increasing v' (up to $v'=6$). The deperturbation analysis of the complex spectral region in the (6, 5) and (6, 4) bands of the Swan system $d^3\Pi_g - a^3\Pi_u$ unveils the presence of the energetically lowest high-spin state of C_2 molecule in the vicinity of the $d^3\Pi_g$, $v'=6$ state (Bornhauser et al., 2011). Thus the $v'=6$ level cannot possibly be influenced by pre-dissociation effects. It should be noted that swan bands originating from $v' > 6$ are extremely weak and no heads appear in the range of observed lines or the head appears in the R branch in contrast to the other bands (which have P branch heads), if present at all, in spectrum recordings at low pressure. Hence the band (7, 9) was observed in the absorption by using a dye laser as a radiation source (Tanabashi and Amano, 2002). Further, the oscillator band strengths for Swan bands are calculated from well estimated FC factors and electronic transition moments. Thus the oscillator strength ($f_{v',v''}$) can be written as

$$f_{v',v''} = 1.499 A_{v',v''} \bar{r}_{v',v''}^{-2} \quad (3)$$

The computation of f_{00} from equation (1) with $R_e^2(\bar{r}_{v',v''})$ gives a constant, that is $f_{00} = 0.0358$. However the calculated oscillator band strength is almost the experimental value 0.035 at wavelength region 5165 Å as reported by Arnold (1968), 0.029 by Kokkin et al. (2007) and 0.0261 by Curtis, Engman, and Erman (1976). The computed oscillator strengths for Swan bands are given in Table 4 with experimental values. These f -values from the C_2 Swan bands are useful to determination of

carbon abundance in the different layers of umbrae and other celestial objects. One can obtain the vibrational temperature from calculating the overlap integrals for the observed bands vibrational energy $G(v')$ of the molecule in the level v' using the procedure detailed by Sriramachandran and Shanmugavel (2013). Therefore the effective vibrational temperature of the source using C_2 molecule

has been determined from a graphical plot of $\log \left[\sum_{v''} (I\lambda^4)_{v'v''} / \sum_{v''} S_{v'v''} \right]$ versus $G(v')$ for Swan band

system in Figure 2 and the straight line was obtained by using the method of least square fit. From the slope of the fit for Swan band system of C_2 molecule, the effective vibrational temperature 5530 ± 1400^0K was obtained assuming the electronic transition moment as varied over the range of r-centroids. The uncertainty on the calculated effective vibrational temperature is nearly 25%, it is due to taking account of uncertainty of the few experimental bands, variation of electronic transition moment and predissociation energy of molecule. Vibrational temperatures were previously reported for cometary C_2 molecular lines of 3500^0K by Lambert and Danks (1983). Hence, the estimated effective vibrational temperature of C_2 molecule provide further evidence to ascertain the possible presence of C_2 molecule in higher temperature regions like star forming regions and solar atmosphere.

The atlas of sunspot spectra which contain photosphere, hot umbra and cold umbra layers of spectrum in the visible and red region were used in the search for the coincidences with laboratory rotational-line wave numbers of the transition (0, 0) Swan band of the C_2 molecule. By the method of coincidence described in detail by Sriramachandran and Shanmugavel (2011), a partial number of only 57 lines of the C_2 molecule referred from Tanabashi et al. (2007) was carefully searched and classified. The value of I -parameter is 30, and is convincingly higher than the C -index value of nearly 18 lines in searched wavenumber range for (0,0) Swan band transition by the method of coincidence with those of sunspot-umbra (in three layers of spectrum-see sample spectrum in Figure 3) suggests that C_2 molecule appears to be a non-negligible component of sunspot umbrae. Stankiewicz (1967) has reported using the quality molecular lines that the C_2 lines are insensitive to the magnetic field strength, whereas MgH and TiO lines are stronger in the cooler sunspots (i.e. stronger magnetic field). A significant number of lines from the exactly coincident lines has met the requirement of Swan (0, 0) band. The Triangular profile approximation method described in Sriramachandran et al. (2008) was used to measure the equivalent widths for spectrally well resolved lines. A list of well resolved C_2 (0, 0) spectral lines and their measured equivalent widths for respective surfaces have been highlighted in Table 5.

By assuming a constant effective rotational temperature through the line-forming layer, for optically thin, faint lines within the same band, the equivalent width may be expressed (Wöhl, 1970) as

$$\log(W_{J''}/S_{J''}) = \log(W_0/S_0) - 0.625B_{v''}J''(J''+1)/T_r \quad (4)$$

where, $B_{v''}$ is the rotational constant and T is the effective rotational temperature of the source. The rotational temperature is determined by plotting $\log(W_{J''}/S_{J''})$ against $J''(J''+1)$ for Swan (0, 0) band. In Figure 4, one can note a large scatter of the representative points. The method of least-square fit is used to obtain the slope of the resulting straight line. This slope is equal to $0.625B_{v''}/T_r$. Several lines were found clearly blended with strong lines and could not be included in the calculation of the rotational temperature. The average rotational temperatures obtained from the straight line fit for the solar photosphere, hot umbra, and cold umbra from the lines of Swan (0, 0) band are 4630^0K , 3014^0K and 2546^0K respectively. The estimated rotational temperatures may have a possible error of the order

of 25 per cent, because the observed intensities of some lines have probably been under estimated. The large error of the derived rotational temperature for the Swan bands of C_2 molecule is caused by smaller statistics when excluding the blended lines. Schadee (1964) has reported that the rotational temperature increases in isothermal regions of solar photospheric spectrum from 4120 $^{\circ}K$ to 5600 $^{\circ}K$ from Hubenet II model, while the average temperature of formation of C_2 is 4610 $^{\circ}K$. It is known that even in the photosphere, temperature as low as 3800 $^{\circ}K$ is measured from CO molecular lines. This is considered to be explainable by the cooling of photospheric plasma during the expansion phase of simple waves propagating upward through these layers (Foukal, 2004). Sotirovski (1971) has estimated the temperatures using rotational lines of such molecules, 2980 ± 200 $^{\circ}K$ for TiO, 3030 ± 200 $^{\circ}K$ for MgH and 3300 $^{\circ}K$ for CN in sunspot umbrae. In the present study, the estimated effective temperatures are the evidences for the existence of C_2 Swan (0, 0) band molecular lines in sunspots umbrae spectra and for their strengthening compared with the photospheric spectrum. Hence the presence of C_2 molecular lines in solar spectrum offers the likelihood to study the different layers in the solar atmosphere and their relative abundances of molecule would be very useful diagnostic of the umbral oscillations.

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Table 1. Spectroscopic equilibrium constants for the electronic states of C_2 molecule

Electronic state	Molecular constants					
	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	$\omega_e y_e$ (cm^{-1})	α_e (cm^{-1})	B_e (cm^{-1})	r_e (Å)
$d^3\Pi_g$	1789.094	17.367	-0.13603	0.0196	1.7554	1.265
$a^3\Pi_u$	1641.341	11.658	-0.00083	0.0165	1.6323	1.312

Table 2. FC factors, r-centroids and wavelength for $d^3\Pi_g - a^3\Pi_u$ band system of C_2 molecule.

v'/v''		0	1	2	3	4	5	6	7	8	9
0	a	0.727	0.219	0.046	0.008						
	b	1.294	1.224	1.169	1.118						
	c	5166.68	5637.04	6192.98							
1	a	0.248	0.349	0.280	0.096	0.024					
	b	1.369	1.308	1.231	1.175	1.124					
	c	4738.41	5130.77	5587.04							
2	a	0.026	0.369	0.151	0.267	0.133	0.042	0.011			
	b	1.467	1.381	1.327	1.237	1.180	1.129	1.081			
	c	4383.32	4716.60	5099.08	5542.235						
3	a		0.063	0.420	0.055	0.225	0.154	0.061	0.018		
	b		1.481	1.393	1.361	1.244	1.185	1.135	1.086		
	c		4372.67	4698.91	5072.32	5503.47	6006.59	6601.02			
4	a			0.101	0.432	0.014	0.177	0.161	0.077	0.027	
	b			1.493	1.405	1.439	1.250	1.190	1.139	1.091	
	c				4686.28		5471.73	5960.41			
5	a				0.138	0.427		0.133	0.158	0.090	0.036
	b				1.507	1.419	---	1.257	1.195	1.144	1.096
	c					4679.89		5448.58	5925.09		
6	a					0.171	0.416		0.097	0.148	0.098
	b					1.522	1.434	---	1.262	1.199	1.148
	c						4681.64			5901.02	
7	a						0.199	0.404		0.068	0.135
	b						1.538	1.449	---	1.268	1.203
	c										5892.81
8	a							0.222	0.396	0.011	0.048
	b							1.554	1.465	1.089	1.274
	c							4395.00*			
9	a								0.240	0.392	0.016
	b								1.571	1.482	1.015
	c									4734.00*	
10	a									0.250	0.386
	b									1.588	1.498
	c										4771.36

*Phillips (1948)

a) FC factor ($q_{v',v''}$)

b) r-centroids ($\bar{r}_{v',v''}$)

c) wavelength ($\lambda_{v',v''}$)

Table 3. Radiative transition parameters for $d^3\Pi_g - a^3\Pi_u$ band system of C_2 molecule

ν', ν''	$q_{\nu'\nu''}$	$\bar{r}_{\nu'\nu''}$	$\bar{\nu}_{\nu'\nu''}$ (cm^{-1})	$\lambda_{\nu'\nu''}$ ($\text{\AA}$)	$I_{\nu'\nu''}$	$R_e(\bar{r}_{\nu'\nu''})$	$P_{\nu'\nu''}$	$S_{\nu'\nu''}$	$A_{\nu'\nu''}$ ($\times 10^6 \text{s}^{-1}$)	$f_{\nu'\nu''}$ ($\times 10^{-2}$)	$\tau_{\nu'}$ (ns)
0,0	0.727	1.294	19354.781	5166.68	7.27	0.915	0.609	0.999	8.941	3.580	
0,1	0.219	1.224	17739.749	5637.04	2.19	1.042	0.238	0.390	2.689	1.282	
0,2	0.046	1.169	16147.247	6192.98	0.46	1.142	0.060	0.099	0.512	0.294	82.358
1,0	0.248	1.369	21104.144	4738.41	2.48	0.778	0.150	0.246	2.859	0.963	
1,1	0.349	1.308	19490.226	5130.77	3.49	0.889	0.276	0.453	4.137	1.634	
1,2	0.280	1.231	17898.573	5587.04	2.80	1.030	0.297	0.488	3.451	1.616	95.723
2,0	0.026	1.467	22813.757	4383.32	0.26	0.600	0.009	0.015	0.225	0.065	
2,1	0.369	1.381	21201.680	4716.60	3.69	0.757	0.211	0.347	4.083	1.362	
2,2	0.151	1.327	19611.372	5099.08	1.51	0.855	0.110	0.181	1.687	0.658	
2,3	0.267	1.237	18043.263	5542.23	2.67	1.019	0.277	0.455	3.299	1.520	107.592
3,1	0.063	1.481	22869.289	4372.67	0.63	0.576	0.021	0.034	0.507	0.145	
3,2	0.420	1.393	21281.549	4698.91	4.20	0.735	0.227	0.373	4.431	1.467	
3,3	0.055	1.361	19714.855	5072.32	0.55	0.739	0.030	0.049	0.466	0.180	
3,4	0.225	1.244	18170.342	5503.47	2.25	1.006	0.228	0.374	2.768	1.257	
3,5	0.154	1.185	16648.361	6006.59	1.54	1.113	0.191	0.313	1.783	0.965	
3,6	0.061	1.135	15149.182	6601.02	0.61	1.204	0.088	0.145	0.623	0.407	105.84
4,3	0.432	1.405	21338.909	4686.28	4.32	0.713	0.220	0.361	4.323	1.424	
4,5	0.177	1.250	18275.753	5471.73	1.77	0.995	0.175	0.288	2.167	0.973	
4,6	0.161	1.190	16777.390	5960.41	1.61	1.104	0.196	0.322	1.877	1.001	119.504
5,4	0.427	1.419	21368.012	4679.89	4.27	0.687	0.202	0.331	3.984	1.309	
5,6	0.133	1.257	18353.387	5448.58	1.33	0.982	0.128	0.211	1.606	0.715	
5,7	0.158	1.195	16877.390	5925.09	1.58	1.095	0.189	0.311	1.845	0.972	134.495
6,5	0.416	1.434	21360.017	4681.64	4.16	0.660	0.181	0.298	3.578	1.176	
6,8	0.148	1.199	16946.214	5901.02	1.48	1.088	0.175	0.288	1.727	0.902	[188.493]*
7,9	0.135	1.203	16969.830	5892.81	1.35	1.081	0.158	0.259	1.562	0.814	[640.240]*
10,9	0.386	1.498	20958.384	4771.36	3.86	0.564	0.123	0.202	2.290	0.782	[436.658]*

Note:

[]* uncertain value

$q_{\nu'\nu''}$ - FC factor; $\bar{r}_{\nu'\nu''}$ - r-centroid; $\lambda_{\nu'\nu''}$ - wavelength ($\text{\AA}$); ν', ν'' - transition band;

$\bar{\nu}_{\nu'\nu''}$ - wavenumber (cm^{-1}); $I_{\nu'\nu''}$ - band intensity; $P_{\nu'\nu''}$ - band strength; $S_{\nu'\nu''}$ - relative band strength;

$R_e(\bar{r}_{\nu'\nu''})$ - electronic transition moment (a.u); $\tau_{\nu'}$ - radiative lifetime (ns); $A_{\nu'\nu''}$ - spontaneous emission rate (s^{-1}); $f_{\nu'\nu''}$ - absorption band oscillator strength

Table 4. Computed oscillator strength $f_{v',v''} \times 10^{-2}$ and lifetime (ns) for various bands of the $d^3\Pi_g - a^3\Pi_u$ system in C_2 molecule compared with experimental data

v', v''	$f_{v',v''} \times 10^{-2}$			$\tau_{v'} \text{ (ns)}$				
	Cal.	Exp. ^c	Cal. ^a	Cal.	Cal. ^d	Exp. ^b	Exp. ^c	Cal. ^a
0,0	3.580	2.610	3.045					
0,1	1.282	0.660	1.015					
0,2	0.294	0.110	0.219	82.35	95.70	101.80	123	98.00
1,0	0.963	1.000	0.945					
1,1	1.634	1.140	1.350					
1,2	1.616	0.770	1.283					
1,3		0.220	0.464					
1,4		0.050	0.117					
1,5		0.010	0.024	95.72	99.21	96.70	124	99.80
2,0	0.065	0.150	0.080					
2,1	1.362	1.400	1.355					
2,2	0.658	0.410	0.493					
2,3	1.520	0.640	1.180					
2,4		0.280	0.642					
2,5		0.070	0.211					
2,6		0.010		107.59	104.56	104.00	130	102.40
3,1	0.145	0.340	0.183					
3,2	1.467	1.450	1.460					
3,3	0.180	0.130	0.124					
3,4	1.257	0.470	0.936					
3,5	0.965	0.290	0.729					
3,6	0.407	0.010		105.84	111.50		128	106.00
4,3	1.424		1.412					
4,5	0.973		0.676					
4,6	1.001			119.50	120.57		131	110.90
5,4	1.309		1.311					
5,6	0.715							
5,7	0.972			134.49	132.88		137	118.20

^aBrooke *et al.* (2013); ^bNaulin *et al.* (1988);

^cCurtis *et al.* (1976); ^dKokkin *et al.* (2007)

Table 5. Estimated equivalent width values for the $d^3\Pi_g - a^3\Pi_u$ (0, 0) transition lines of the C_2 molecule.

Branch	J	Wavelength λ (Å)	Wavenumber (cm^{-1})	PS Cat	W (mÅ)	HU Cat	W (mÅ)	CU Cat	W (mÅ)
P3	1	5160.230	19373.650	p	9.968	b		b	
	2	5161.158	19370.171	p	8.722	p	5.607	b	
	3	5161.937	19367.245	b		b		b CrI	
	4	5162.633	19364.636	m		m		m	
	5	5163.210	19362.473	m		m		m	
	6	5163.731	19360.517	b		b		b	
	7	5164.144	19358.970	s		s		p	22.428
	8	5164.497	19357.645	m		m		m	
	9	5164.799	19356.514	s		m		m	
	10	5191.863	19355.613	p	41.118	p		p	43.860
R3	0	5158.065	19381.784	m		m		m	
	1	5156.796	19386.556	m		m		m	
	2	5155.600	19391.051	m		m		m	
	3	5154.244	19396.155	m		p		p	13.083
	4	5152.966	19400.963	s		p	12.460	p	11.214
	5	5151.531	19406.367	s		p		p MgH	
	6	5150.151	19411.568	m		b		b	
	7	5148.621	19417.337	m		m		m	
	8	5147.127	19422.973	p FeI		P		s	
	9	5145.489	19429.154	p TiI		m		m	
	10	5143.877	19435.244	p	7.476	m		m	
P2	2	5160.583	19372.330	b		b		b	
	3	5161.295	19369.655	s		s		s	
	4	5161.996	19367.026	b		m		m	
	5	5162.577	19364.846	m		p	14.454	p	13.457
	6	5163.157	19362.670	b		p	5.482	p	15.326
	7	5163.617	19360.944	p	11.962	m		m	
	8	5164.051	19359.317	P		b		b	
	9	5164.395	19358.029	p	13.706	p	27.911	p	14.952
	10	5164.683	19356.949	p FeI		p	21.930	m	
R2	1	5157.172	19385.141	m		b		b	
	2	5156.105	19389.152	p Si2		m		m	
	3	5155.004	19393.294	m		m		m	
	4	5153.782	19397.892	b		b		b	
	5	5152.528	19402.615	b		m		m	
	6	5151.184	19407.676	P	2.990	p	15.700	p	13.457
	7	5149.797	19412.903	p CoI		p MgH		p MgH	
	8	5148.336	19418.410	m		m		m	
	9	5146.824	19424.115	p CoI		m		m	
	10	5145.245	19430.079	b		b		b	

Table 5. Continued...

Branch	J	Wavelength λ (Å)	Wavenumber (Cm^{-1})	PS Cat	W (mÅ)	HU Cat	W (mÅ)	CU Cat	W (mÅ)
P1	3	5160.734	19371.762	b		b		b	
	4	5161.385	19369.317	b		b		b	
	5	5161.996	19367.026	b		m		m	
	6	5162.577	19364.846	m		p		p	
	7	5163.329	19362.974	p	7.476	m		m	
	8	5163.343	19361.195	m		m		m	
	9	5163.951	19359.692	m		m		m	
	10	5164.297	19358.395	p		b		b	
R1	2	5156.151	19388.978	m		m		m	
	3	5155.209	19392.523	m		m		m	
	4	5154.189	19396.362	m		m		m	
	5	5153.093	19400.487	m		m		m	
	6	5151.917	19404.915	p Fe I		m		m	
	7	5149.342	19414.619	p		m		m	
	8	5150.666	19409.629	p		b		b	
	9	5148.046	19419.505	m		m		m	
	10	5146.479	19425.417	m		m		m	

Note:

PS – Photosphere spectrum; HU – Hot umbra spectrum; CU – Cold umbra spectrum

W – equivalent width (mÅ)

Figure 1. Electronic transition moment versus r-centroid for the Swan system of C_2 molecule

Figure 2. Graph showing the straight line is obtained by plotting of $\log \left[\frac{\sum (L\lambda^4)_{v'v''}}{\sum S_{v'v''}} \right]$ versus $G(v')$ for the Swan band system of C_2 molecule.

Figure 3. Section of the sunspot umbral spectrum with identified for the (0, 0) Swan system of C_2 molecular rotational lines.

Figure 4. Graph showing the straight lines are obtained by plotting of $\log(W_{J''}/S_{J''})$ against $J''(J''+1)$ for the Swan (0, 0) band system from photosphere (PS), hot umbra (HU) and cold umbra (CU) data's.

Figure 1

Figure 2

Figure3

Figure4