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Presence of C_2 molecular Lines in Sunspot Umbral Spectra

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HIGHLIGHTS

- The newly identified C_2 molecular lines are non-negligible components in the sunspot umbrae.
- The radiative lifetime of the band helps to determination of C_2 molecular abundance in celestial objects.
- The effective temperatures help to ascertain the presence of C_2 molecule in the solar atmosphere.
- The bands oscillator strength of C_2 are useful to determination of carbon abundance in the sunspot.

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ABSTRACT

The C_2 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 C_2 molecule for experimentally observed vibrational levels using RKR (Rydberg–Klein–Rees) potential energy curve. The lifetime for the $d^3\Pi_g$ state of C_2 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 C_2 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 C_2 molecule in the interstellar medium, photosphere and sunspots.

1. Introduction

The spectra of the C_2, 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

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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 15,149–22,869 cm^{-1} region. In the sequence $\Delta v = 0$ is located in the 19,350–19,950 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 20,800–21,700 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 17,740–18,600 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 22,600–23,100 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 et al. (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). Nicholls (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 8900–15,050 cm^{-1} and 15,000–25,500 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 re-