**Short Research Communications :**

# SULPHUR MOLECULES ON THE SUN

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## 1. INTRODUCTION

To date no sulphur molecule has been detected in the solar atmosphere. The principal difficulty lies in the fact that most of the electronic transitions are either in the rocket UV or in a region for which ground based observations are somewhat difficult. Moreover, in the crowded UV region of solar spectrum the uncertainties in the location of the true continuum and the correct assesment of the role of blending make detection of weak lines difficult.

On the theoretical side, the run of continuous opacity with depth is open to question. For this reason Pande et al. (1967) could not pursue their investigation further, inspite of the fact that for the solar photosphere molecular abundances of SH, CS and SO were found larger than that for MgH which is already detected in the solar spectrum (Laborde 1961 ; Schadee 1964). Matsushima (1968) and Travis and Matsushima (1968) have given empirical relationships for the solar continuous opacity in UV which satisfactorily explain observed centre-to-limb behaviour of the UV continuum radiation. This prompted us to theoretically investigate the question of presence or absence of the molecules SH, CS, SO, NS and $S_2$.

## 2. CALCULATIONS AND FORMULATIONS

The formulation for the equivalent widths of a weak line is the same as used by Sinha (1977), a modification of the formulation used by Waddell (1958). For the computation of the free partial pressures, the HSRA model (Gingerich et al. 1971) and the abundances quoted therein were used except for nitrogen taken from Boyer and Sotirovski (1973). Internal partition functions, the dissociation constants and the molecular constants are from the formulae and the tables of Glushko (1962). The UV opacity in continuum is obtained through the works of Travis and Matsushima (1968), Matsushima (1968) and Tsuji (1964). The small contributions of Thomson and Rayleigh scatterings were ignored. The rotational line intensity factors for CS and SH were calculated according to Schadee (1964). The oscillator strengths are from Smith (1969) and from Henneker and Popkie (1971).

## 3. RESULTS AND DISCUSSION

The Franck-Condon factors for the molecules CS and SH are tabulated by McCallum et al. (1971) and Nicholls et al. (1960) respectively. A consideration of the molecular rotational constants tabulated by Glushko (1962) shows tnat for the strongest (0-0) bands, the most intense lines would be originating from $J = 46$ for CS and from $J = 13.5$ for SH.

The SH band oscillator strength, $f_{0\text{-}0} = 1.63 \times 10^{-3}$ used in the present investigation is derived by Henneker and Popkie (1971) through the construction of Hartree-Fock wave functions. In the absence of any other estimate, observational or theoretical, a comparison is not possible. However, the band oscillator strength for MgH, $f_{0\text{-}0} = 0.250$ derived in a similar manner by these authors, is in excellent agreement with the recent experimental result, $f_{0\text{-}0} = 0.257$ due to Balfour and Cartwright (1976), whereas that for OH ($f_{0\text{-}0} = 20.6 \times 10^{-4}$) is higher than an average value $f_{0\text{-}0} = (8.0 \pm 2.5) \times 10^{-4}$ given by Grevesse and Sauval (1973). A laboratory determination of the SH oscillator strength is therefore required to assess the reliability of the oscillator strength used here. Equivalent widths were calculated for the $Q_2$ branch lines of SH with J values in the range 1.5 to 11.5. The maximum equivalent width is 4.4 mÅ for $J = 11.5$. The wave numbers for all the lines belonging to the (0-0) band are given by Ramsay (1952). The rotational intensity factors were obtained through the formulation of Earls (1935) quoted by Schadee (1964) for the transition ${}^2\Sigma - {}^2\pi_i$. However, the formulation due to Kovacs (1969) yields two times higher values. This is apparently due to the use of $(2S + 1)(2J + 1)$ as the normalising factor used by the latter author. The use of different normalisation factors have been accounted for in the calculations. The equivalent widths together with wave-lengths are given in Table 1. The centre-to-limb behaviour for the strongest line (in our investigation) $\lambda = 3293.015$ Å is presented in Figure 1. An inspection of the identification tables due to Moore et al. (1966) shows that features as weak as 0.5 mA can also be identified in the spectral range occupied by the SH molecules in the solar spectrum. However, judicious corrections for blending and the true location of the continuum have to be made.

The laboratory measurements of wavenumbers for CS do not extend to high J values. The formulation due to Herzberg (1950) and the molecular constants due to Glushko et al. (1962) were used to obtain the wave numbers for the Q branch lines originating from the J values in the range 41 to 51 of the (0-0) band. For a comparison with the laboratory observations of Crawford and Shurcliff (1934), wave numbers for the (0-1) and the (0-2) bands were obtained. It is found that the calculated values differ by $\sim 5.5 \mathrm{cm}^{-1}$ for small J values and by 1.5 $\mathrm{cm}^{-1}$ at $J=40$. The calculated wave numbers are unsuitable for identifications particularly in a crowded region of spectrum where tolerances within 0.03 Å are required. However, they can be used for equivalent width calculations. Using $f_{o-o} = 5.91 \times 10^{-3}$ (Smith 1959), equivalent widths are found to be $\backsim$ 1mÅ. Due to small changes in the rotational intensity factor $S_J$ for different lines, all the lines originating from J values in the range 41 to 51 have about the same intensity.

In Figure 1 the centre-to-limb behaviour of a line ($\lambda=2583.35$ Å) is presented. It shows maximum intensity around $\cos\theta=0.3$. The near limb decline in equivalent width (compared with SH) is due to larger contribution by the unknown opacity source due to Matsushima (1968). The molecule SO has an abundance smaller by about two orders of magnitude than that for CS. Consequently, taking an equivalent width of 1 mÅ as the limit for detectibility in UV region, the desired transition of SO will be detectable only if it has an oscillator strength around 0.59. However, no precise oscillator strengths are available for SO. Smith (1959) has given

TABLE 1

Equivalent widths for the SH molecules ($A^2\Sigma - X^2\pi_i$) in HSRA

| J | λ(Å) | W(mÅ) |
|---|---|---|
| 1.5 | 3280.314 | 0.8 |
| 2.5 | 3280.201 | 1.2 |
| 3.5 | 3280.356 | 1.6 |
| 4.5 | 3280.849 | 2.1 |
| 5.5 | 3281.636 | 2.5 |
| 6.5 | 3282.742 | 2.8 |
| 7.5 | 3284.153 | 3.3 |
| 8.5 | 3285.891 | 3.6 |
| 9.5 | 3287.941 | 4.0 |
| 10.5 | 3290.315 | 4.2 |
| 11.5 | 3293.020 | 4.4 |

TABLE 2

$f_{el} \cdot f_{vib}$ for the (8-0) band of SO molecule ($B^3\Sigma^- - X^3\Sigma^-$)

| No. | Band used | $f_{el} \cdot f_{vib}$ for the (8-0) band |
|---|---|---|
| 1 | (0—6) | $28.9 \times 10^{3}$ |
| 2 | (0—7) | $76.2 \times 10^{-3}$ |
| 3 | (0—8) | $139.0 \times 10^{-3}$ |
| 4 | (0—9) | $178.4 \times 10^{-3}$ |
| 5 | (0—10) | $172.5 \times 10^{-3}$ |

some observational estimates for a few bands of the B $^3\Sigma^-$—X$^3\Sigma^-$ transition in SO and has also enumerated the difficulties encountered in his determinations. The formulation for the oscillator strength given in the referred paper was used to obtain the oscillator strength for the (8-0) band of the aforesaid transition of SO molecule. The results are presented in Table 2. Since we get different values for the oscillator strength when different bands are utilised by us, it appears that a variation in the electronic transition moment with internuclear distance may be involved. In such a case, the formulation used here will not hold. Therefore, we are unable to say something definite regarding the observability of this molecule in the photospheric spectrum. The fairly strong (8-0) band was chosen because it originates from the lowest vibrational level of the ground electronic state and also the diffuseness that sets in due to predissociation in some other bands is entirely absent in this band (Collin 1969). The Franck-Condon factor for this band is taken from Smith and Lyszt (1971).

The abundances for the molecules NS and $S_2$ are several orders of magnitude smaller in photosphere as compared to that of CS. So it is inferred that NS and $S_2$ may not show up in the photospheric spectrum.

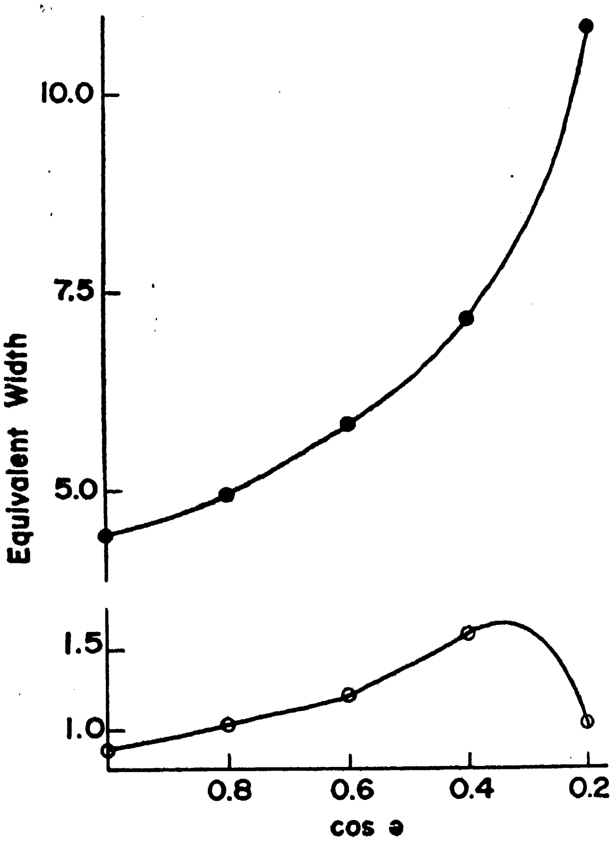

Fig. 1. Centre to limb behaviour of CS ( -o- ) and SH ( -●- )

Gaur (1976) calculated the equivalent widths for the $R_1$ (26.5) line of the (1-0), (2-1) and (3-2) vibrational-rotational bands of NO in two sunspot models. The results lie in the 9 to 21 mA range, for the centre of the solar disc. It is interesting to compare the umbral SH and SO abundances with that of NO. For this purpose we chose a sunspot model due to Zwaan (1965). The molecule SH is an order of magnitude more abundant than NO while SO is less abundant by the same amount. Now, since the vibrational-rotational oscillator strengths of SH and SO can reasonably be taken to be the same as in the case of NO, weak lines belonging to these molecules may show up in the infrared sunspot spectrum. Therefore, it is necessary to have a precise knowledge of the vibrational-rotational oscillator strengths as well as that of the infrared spectra of the SH and SO molecules.

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