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On detection of BO molecules in the sunspot spectrum

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Abstract. The boron atoms for which the solar abundance is as low as 2.6 ± 0.3 form a stable molecule BO (D_0^0 = 8.28 eV) in association with the oxygen atoms. The detectibility of BO lines in the spectra of the relatively cool atmosphere of sunspots has been investigated in detail by several authors but with a negative result. In the present communication, the whole problem has been examined afresh in view of the latest developments in molecular spectroscopy and model atmospheres. However, our conclusions are in agreement with the earlier investigators and it is found that even if the most favourable parameters are "chosen" for computations, the predicted intensities of the BO lines remain well below the limits of detectibility in sunspots. We also examine the possibility of detecting BO lines in the spectra of stars with effective temperatures of ≃ 4000 K.

Key words : sunspot spectra, BO molecules, oscillator strengths, Franck-Condon factors

1. Introduction

The stellar abundances of the light elements such as lithium, beryllium and boron have often been an area of special interest as they provide valuable information on stellar evolution. In the solar spectra, the lines due to these elements have been studied with special emphasis. However, since the number of lines of these atomic species in a spectral interval such as the visible region are small, the derived abundances are subject to close scrutiny. In the case of boron, the solar and the meteoritic abundances are 2.6 ± 0.3 and 2.88 ± 0.04 respectively (Anders and Grevesse, 1989). In view of the large uncertainty limit in the solar abundance, it is difficult to say whether the two abundances are in agreement. The great advantage with the solar molecular spectroscopy has been a dependable derivation of elemental abundances from a large number of unblended and pure lines for even such low abundance elements. These elements combine with a more abundant element such as hydrogen and form a stable compound e.g., HF and HCL (Sinha, 1991; Grevesse and Sauval, 1994; Jaschek and Jaschek, 1995). The sunspot atmosphere with lower than photospheric temperatures, helps in molecule

formation and offers a unique opportunity for a study of boron containing molecules such as BO (D_0^0 = 8.28 eV), BH (D_0^0 = 3.42 eV) and BN (D_0^0 = 4.9 eV) for a derivation of abundances, provided these molecules form insufficient numbers and show detectable lines. In the present paper, we concentrate upon the molecule BO which is more stable than the other two molecules.

1.1 Historical perspective

As far back as in 1956, in their classic paper "Molecules in the Solar Spectrum", Broida and Moore (1957) did consider the then reported identification of BO by Tanaka et al. (1939) and Nicholson and Perrakis (1928) and commented that the reported identification was least sure. Schadee (1964) did some computations and concluded on theoretical grounds that some molecules including BO, BH and BN could not be expected to show observable lines between $\lambda\lambda$ 3400 - 8000 Å.

Examining the sunspot spectra, Engvold (1970) remarked as follows :

(a) At the wavelengths of the (1,1) and (0,2) bands, the problem with scattered light is less serious. These bands are thus the most favourable for a search of BO in the spectra of sunspots.

(b) It is concluded that the (1,1) and the (0,2) bands of the BO alpha system are not observed in the studied sunspot spectrograms. In the spectrograms one could detect the BO lines, if their residue intensities exceeded about 1.5% and (c) The ultraviolet (2,0) band was searched for and not found in the spectrum of a great sunspot of May 22, 1968. Furthermore, there was no evidence for the (1,0) band in the spectrum of the spot of December 31, 1967. Looking for 122 lines of the (0,0), (0,1) and the (0,2) bands, Wöhl (1971) found wavelength coincidences for only 60 lines and commented that with a low W-index (0.1-0.2), the presence of these bands in sunspots is questionable. The W-index has been defined and explained in his paper. Sotirovski (1971) reported that his attempt to detect the (0,3) band of the molecule BO failed in sunspot spectra.

Against this backdrop, we found an interesting paper by Singh et al. (1996) claiming, "Our results presented in last column of Table 5 with question mark indicate that laboratory bandheads of A - X system of BO could also be present in the umbral spectrum of the sun, since the corresponding transition probabilities are appreciable". In the footnotes to Table 5, the authors seem positive about the presence of the (0,2), (0,1) and the (0,0) bands of this molecule in the umbral spectrum of the sun without actually calculating the oscillator strengths and the umbral line intensities. Considering the implication of these results and statements, we decided to survey the available literature and calculate the line intensities on the basis of the latest laboratory data and model atmospheres. We also wished to assess the possibility of detecting BO molecules in stars with effective temperatures of about 4000 K and different surface gravities.

1.2 Spectroscopic data

The molecule BO offers two strong transitions in laboratory spectra viz., the α and the β systems of bands. The β system of bands (B $^2\Sigma^+$ - X $^2\Sigma^+$) falls in the UV region, mostly

inaccessible to ground based observations of celestial bodies. Important developments in laboratory investigations on the α system of bands ($A\ ^2\Sigma_i$ - $X\ ^2\Sigma^+$) which fall in the visible region of spectrum have been the object of previously mentioned solar studies, important for night time observers as well, can briefly be summed up as follows :

(a) *Wavelength measurements and molecular constants* : Lot of work related to BO has been reported in literature after the publication of a critical and monumental work by Huber and Herzberg (1979). Accurate molecular constants have been derived by Coxon et al. (1984), Melen et al. (1995) and Tamimoto (1986). Additionally a detailed listing of accurate wavenumbers for 17 band systems have been reported in Coxon et al. (1984) and they are available from the authors on request.

(b) *The Frank-Condon factors* : The calculation of 5 × 5 array of the Franck-Condon factors (abbreviated as FCFs) based on the Morse potential have been reported by Nicholls et al. (1960) and Robinson and Nicholls (1960). Also Listz and Smith (1971) provide a 13 × 22 array based on realistic RKR potential energy curves. Mummigatti and Jyoti (1977) provide the same using a more realistic RKRV potential

(c) *Lifetime measurements and the transition moment* : Lifetime measurements for the $A\ ^2\Pi$ system, the upper electronic state involved in the alpha bands of BO, have been commented upon by Schamps (1994) and it appears that the results due to Huie et al. (1978) and Kozlov et al. (1994) are in agreement with each other. However, the variation of the square of the transition moment with internuclear distance has been a subject of controversy. In the first place, Robinson and Nicholls (1960) made accurate photoelectric measurements and gave a unique relationship between R_e ($\bar{r}$) and $\bar{r}$ on the basis of Morse potential The work was followed up with investigations by Walvekar (1969) and Mummigatti (1987) and these authors report different results, inconsistent with the work by Robinson and Nicholls (1960).

Taking advantage of the vast source of literature available now and considering the importance of the BO molecules in the context of the above scenario, we decided to do calculations and see for ourselves what could be the maximum intensity of the BO lines in solar umbral atmospheres and in the spectra of low temperature stars.

2. Formulations and calculations

At sunspot temperatures of about 3000 K, the well known formula,

$$J_{max} = 0.59\ (\ T/B_{\upsilon''})^{½} - 0.5$$

gives $J_{max} \simeq 27.5$ as the most populated level for the molecule BO with $B_e = 1.4018$; the symbols have the usual meanings. Also, it is expected that most of the BO molecules should be in the lower most vibrational state, i.e., $\upsilon'' = 0$ of the ground electronic state. A consideration of the FCFs (cf. Listz and Smith, 1971) gives (2,0), (1,0), (1,1), (0,1), (0,2) and (0,3) bands as the best candidates for a search in solar studies. It may be remarked here that these bands were included in earlier investigations described in section 1.1. The rotational intensity factors for all the lines reported by Coxon et al. (1984) for these bands were calculated by us, utilizing the formulae given by Schadee (1964). The different normalisations used and

suggested by other investigators such as Whitting et al. (1980) do not affect the results reported here. It may be pointed out that a $^2\Pi$ - $^2\Sigma$ transition gives 12 branches of lines as in the present case and we found that the rotational line intensities for the Q^1 and the Q^2 branches were larger than those for other bands.

The problem of variation of the square of the transition moment with internuclear distance was reinvestigated by us. The accurate photoelectric intensity measurements from Robinson & Nicholls (1960) and the RKR, FCFs and r-centroids from Listz and Smith were preferred by us. We closely followed Robinson and Nicholls (1960) and utilizing least square solutions for line fits, we could reproduce the results due to Robinson and Nicholls (1960); in contrast to the claims by Walvekar (1967). We do not depend heavily upon the RKRV results from Mummigatti and Jyoti (1977) for we fear some typographic errors. However, it must be remembered here that use of Morse, RKR, RKRV or any other potential is inconsequential here as we are dealing with low vibrational states. Our results for $R_e(\bar{r})$ dependence on $\bar{r}$ are :

$$R_e(\bar{r}) = k(1 - \bar{r}\,(0.58 \pm 0.11)),\ \textit{Robinson \& Nicholls data, Morse potential} \quad (1)$$

$$R_e(\bar{r}) = k(1 - \bar{r}\,(0.58 \pm 0.16)),\ \textit{Walvekar data, Morse potential} \quad (2)$$

$$R_e(\bar{r}) = k(1 - \bar{r}\,(0.61 \pm 0.07)),\ \textit{Listz \& Smith data, RKR potential} \quad (3)$$

$$R_e(\bar{r}) = k(1 - \bar{r}\,(0.58 \pm 0.17)),\ \textit{Mummigatti \& Jyoti data, RKRV potential} \quad (4)$$

Similarly for the β bands, we obtain

$$R_e(\bar{r}) = k(1 - \bar{r}\,(1.22 \pm 0.25)),\ \textit{Robinson \& Nicholls data, Morse potential} \quad (5)$$

$$R_e(\bar{r}) = k(1 - \bar{r}\,(1.22 \pm 0.34)),\ \textit{Listz \& Smith data, RKR potential} \quad (6)$$

$$R_e(\bar{r}) = k(1 - \bar{r}\,(0.37 \pm 0.25)),\ \textit{Mummigatti \& Jyoti data, RKRV potential} \quad (7)$$

Utilizing equation (3), the formulae for the band strengths from Schadee (1967) and the life times from Huie et al. (1978) and Kozlov et al. (1990), we calculate the oscillator strengths in absorption and present the same in Table 1. An inspection clearly indicates that

Table 1. Absorption band oscillator strengths for the alpha system of bands of the molecule BO.

v'' / v'	0	1	2	3
0	2.83(-3)*	8.21(-3)*	1.09(-2)*	8.76(-3)*
1	8.18(-3)* 1.37(-2)#	1.21(-2)* 2.03(-2)#	5.05(-3)* 8.48(-3)#	
2	1.38(-2)* 2.86(-2)#	8.09(-3)* 1.68(-2)#		

* lifetime from Kozlov et al. (1990).
\# lifetime from Huie et al. (1978).

the absorption oscillator strengths are largest for the (2,0) and the (1,1) bands of the alpha system of BO. The selection of these bands is important from one more point of view that one of the bands originate from the most populated $\upsilon'' = 0$ state.

Considering the above mentioned facts for the BO molecules, in brief, we expect the Q_1 and the Q_2 branch lines of the (2,0) and the (1,1) bands originating from J $\simeq$ 27.5 to be stronger in sunspots as compared to the other lines.

For a calculation of equivalent widths, we chose the sunspot models HSM (Henoux, 1969), ZSM (Zwaan, 1974), SWSM (Stellmacher and Wiehr, 1975), BSM (Boyer, 1980) and MACKKLSM (Maltby et al., 1986) and the oscillator strengths as $f_{2,0} = 2.86 \times 10^{-2}$ and $f_{1,1} = 2.03 \times 10^{-2}$ (cf., Table 1). We would like to repeat here that the different normalisation procedures for the rotational line strengths (Whitting et al. 1980) and for the oscillator strengths (Larsson, 1983), have no effect on the equivalent widths (abbreviated as EW) reported here as they have been duly accounted for by us.

3. Results and discussions

As it is clear from the above, we have deliberately chosen such parameters that should yield the maximum possible equivalent widths for the BO lines. The results for the Q_1 and the Q_2 branch lines of the (2,0) and the (1,1) bands are presented in Fig. 1. It can easily be seen from the figure that even under the most favourable circumstances the best possible band (2,0) has an EW less than a quarter of a mÅ. Detection of such lines in a sunspot spectrum is

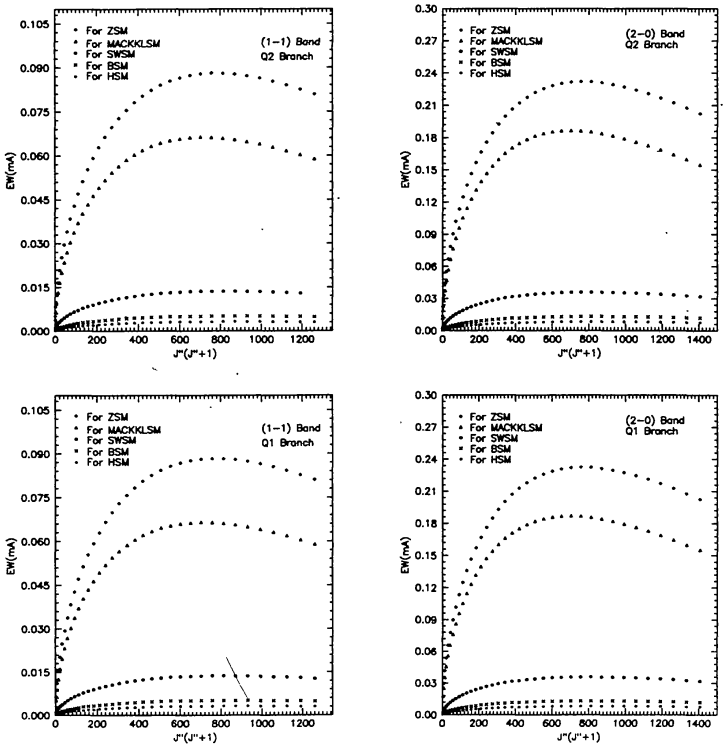

Figure 1. The predicted line intensities of the Q_1 and Q_2 branch of the (1,1) and (2,0) bands of the alpha system of BO molecules plotted in different sunspot models against $J''(J''+1)$.

extremely difficult. It may be added here that the f_{el} based on the assumption of a constant $R_e(\bar{r})$ (cf. Popkie and Henneker, 1971) yields even smaller values of oscillator strengths e.g., $f_{2,0} = 4{,}55 \times 10^{-3}$ and $f_{1,1} = 5.49 \times 10^{-3}$ and thus smaller EWs.

We repeated our calculations with the higher meteoritic value of boron abundance but the conclusion related to the absence of alpha bands of BO lines in sunspot spectra remains unchanged. We also checked the accuracy of the wavelengths used by Engvold (1970) for the (1,1) and the (0,2) bands with those reported by Coxon et al. (1984) and found them to be very accurate. Though Engvold (1970) could not look for lines originating from as high a J value as 27.5, the conclusion reached in his paper cannot be contrasted.

The EWs for the infrared lines of atomic boron lines at wavelengths 16240.36, 16244.62, 11660.04 and 11662.47 Å were calculated for sunspot and photospheric model atmospheres and the maximum result was found as 0.073 mÅ for the 11660.04 Å line in photosphere. Thus, these infrared lines suggested by Engvold (1970) are not suitable for a solar determination of boron abundance. We also computed EWs for the (2,0) and the (1,1) bands in the spectra of stars with effective temperatures $\simeq$ 4000 K and different surface gravities. The models given by Bell et. al (1976) were updated for the present day solar values of abundances. The results for EWs are presented in Fig. 2. We do not feel sure if lines as strong as 4 mÅ can

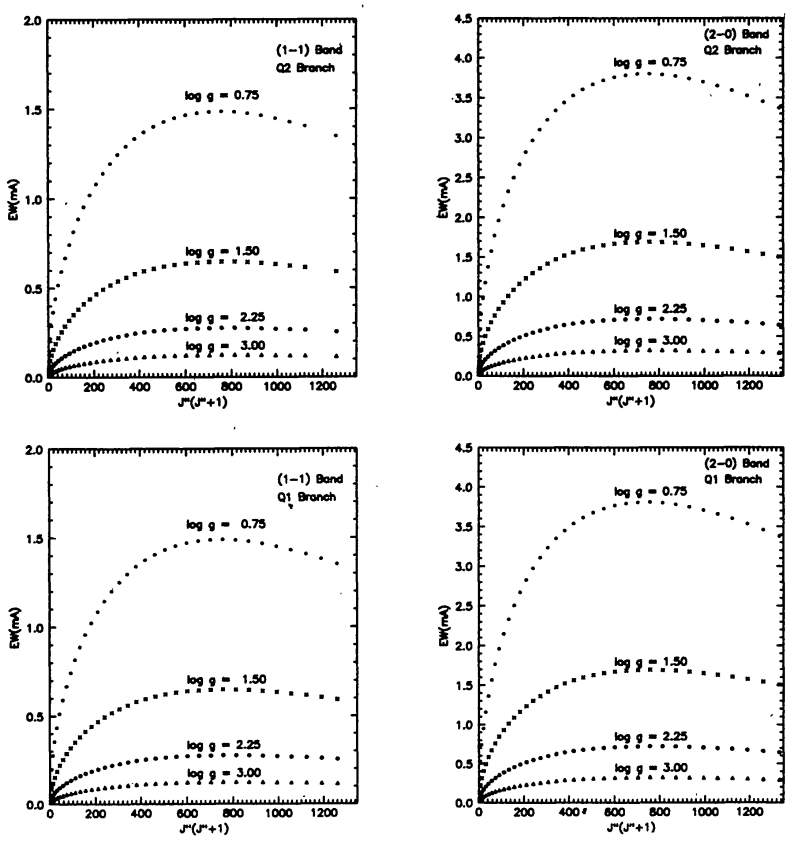

Figure 2. The predicted line intensities of the Q_1 and Q_2 branch of the (1,1) and (2,0) bands of the alpha system of BO molecules calculated using Bell et al model for T_{eff} = 4000 K and different log g plotted against J ″(J ″+ 1).

be easily detected in the spectra of giant stars. As the calculations of continuous opacity become quite uncertain at low temperatures, due to increased contributions from several molecular lines, we took this effective temperature as the lower limit.

In conclusion, we may say that using the most favourable conditions, the EWs obtained here rule out the possibility of presence of the α system of bands of BO in sunspots. It is also suspected whether the same bands can show up in other stars with different surface gravities.

4. Conclusions

On the basis of the latest laboratory data and sunspot model atmospheres, the α system of the BO molecule is too weak for identification in sunspot spectra.

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