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*A. Krüger*  
 see the heading of the paper

*J. Olmr*  
 Astronomical Observatory  
 251 65 Ondřejov  
 Czechoslovakia

## IONISED MOLECULES IN BCA PHOTOSPHERIC MODEL

*M. C. Pande, V. P. Gaur*, Uttar Pradesh State Observatory, Naini Tal, India.

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The dissociation equilibrium of ionised diatomic molecular species  $\text{CO}^+$ ,  $\text{NO}^+$ ,  $\text{OH}^+$ ,  $\text{O}_2^+$ ,  $\text{N}_2^+$ ,  $\text{H}_2^+$  in BCA photospheric model is considered. The abundances of these species are in the order  $\text{H}_2^+$ ,  $\text{CO}^+$ ,  $\text{OH}^+$ ,  $\text{NO}^+$ ,  $\text{O}_2^+$  and  $\text{N}_2^+$ . The equivalent width of  $R_1$  ( $K=30$ ) line of the (0—3) band belonging to the transition  $A^2\Pi_i - X^2\Sigma^+$  of  $\text{CO}^+$  is either 0.042 or 0.084 mÅ (cf. text) which shows that no detectible lines of  $\text{CO}^+$  occur in the photospheric spectrum.

### Ионизированные молекулы в фотосферной модели ВСА

Обсуждаются диссоциативные равновесия двухатомных ионизированных молекул  $\text{CO}^+$ ,  $\text{NO}^+$ ,  $\text{OH}^+$ ,  $\text{O}_2^+$ ,  $\text{N}_2^+$ ,  $\text{H}_2^+$  в фотосферной модели ВСА. Их численность убывает в последовательности  $\text{H}_2^+$ ,  $\text{CO}^+$ ,  $\text{OH}^+$ ,  $\text{NO}^+$ ,  $\text{O}_2^+$ ,  $\text{N}_2^+$ . Эквивалентная ширина линий  $R_1$  ( $K=30$ ) из полосы (0—3) соответствующей переходу  $A^2\Pi_i - X^2\Sigma^+$  молекулы  $\text{CO}^+$  равна 0,042 или 0,084 мÅ (см. текст), из чего следует, что в спектре фотосферы не могут быть наблюдаемые линии  $\text{CO}^+$ .

### 1. Introduction

Ionised molecular species occur in comets and interstellar medium and show up in their emission and absorption spectra respectively. In both cases, the physical conditions for the formation of these molecular species and their spectra correspond to non-LTE conditions. However, recent detection of  $\text{SiH}^+$  lines in the photospheric spectrum by Grevesse and Sauval (1970, 1971) shows that even under conditions close to LTE, some diatomic ionised molecular species may form in the solar atmosphere in particular and in stellar atmospheres in general. Excepting  $\text{SiH}^+$  mentioned above, the general problem concerning the presence of ionised molecular species in stellar atmospheres and their detection in stellar spectra has not received

proper attention. In identifying other ionic species in the photospheric spectrum, the fact that such lines may be intrinsically very weak should be borne in mind. For example, in the photospheric spectrum  $\text{SiH}^+$  molecules show absorption lines belonging to the (0—0) and (0—1) bands of the transition  $A^1\Pi - X^1\Sigma$  with maximum equivalent widths of about 2.5 and 1.3 mÅ respectively. Such weak lines make the identification very difficult and so the best way is to predict the equivalent widths of some strongest selected lines of the considered ionic species based on some representative photospheric model. The probable species thus selected out should then be subjected to a careful spectroscopic identification in the photospheric spectrum. In view of this we have selected the species  $\text{CO}^+$ ,  $\text{NO}^+$ ,  $\text{OH}^+$ ,  $\text{O}_2^+$ ,  $\text{N}_2^+$  and  $\text{H}_2^+$  for obtaining

their concentration-optical depth curves in BCA. The concentration-optical depth curve for  $\text{CO}^+$  in BCA model has been used for predicting the equivalent width of a selected line of the comet tail band. Here we discuss the results of such an investigation.

## 2. Dissociation Equilibrium Calculations

By an approach similar to our earlier work (Pande et al., 1969), the concentration-optical depth curves of  $\text{CO}^+$ ,  $\text{NO}^+$ ,  $\text{OH}^+$ ,  $\text{O}_2^+$ ,  $\text{N}_2^+$  and  $\text{H}_2^+$  in BCA were obtained. Excepting  $\text{H}_2^+$ , the dissociation constants were taken from Glushko et al. (1962). For  $\text{H}_2^+$  a polynomial formulation of the dependence of equilibrium constant on temperature by Vardya (1961) was used. Each concentration-optical depth curve was subjected to numerical integrations to obtain the value of  $I(\text{AB}^+)$  i.e. the number of  $\text{AB}^+$  in one  $\text{cm}^2$  column extending between  $\tau = 0$  to  $\tau = 3.16$  and also  $\bar{Z}(\text{AB}^+)$  the average geometrical depth of formation of  $\text{AB}^+$  as described in Pande et al. (1971). The results are summarised in Table I.

Table I  
Results of Dissociation Equilibrium Calculations

Molecule	$I(\text{AB}^+)$ ( $E + n$ means $\times 10^n$ )	$\bar{Z}(\text{AB}^+)$ Km.
$\text{H}_2^+$	8.58 E + 16	+ 19.8
$\text{CO}^+$	1.81 E + 15	-110.0
$\text{OH}^+$	8.85 E + 14	+ 7.0
$\text{NO}^+$	4.81 E + 14	- 90.0
$\text{O}_2^+$	1.26 E + 12	- 29.0
$\text{N}_2^+$	3.81 E + 11	- 83.0

## 3. Equivalent Width Calculations for a $\text{CO}^+$ Line

The ionised molecule  $\text{CO}^+$  is the second most abundant species amongst the six species considered by us. Moreover, the transition  $A^2\Pi_i - X^2\Sigma^+$  of  $\text{CO}^+$  has long been observed in comet tail spectra. This led us to investigate the presence of this transition in the photospheric spectrum. Inspection of the Franck-Condon factors suggests that the (0-3) band of this system will be the strongest band. Further, under photospheric conditions the rotational level with  $K = 30$  is expected to have maximum population. For these reasons we picked up the  $\lambda$  7296.937 Å line of  $\text{CO}^+$  belonging to  $R_1$  ( $K = 30$ ) branch of the (0-3) band of the above transition for equivalent width calculations in BCA

adopting the same approach as outlined earlier (Gaur et al., 1971). The laboratory spectroscopic data needed for the present calculations have been borrowed from Rao (1950) and Krupenie (1966).

The continuous opacity was calculated as outlined by Tsuji (1966) taking  $\text{H}^-$  ion, neutral hydrogen, electron scattering and the Rayleigh scattering by neutral hydrogen atoms as the possible sources. For the (0-3) band of the comet tail system of  $\text{CO}^+$ , an oscillator strength  $f_{e1} \cdot f_{vib} = 5.534 \times 10^{-4}$  (Krupenie, 1966) was accepted. With the coupling constant  $A = -117.5 \text{ cm}^{-1}$ , a rotational line strength factor of 7.037 for the  $R_1$  ( $K = 30$ ) line was obtained from Schadee's (1964) formulation. The  $p(\text{CO}^+)/P(\text{H})$  values were obtained from the already mentioned dissociation equilibrium calculations. The internal partition function,  $Q_{\text{int}}$ , values at various temperatures  $T$  were obtained from  $\Phi^*(T)$  values tabulated by Glushko et al., (1962) using the following formula given therein:

$$(1) \quad \Phi^*(T) = 2.28792[2 \log Q_{\text{int}} + 3 \log M + 5 \log T] - 7.28355,$$

where  $\Phi^*(T) = \Phi_{\text{trans}} + \Phi_{\text{int}}$  represents the effective thermodynamic potential which is the sum of the two parts corresponding to the translational and the internal degrees of freedom and  $M$  is the molecular weight. The rotational and vibrational energies  $F_v(J)$  and  $G_0(v)$  were calculated from the usual expressions:

$$(2) \quad F_v(J) = B_v K(K+1) - D_v K^2(K+1)^2 - \frac{1}{2}\gamma(K+1)$$

$$(3) \quad G_0(v) = w_0 v - w_0 x_0 v^2 + w_0 y_0 v^3 - \dots$$

The Doppler width values were obtained with the help of the temperature structure of BCA model and the turbulence velocity as in URP (Heintze et al., 1964). For the center of the disk, we obtained an equivalent width of 0.042 mÅ for the selected line.

## 4. Concluding Remarks

Table I shows that the abundances of six selected ionised molecular species decrease in the order  $\text{H}_2^+$ ,  $\text{CO}^+$ ,  $\text{OH}^+$ ,  $\text{NO}^+$ ,  $\text{O}_2^+$  and  $\text{N}_2^+$ . For  $\text{H}_2^+$  the equilibrium constants available for  $\text{H} + \text{H}^+ = \text{H}_2^+$  were used, while for other species the process of the type  $\text{AB} = \text{AB}^+ + e$  was used. However, in the latter cases equilibrium constants for a process of the type  $\text{A} + \text{B}^+ = \text{AB}^+$  are also available. Elsewhere we have shown that these two processes are equally effective

in forming species  $AB^+$  in the temperature range 3000–10 000 K in case of species  $CO^+$ ,  $OH^+$ ,  $NO^+$ ,  $O_2^+$  and  $N_2^+$  (Gaur et al., 1972). Therefore, if these two processes operate independently under LTE the abundances of these species should be doubled at each optical depth in BCA and so also the  $I(AB^+)$  values in Table I. As a result of this, the equivalent width of the considered  $CO^+$  line will become 0.084 mÅ.

The obtained contribution function shows that in BCA the layers above and near the temperature minimum contribute maximum to the line formation. In fact, the maximum of the contribution function falls at  $\log \tau = 5.6998$  corresponding to a temperature  $T = 4750$  K and electron pressure  $\log P_e = 2.7461$ . Thus, the  $CO^+$  line originates essentially in the transition region between chromosphere and photosphere.

As the yellow supergiants may possess relatively more extended photosphere to chromosphere transition region,  $CO^+$  lines may gain strength as one goes from G2 dwarfs to supergiants. However, without a detailed investigation it is rather difficult to predict the extent to which the equivalent widths of  $CO^+$  line will increase from G2V to G2I.

Taking the lines with equivalent widths of about 1 mÅ as detectable in the solar spectrum, we can say that the selected  $CO^+$  line is not present in the photospheric spectrum. Even if reasonable changes in the photosphere to chromosphere transition region are incorporated in BCA model, as was done by Elste (1968), one cannot expect to gain a factor of 100 in the equivalent width of the mentioned line.

Thus, for reasonable photospheric models the considered (0–3) band will not show detectable lines. The Franck-Condon factors suggest that the (0–3) band is the strongest band of  $A^2\Pi_i - X^2\Sigma^+$  transition of  $CO^+$ . Consequently, the other bands belonging to this

transition should also be absent in the photospheric spectrum. A comparison of the oscillator strengths of  $B^2\Sigma^+ - X^2\Sigma^+$  with the comet tail band of  $CO^+$  indicates that the former band will also not produce any detectable lines in the photospheric spectrum.

It is desirable to carry out similar investigations for other ionised species of our list so as to reach a definite conclusion about their detectability in the photospheric spectrum.

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M. C. Pande, V. P. Gaur  
 Uttar Pradesh State Observatory  
 Manora Peak  
 Naini Tal  
 U. P. 263 129, India