

Ionized molecules in facula models

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Abstract. Equivalent widths for the lines of ionized molecules AlH^+ , CH^+ , CN^+ , CO^+ , MgH^+ , N_2^+ , NH^+ , OH^+ and SiH^+ have been calculated in five facular and two photospheric models. The calculations suggest that CH^+ should show up in facular spectrum. MgH^+ , OH^+ and SiH^+ may also be present while AlH^+ , CN^+ , CO^+ , N_2^+ and NH^+ should be absent.

Key words : ionized molecules—equivalent widths—facula models

1. Introduction

The detection of SiH^+ lines in the photospheric spectrum by Grevesse & Sauval (1970, 1971) suggests that ionized diatomic species may form in the solar atmosphere. However, the lines of ionized molecules may be very weak and consequently difficult to identify. So the best way is to first predict the equivalent widths of various ionized molecules to know whether these molecules at all show detectable absorption lines. With this in view, we have carried out equivalent width calculations of some strong lines belonging to molecules AlH^+ , CH^+ , CN^+ , CO^+ , MgH^+ , N_2^+ , NH^+ , OH^+ and SiH^+ in five facular and two photospheric models. The facular and photospheric models used by us in these calculations are Schmahl (1967), Stellmacher & Wiehr (1973), Shine & Linsky (1974), Stenflo (1973), Chapman (1979), Holweger & Müller (1974) and Vernazza *et al.* (1976). Hereinafter these models are abbreviated respectively as SF, SWF, SLF, StF, 7B14, HM and VAL. The reason for selecting many facular and photospheric models is to assess the effect of the model on the predicted equivalent widths.

2. Equivalent width calculations

For calculating the equivalent widths of the ionized molecular lines we have adopted the method outlined by Sinha (1978). The elemental abundances were taken from Hauge & Engvold (1977) except for elements C, N and O which were adopted from Lambert (1978). Atomic partition functions for the constituent elements of these ionized molecules have been adopted from Glushko *et al.* (1962). The chosen

electronic transitions, bands, oscillator strengths *etc.* are given in Table 1 along with the range of computed equivalent widths in the photospheric and facular models. The spectroscopic constants and dissociation energies required for the calculations were taken from Huber & Herzberg (1979).

Table 1. Molecular data used in the present work and results

Molecule	Electronic transition	(v', v'')	$\lambda_{v'v''}$	No.	$f_{v'v''}$	Range of W (mÅ) in	
						Photospheric models	Facular models
AlH ⁺	A ² Π _r –X ² Σ ⁺	(0, 0)	3690	15	1.0 E–2	0.1 to 0.4	0.11 to 0.7
		„ (1, 1)	3590	10	„ (Sauval <i>et al.</i> 1977)	0.1 to 0.27	0.07 to 0.46
CH ⁺	A ¹ Π–X ¹ Σ ⁺	(0, 0)	4225	10	1.2 E–3 (Grevesse & Sauval 1971)	1.2 to 2.9	1.2 to 19.6
CN ⁺	c ¹ Σ–a ¹ Σ	(1, 0)	3063	9	unity (assumed value)	0.028 to 0.039	0.032 to 0.25
CO ⁺	A ² Π _i –X ² Σ ⁺	(0, 3)	7191.7	9	5.534 E–4 (Krupenie 1966)	0.015 to 0.027	0.017 to 0.25
MgH ⁺	A ¹ Σ ⁺ –X ¹ Σ ⁺	(2, 0)	2641	10	5.0 E–3 (assumed value)	3.4 to 4.3	2.3 to 6.5
N ₂ ⁺	A ² Π _{ui} –X ² Σ _g ⁺	(2, 0)	7875	8	6.9 E–4	3.0 E–5 to 9.0 E–5	4.1 E–5 to 8.6 E–4
		„ (3, 1)	8105	9	1.01 E–3 (Lofthus & Krupenie 1977)	4.0 E–5 to 16.9 E–5	5.2 E–5 to 15.6 E–4
NH ⁺	A ² Σ [–] –X ² Π _r	(0, 0)	4627	10	unity (assumed value)	0.23 to 1.02	0.25 to 4.84
		(0, 0)	4349	10	unity	0.14 to 0.90	0.15 to 4.401
OH ⁺	A ³ Π _i –X ³ Σ [–]	(0, 0)	3565	5	4.39 E–3 (calculated value)	0.6 to 3.3	0.6 to 4.4
SiH ⁺	A ¹ Π–X ¹ Σ ⁺	(0, 0)	3993	10	5.0 E–4	0.6 to 2.0	0.3 to 3.1
		„ (0, 1)	4356	9	4.0 E–4 (Grevesse & Sauval 1970)	0.3 to 1.2	0.2 to 4.8

$\lambda_{v'v''}$: Band origin.

W (mÅ) : Solar equivalent width.

$f_{v'v''}$: Oscillator strength.

No. : Number of lines included in this study.

3. Results and Discussions

It is obvious from Table 1 that molecules AlH^+ , CO^+ and N_2^+ should be absent in both photospheric and facular spectra. CN^+ and NH^+ should also be considered as absent since the calculated equivalent width ranges shown in Table 1 are based on highly exaggerated assumed $f_{\nu'\nu''} = 1$.

Ten lines of CH^+ molecule were taken for calculations following Grevesse & Sauval (1971) who had tentatively identified CH^+ in photospheric spectrum. For this molecule Brooks & Smith (1975) recommended a measured value of f_{00} to be 0.0136 which is a mean of their value and that of Brzozowski *et al.* (1974). This value of f_{00} is about an order more than the value of f_{00} ($= 0.0012$) derived from solar data by Grevesse & Sauval (1971). We have used Grevesse & Sauval's (1971) value of f_{00} in our calculations. Our results show that the lines of CH^+ get strengthened in all facular models relative to the selected photospheric models. StF model predicted unexpectedly high values of equivalent widths. Even the 7B14 model where the equivalent widths turned out to be the least ($\sim 1.2 \text{ m}\text{\AA}$) show that lines of CH^+ can be detected in the facular spectrum. For facular models other than chosen here Tripathi (1978) reached the same conclusion regarding CH^+ .

Balfour (1972) suggested that the $\text{A}^1\Sigma^+ - \text{X}^1\Sigma^+$ transition of MgH^+ should be searched in the solar spectrum as MgH and SiH molecules have similar ionization potentials and the abundances of Mg and Si in sun are about the same. With this in view, ten lines of (2, 0) band of this transition of MgH^+ around $J_{\text{max}} = 16$ were chosen for equivalent width calculations. The oscillator strength $f_{20} = 5 \times 10^{-3}$ was assumed which is the same as used by Sauval *et al.* (1977) for (0, 2) band. Our calculations show that equivalent widths get enhanced in SF, SWF and SLF as compared to the HM and VAL models, while models StF and 7B14 lead to lesser equivalent widths ($\sim 2 \text{ m}\text{\AA}$). Sauval *et al.* (1977) obtained a maximum equivalent width of $2 \text{ m}\text{\AA}$ for a line of the (0, 2) band in the photospheric models. This difference in equivalent widths is mainly because of the use of higher oscillator strength by us. The experimental oscillator strengths of MgH^+ bands are not known. If our oscillator strength value is modified with the help of known Franck-Condon factors (Balfour 1972), the equivalent widths of about $2 \text{ m}\text{\AA}$ will be found for the photospheric models. The difference will also occur if different photospheric models and different dissociation energies are used for these calculations. The dissociation energy and photospheric models used by Sauval *et al.* (1977) are not known to us. The results suggest that the lines of MgH^+ may show up in the photospheric and facular spectra.

Most intense lines of the $\text{A}^3\Pi_i - \text{X}^3\Sigma^-$ system of OH^+ should be the lines of the (0, 0) band (Merer *et al.* 1975). 5 lines of this band around J_{max} were selected for the present calculations. The oscillator strength was calculated from the life time measurement [$\tau(\nu' = 0) = 0.89 \times 10^{-6} \text{ sec}$] given by Huber & Herzberg (1979). In the models SF, SWF, SLF and StF predicted equivalent widths of the selected lines resulted in the range $1 \text{ m}\text{\AA}$ to $4.4 \text{ m}\text{\AA}$, while in the model 7B14 the range turned out to be $0.6 \text{ m}\text{\AA}$ to $1.4 \text{ m}\text{\AA}$. The model HM predicted higher equivalent widths than the VAL model. Two lines $Q_{11}(14)$ and $Q_{11}(16)$ showed equivalent widths larger than $1 \text{ m}\text{\AA}$ in all the photospheric and facular models. For molecule OH^+ we obtained a maximum equivalent width of $3.3 \text{ m}\text{\AA}$ in HM and $1.3 \text{ m}\text{\AA}$ in

VAL as compared to the calculated value of 0.6 mÅ by Sauval *et al.* (1977). Here again the models and dissociation energy used by Sauval *et al.* (1977) are not given by them and the difference in equivalent widths may be a result of model effect and the dissociation energy selected by them. Since we found higher equivalent widths in the facular models as compared to the photospheric models it seems that the chances of detection of OH⁺ lines are more favourable in the facular case. Therefore, OH⁺ molecular lines should be searched for in the photospheric as well as in the facular spectrum. If an experimental value of $f_{00} = 4.6 \times 10^{-3}$ given by Sauval *et al.* (1977) is chosen slightly higher equivalent widths will result.

For the transition A¹Π — X¹Σ⁺ of SiH⁺ we have selected the most intense (0, 0) and (0, 1) bands. Ten lines of the (0, 0) band and nine lines of the (0, 1) band around J_{\max} were chosen for calculations. Our results show that the lines get strengthened in the SF and SWF models as compared to the HM and VAL models, while the weakening of lines was found to occur for SLF, StF and 7B14 models. Model SLF predicted unexpectedly small equivalent widths (not included in Table 1). The maximum equivalent width obtained for photospheric models is about 2 mÅ for the Q(15) line of the (0, 0) band. As this molecule has already been identified in the photosphere (Grevesse & Sauval, 1970) and models SF and SWF show strengthening, the presence of SiH⁺ lines in facular spectrum cannot be ruled out. However, definite conclusions regarding the presence of SiH⁺ in the facular spectrum cannot be drawn.

In brief, CH⁺, MgH⁺, OH⁺ and SiH⁺ molecules may show up in the facular spectrum. Low noise high resolution spectra of faculae are required for comparing the predictions against observations. As per our calculations molecules AlH⁺, CN⁺, CO⁺, N₂⁺ and NH⁺ should be absent in both the photospheric and facular spectra.

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