ON THE POSSIBILITY OF FAINT MOLECULAR LINES OF PO, PH, MgH^+, AND CN IN THE SOLAR SPECTRUM

K. SINHA[2], B. M. TRIPATHI[2], R. M. ATALLA[1], and P. D. SINGH[1]

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Abstract. Equivalent width calculations for some electronic and vibration-rotation transitions of the molecules PO, PH, MgH^+, and CN have been carried out for a few umbral, photospheric, and facular model atmospheres. It appears that a few weak lines of these molecules might show up in the umbral spectrum. Le Blanc bands of CN are too weak for detection in the solar spectrum.

1. Introduction

The solar spectrum is known to exhibit a host of weak and strong molecular lines (Grevesse and Sauval, 1973; Mallia, 1974; Lambert, 1977) and identification of Fraunhofer lines with known molecular lines continues to be an important area of research (Porfire'va, 1982; Sinha and Mehrotra, 1985). A method usually employed for this purpose consists of absorption line intensity (equivalent widths) calculation, utilizing a suitable model atmosphere, opacity code, and molecular parameters like oscillator strengths and dissociation energies. It is possible now to identify lines as weak as 1 mÅ and even less (Brault *et al.*, 1982).

Sauval *et al.* (1977), utilizing high-resolution solar spectra, investigated the possibility of detecting some faint molecular lines in the photospheric spectrum. Continuing the same approach, we report here the results of our calculations for the $A^3\pi_i - X^3\Sigma^-$ transition of PH, the $A^1\Sigma^+ - X^1\Sigma^+$ transition of MgH^+, the $B^2\Sigma^+ - X^2\pi_r$ transition (beta bands) of PO, the $B^2\Sigma^+ - A^2\pi_i$ transition (Le Blanc bands) of CN molecules and for vibration-rotation lines of the (1, 0) band of the MgH^+ and PH molecules.

2. Formulation and Calculations

The method of equivalent width calculations for weak molecular lines are well known (see, for example, in Schadee, 1964; Lambert, 1968; and Sotirovski, 1971). The calculations were performed for the photospheric model due to Holweger and Müller (1974), umbral model atmospheres due to Hénoux (1969), Zwaan (1974), and Avrett (1981) and the facular model atmospheres due to Shine and Linsky (1974) and Stenflo (1975). A comparison of the chosen model atmospheres is made in Figure 1. The selection of these representative models is based on studies already carried out by us (Sinha, 1982, 1984; Tripathi and Sinha, 1986). It may be remarked here that Hénoux

[1] Department of Astronomy, Institute of Astronomy and Geophysics, University of São Paulo, Av. Miguel Stefano, 4200, (Caixa Postal 30.627) 04301, São Paulo, Brazil.
[2] Uttar Pradesh State Observatory, Manora Peak, Naini Tal, 263 129, India.

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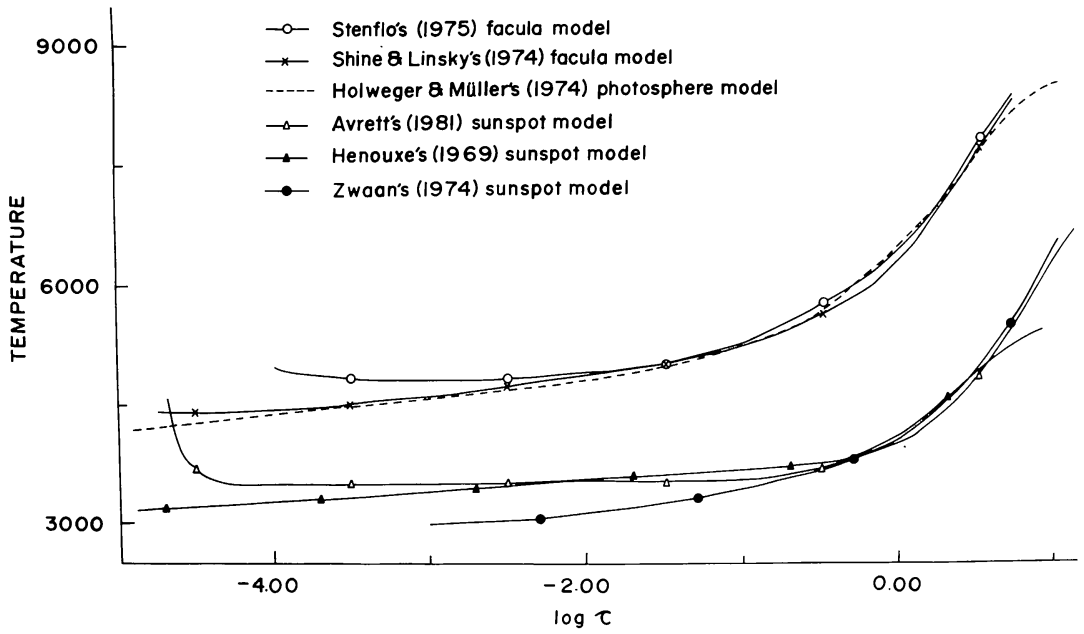

Fig. 1. Temperature versus optical depth plot for the considered facular, photospheric, and umbral model atmospheres.

(1969) and Zwaan (1974) umbral models represent the two extremes in the available range of model atmospheres (Sinha, 1982). The opacity code was borrowed from Tsuji (1966). The molecular line haze opacity introduced by Gaur, Pande, and Sah (1979) and Joshi, Punetha, and Pande (1979) in the case of sunspot umbrae was not used by us.

TABLE I

Parameters used in the calculation of equivalent widths

Molecule	Transition	D_0^0 (eV)	Oscillator strength $fv'v''$	Wavelength and branch identification
PO	$B^2\Sigma^+ - X^2\pi_r$ (0–0) band	6.15 (Huber and Herzberg, 1979)	2.79(−3) (Atalla and Singh, 1987)	Atalla (1984)
PH	$A^3\pi_i - X^3\Sigma^-$ (0–0) band	3.02 (Huber and Herzberg, 1979)	7.5(−3) (DeGouveia and Singh, 1984)	DeGouveia and Singh (1984)
MgH^+	$A^1\Sigma^+ - X^1\Sigma^+$ (0–2) band	2.08 (Huber and Herzberg, 1979)	5(−3) (Sauval *et al.*, 1977)	Singh (1984)
	(0–3) band		3.1(−3) (This study)	
CN	$B^2\Sigma^+ - A^2\pi_i$ (0–0) band	7.76 (Huber and Herzberg, 1979)	4.0(−4) (Halpern and Tang, 1983)	

Notation: $2.79(-3) = 2.79 \times 10^{-3}$.

It seems to yield too large opacities (Stellmacher and Wiehr, 1981; Zeidler and Koester, 1982). The atomic partition functions are from Irwin (1981), the dissociation constants are from Tsuji (1973) and Tarafdar (1977) and the molecular constants are from Huber and Herzberg (1979). A depth independent micro-turbulence velocity of 1 km s^{-1} was assumed. A different value like 2.1 km s^{-1} (Porfire'va, 1986) does not affect the results for faint lines reported here. The atomic abundances N(C) = 8.67, N(O) = 8.92, N(N) = 7.99, N(P) = 5.45, and N(Mg) = 7.62 on the usual scale of N(H) = 12.00 were adopted from Lambert (1978) and Lambert and Luck (1878). Other important parameters used in the calculations are given in Table I. It should, however, be pointed out that the Honl–London factors were obtained from Kovacs (1969) and they were normalised according to Whiting *et al.* (1980). The expressions given by Schadee (1978) and Larsson (1983) for oscillator strengths were used while writing the line opacity.

3. Results and Discussions

The partial pressures of PO, PH, and MgH^+ computed for different models are compared in Figure 2. The results of our equivalent width calculations are presented in

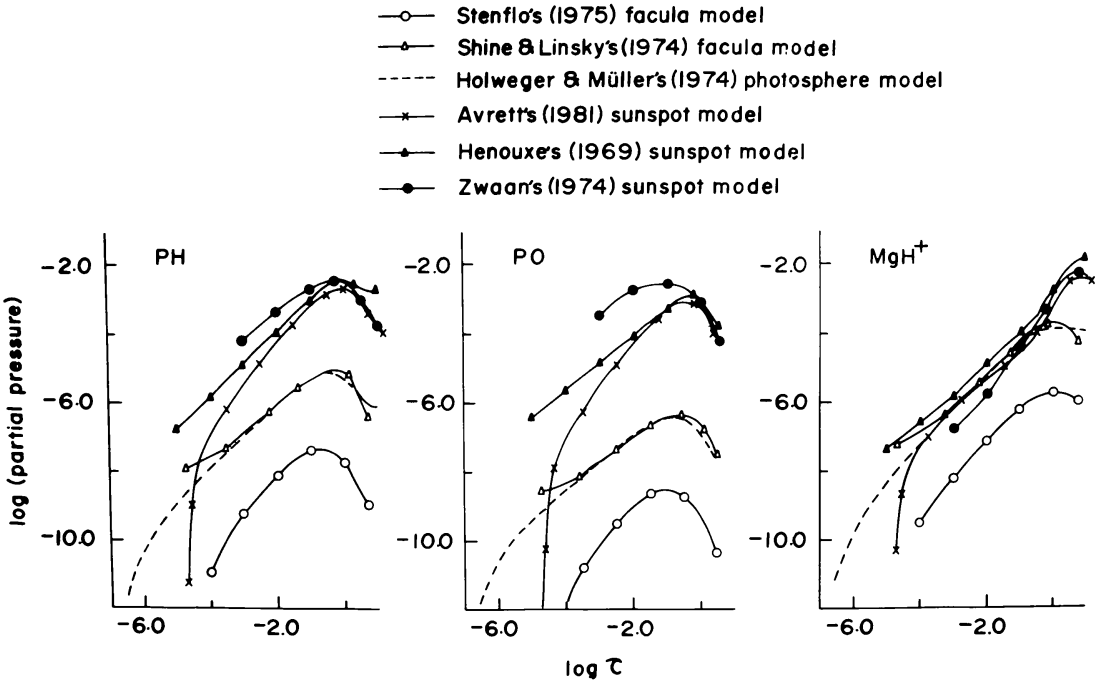

Fig. 2. Partial pressure of the molecules PH, PO, and MgH^+ in the six considered models as functions of optical depth.

Table II. It may be noted from this table, that like other average facula models, the model of Shine and Linsky (1974) gives equivalent widths higher than the corresponding photospheric value. This was noted earlier also in case of CN lines (Tripathi and Sinha,

TABLE II

Predicted equivalent widths of $B^2\Sigma^+ - X^2\pi_r$ transition of PO, $A^3\pi_i - X^3\Sigma^-$ of PH, $A^1\Sigma^+ - X^1\Sigma^+$ of MgH^+, and $B^2\Sigma^+ - A^2\pi_i$ of CN in solar atmosphere

λ pred. (Å)	Branch identification	Equivalent width (mÅ)					
		Sunspot models			Photosphere model	Facula models	
		Zwaan (1974)	Avrett (1981)	Hénoux (1969)	Holweger and Müller (1974)	Shine and Linsky (1974)	Stenflo (1975)
PO (0, 0) band							
3240.93	$rQ_{21}(32.5)$	13.0	4.8	3.1	1.6 (−3)	2.1 (−3)	4.6 (−4)
3241.58	$rQ_{21}(28.5)$	12.8	4.7	3.0	1.5 (−3)	2.0 (−3)	4.4 (−4)
3245.79	$Q_{11}(11.5)$	9.4	3.2	2.1	9.4 (−4)	1.2 (−3)	2.8 (−4)
3263.01	$Q_{22}(46.5)$	19.1	7.9	5.1	2.9 (−3)	4.0 (−3)	8.6 (−4)
3263.17	$Q_{22}(45.5)$	19.1	7.9	5.1	2.9 (−3)	3.9 (−3)	8.6 (−4)
3263.78	$Q_{22}(41.5)$	19.1	7.8	5.1	2.8 (−3)	3.8 (−3)	8.2 (−4)
3263.93	$Q_{22}(40.5)$	19.1	7.8	5.1	2.8 (−3)	3.7 (−3)	8.1 (−4)
3273.31	$oP_{12}(21.5)$	6.4	2.1	1.4	6.3 (−4)	8.4 (−4)	1.9 (−4)
PH (0, 0) band							
3418.922	$oP_{23}(3)$	29.2	29.5	28.2	0.15	0.22	0.06
3419.009	$Q_{22}(13)$						
3419.765	$Q_{11}(8)$	30.5	30.7	29.0	0.15	0.21	0.058
3419.803	$R_{12}(6)$						
3427.440	$P_{23}(5)$	23.6	23.4	22.8	0.18	1.3	0.038
3427.474	$Q_{11}(6)$						
3429.167	$Q_{11}(17)$	30.0	30.6	29.2	0.18	0.26	0.071
3431.033	$Q_{11}(18)$	29.2	29.7	28.5	0.18	0.26	0.07
MgH^+ (0, 2) band							
3111.203	$R(16)$	20.9	21.0	21.8	3.0	4.3	1.8
3115.598	$R(17)$	20.8	20.9	21.7	3.0	4.3	1.8
3136.116	$R(21)$	19.7	19.6	20.2	3.0	4.3	1.8
3138.037	$P(16)$	20.1	20.1	21.1	2.9	4.1	1.7
3175.359	$R(27)$	16.2	15.9	16.3	2.5	3.8	1.5
3190.561	$R(29)$	14.7	14.4	14.7	2.4	3.5	1.4
3210.972	$P(26)$	16.6	16.2	16.7	2.6	3.9	1.5
3299.892	$R(41)$	6.4	6.1	5.9	1.2	1.9	0.6
MgH^+ (0, 3) band							
3237.146	$R(9)$	8.4	8.4	9.4	1.1	1.6	0.6
3241.621	$R(11)$	9.3	9.2	10.2	1.2	1.8	0.7
3275.978	$R(20)$	9.8	9.5	10.3	1.4	2.1	0.8
3333.993	$P(23)$	8.9	8.4	9.1	1.3	2.0	0.7
3338.923	$R(30)$	6.7	6.3	6.6	1.1	1.7	0.6
3469.933	$P(38)$	3.8	3.4	3.5	0.7	1.2	0.4
CN (0, 0) band							
5947.984	$P1(22.5)$			0.005	0.083		
5954.808	$P2(21.5)$			0.0047	0.078		
5940.199	$R1(22.5)$			0.0055	0.092		
5946.551	$R2(21.5)$			0.0056	0.092		

$\lambda_{pred} = \lambda_{air} + 10$ mÅ (gravitational red shift).
Notation: $6.0\,(-3) = 6.0 \times 10^{-3}$.

1986). For a brief resume on the molecular transitions considered here we refer to Atalla (1984), Singh (1984), DeGouveia and Singh (1984), Singh, Gomes Balboa, and De Freitas Pacheco (1985), and Atalla and Singh (1987). Now we shall take each transition separately for discussion. As it should be expected the lines in general are strengthened in umbrae atmospheres compared to photosphere and facula. In the light of the following predictions we feel that sunspot observations in the 3000 to 4000 Å region may lead to identification of new molecular lines and to perhaps an improved opacity code. However, blending and scattering effects from photosphere should be taken into account.

3.1. THE $B^2\Sigma^+ - X^2\pi_r$ TRANSITION OF PO (TABLE II)

The oscillator strength $f_{00} = 2.79 \times 10^{-3}$ is based upon lifetime studies carried out by Wong *et al.* (1986). Variation of electronic transition moment with internuclear distance was accounted for. An inspection of Table II leads to the result that the beta bands of PO which have equivalent widths less than thousandth of a mÅ cannot be observed in photosphere and facular spectra. However, the intensities in umbrae are in excess of one mÅ in all the models considered here. It seems likely that the lines are of sufficient strength to register in high quality FTS scans.

3.2. THE $A^3\pi_i - X^3\Sigma^-$ TRANSITION OF PH (TABLE II)

The identification of this transition in the umbral spectrum seems possible. All the lines considered here are stronger than 10 mÅ. In photospheric and facular spectra the lines might lie close to the limit of detectibility. Sauval *et al.* (1977), using $f_{00} = 10^{-2}$ found the maximum photospheric equivalent width of 0.3 mÅ. So this should be considered a border line case only. The oscillator strength used agrees very well with the value $f_{00} = 8.6 \times 10^{-3}$ theoretically obtained by Senekowitsch, Rosmus, and Werner (1986).

Detection of the umbral (1, 0) band of the vibration-rotation lines may be possible but in faculae and photosphere these lines will not appear.

3.3. THE $A^1\Sigma^+ - X^1\Sigma^+$ TRANSITION OF MgH^+ (TABLE II)

The accuracy of the wavelengths (Singh, 1984) was checked with the help of the term values given by Balfour (1972). Sauval *et al.*'s (1977) oscillator strength was used to obtain the same for the (0–3) band from standard expressions. It is clear from Table II that the lines of the electronic transition of this molecule are of detectible strengths in umbra, photosphere and facula. The photospheric equivalent widths obtained are in agreement with Sauval *et al.* (1977). A notable feature of this study is the large equivalent widths of MgH^+ in umbral atmosphere because of the large partial pressures in sunspots (cf. Figure 2). Further, MgH^+ has a low dissociation energy ($D_0^0 = 2.08$ eV) which can perhaps help in resolving problems associated with umbral MgH ($D_0^0 = 1.27$ eV) (Sinha, 1982; Yun and Kim, 1983).

The vibration-rotation line predictions may not be reliable because the dipole moments used here for oscillator strength calculations are not very accurate.

3.4. THE $B^2\Sigma^+ - A^2\pi_i$ TRANSITION OF CN MOLECULES (TABLE II)

The red and the violet band systems of CN molecules are characteristic features of the solar spectrum. In recent years experiments have been carried out to determine the band oscillator strength for the Le Blanc bands of CN. We used the upper limit of oscillator strengths from Halpern and Tang (1983), Lavendy, Gandara, and Robbe (1984), Costes, Naulin, and Dorthe (1985), together with Holweger and Müller (1974) photospheric model and Hénoux (1969) sunspot model. The results clearly indicate (Table II) that this band system is not identifiable in the solar spectrum. In sunspots increased association of carbon atoms in CO formation leads to a depletion of CN molecules resulting in still lower equivalent widths. However, it may be useful to search for these lines in the spectra of carbon stars where CO problem is less severe.

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