On MgH line intensities in sunspot umbrae

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Abstract. The line intensities of the umbral MgH molecules reported by Sotirovski (1971) are re-analysed utilizing the latest laboratory data. It appears probable that because of a neglect of the role of blurring in producing stray light, Sotirovski's (1971) results are under estimated. The need of a laboratory check upon the theoretical oscillator strengths of the weak bands ($\Delta v \neq 0$) calculated by Kirby *et al.* (1979) is stressed.

Key words : sunspot umbrae—MgH

1. Introduction

The MgH lines are a characteristic feature of late-type stars. They have been a subject of study in the solar spectrum also (Schadee 1964; Boyer *et al.* 1971; Lambert *et al.* 1971; Sotirovski 1971; Webber 1971; Grevesse & Sauval 1963; Sinha *et al.* 1979; Sinha 1981). Sotirovski (1971, 1972) has provided detailed tables on the line intensities of molecules, including MgH, observed in sunspot spectra.

Recently the discovery of a low-lying electronic state in the MgH molecule has led to a better evaluation of its dissociation energy (Balfour & Cartwright 1976; Balfour & Lindgren 1978) which helps in a better understanding of the line spectrum observed in different sources. Since the molecular oscillator strengths are crucially dependent upon the dissociation energies, the new result, $D_0^0 (MgH) = 1.27$ eV has been used by Kirby *et al.* (1979) to provide a set of theoretical oscillator strengths for use in the interpretation of line intensities. The theoretical results for the intense (0–0) band and the (1–1) band are in excellent agreement with the laboratory results on life-time measurements (Nedelac & Dufayard 1978). Further, the oscillator strength for the (0–0) band is in agreement with the analyses carried out by Tomkin & Lambert (1980) and Sinha (1981) in the case of the star epsilon Eridani and the solar photosphere respectively.

In the previous studies of MgH lines in sunspot umbrae $D_0^0 (MgH) \simeq 2.2$ eV was used (Boyer *et al.* 1971; Sotirovski 1971; Webber 1971) as against the new value $D_0^0 (MgH) = 1.27$ eV mentioned above. Further, following Main *et al.* (1967), Sotirovski (1971) used the electronic part of the oscillator strength, $f_e (MgH) = 1.5 \times 10^{-3}$ which, however, is in error (Grevesse & Sauval 1973; Sinha 1981).

In the present investigation the MgH line intensities reported by Sotirovski (1971) are re-analysed in the light of the new results on oscillator strength and the dissociation energy.

2. Formulations and calculations

Only good-quality lines of the green band of the MgH molecules were selected from Sotirovski (1971) with the help of the tables given by Sotirovski (1972). The calculated values of equivalent widths, W_{cal}, were compared with the corresponding observed values of equivalent widths, W_{obs}. The various sources for data etc. used in calculations are listed below :

Magnesium abundance : 7.62 (Lambert & Luck 1978)
Dissociation energy : 1.27 eV (Balfour & Lindgren 1978)
Oscillator strengths : Kirby *et al.* (1979)
Hönl-London factors : Kovacs (1969)
Molecular constants : Hüber & Herzberg (1979)
Opacity sources : Tsuji (1966)
Dissociation constants : Tripathi & Gaur (1979)
Reduced equation for $p(Mg)$: Sotirovski (1971) and Gaur *et al.* (1973)
Formula for profile calculation : Gaur *et al.* (1971) and Sotirovski (1971)
Microturbulence velocity : 1 km s⁻¹ (Sotirovski 1971)

It was found that the equation

$$\log K_p = 0.0691021\,\theta^2 - 1.581551\,\theta + 10.73311 \qquad \ldots (1)$$

can reproduce the dissociation constants of Tripathi & Gaur (1979) with an accuracy better than 2.5 per cent. Here $\theta = 5040/T$ with T as temperature.

The sunspot models of Henoux (1969), Zwaan (1974), Stellmacher & Wiehr (1975), Boyer (1980) and Kollatschny *el al.* (1980) abbreviated hereinafter as HSM-69, ZSM-74, SWSM-75, BSM-80 and KSM-80 respectively, were used in the calculations of equivalent widths. These models provide a fairly wide range in the proposed models for sunspot umbrae. HSM-69 is the hottest while ZSM-74 is the coolest in the molecule forming region of an umbra. The model BSM-80 is an improved version of SWSM-75 and has been used by Boyer (1980) to explain the line intensities of the γ and the γ' band systems of TiO in the spectral range 6100–7100Å. KSM-80 explains line intensities due to different atomic species in a wide spectral range when an opacity enhancement factor due to Zwaan (1974) is included in the calculations (Kollatschny *et al.* 1980). In the present calculations the opacity enhancement factor due to Zwaan (1974) was used to derive ZSM-74 and KSM-80 based results.

3. Results and discussions

As emphasized in section 1 the oscillator strength for the (0–0) band is now known with good accuracy. Therefore, in the first attempt 16 lines of the (0–0) band were used to compute W_{cal} in two sunspot models *viz.*, ZSM-74 and KSM-80. Oscillator strengths were chosen as $f_{0-0} = 0.161$ (Kirby *et al.* 1979) and $f_{0-0} = 0.11$ (Tomkin & Lambert 1980). The results are presented in table 1. It may be inferred that (i) the two oscillator strengths and the two models give the same scale factors which are averages of (W_{cal}/W_{obs}) and (ii) the calculated equivalent widths are higher than observations. We felt prompted to extend the investigation to more

lines which, however, does not change the conclusions. Good quality lines of the (1–1), (2–2), (1–2) and (0–1) bands were selected with the help of Sotirovski (1972). The $\Delta\upsilon = 0$ and $\Delta\upsilon = -1$ sequences were treated separately. Also the models HSM-69, SWSM-75 and BSM-80 were included to eliminate uncertainties due to model atmospheres. The results are given in tables 2a and 2b. The scale factors which are suggestive of an increase in the observed equivalent widths were used to scale the W_{obs} values due to Sotirovki (1971) and the resulting values were plotted against W_{cal} for the different model atmospheres in figures 1 through 5. The dotted lines are drawn to indicate the 20 per cent scatter in observations while the solid one shows the 45° line.

Table 1. (0–0) band intensities in ZSM-74 and KSM-80

Wavelength (Å)	Identification	Equivalent width (mÅ)			
		ZSM-74		KSM-80	
		$f_{0-0} = 0.161$	$f_{0-0} = 0.11$	$f_{0-0} = 0.161$	$f_{0-0} = 0.11$
5055.40	$Q_2(38)$	99.2	92.9	94.1	87.2
5055.77	$Q_1(38)$	97.3	90.9	92.0	85.3
5061.54	$Q_2(37)$	101.2	94.9	96.3	89.3
5073.38	$Q_2(35)$	105.0	98.8	100.4	93.4
5073.75	$Q_1(35)$	103.2	97.0	98.5	91.4
5079.51	$Q_1(34)$	105.0	98.9	100.5	93.4
5085.18	$Q_1(33)$	106.8	100.7	102.4	95.4
5095.34	$R_1(18)$	113.3	108.0	109.3	102.8
5101.06	$Q_2(30)$	112.7	107.2	108.9	102.5
5106.21	$Q_2(29)$	114.0	108.6	110.4	104.0
5106.85	$R_2(16)$	114.5	109.3	110.7	104.2
5111.26	$Q_2(28)$	115.2	109.9	111.8	105.4
5125.82	$Q_1(25)$	117.3	112.2	114.5	108.1
5134.20	$Q_2(33)$	109.0	103.0	104.7	97.9
5190.56	$P_2(29)$	103.7	97.4	98.3	91.1
5207.78	$P_2(10)$	110.3	104.6	105.0	98.1
*Scale factor		1.8 ± 0.1	1.7 ± 0.1	1.7 ± 0.1	1.6 ± 0.1

Table 2(a). Calculated intensities of MgH lines in the spectrum of sunspots ($\Delta\upsilon = 0$ band sequences)

Wavelength (Å)	Identification	Equivalent width (mÅ)				
		ZSM-74	KSM-80	HSM-69	SWSM-75	BSM-80
0–0 band; $f_{0-0} = 1.61 \times 10^{-1}$						
5055.40	$Q_2(38)$	99.2	94.1	80 9	84.5	78.9
5055.77	$Q_1(38)$	97.3	92.0	79.6	82.6	77.2
5061.54	$Q_2(37)$	101.2	96.3	82.2	86.3	80.6
5073.38	$Q_2(35)$	105.0	100.4	84.7	89.8	83.7
5073.75	$Q_1(35)$	103.2	98.5	83.4	88.1	82.2
5079.51	$Q_1(34)$	105.0	100.5	84.7	89.8	83.7
5085.18	$Q_1(33)$	106.8	102.4	86.0	91.4	85.2
5095.34	$R_1(18)$	113.3	109.3	91.4	98.3	91.6
5101.06	$Q_2(30)$	112.7	108.9	91.1	97.2	90.8
5106.21	$Q_2(29)$	114.0	110.4	92.2	98 5	92.1
5106.85	$R_2(16)$	114.5	110.7	92.4	99.5	92.8
5111.26	$Q_2(28)$	115.2	111.8	93.3	99.8	93.3
5125.82	$Q_1(25)$	117.3	114.5	95.4	102.0	95.5
5134.20	$Q_2(33)$	109.0	104.7	87.4	93.1	86.8
5190.56	$P_2(29)$	103.7	98.3	82.5	87.5	81.3
5207.78	$P_2(10)$	110.3	105.0	87.0	94.0	87.1

Continued

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Table 2(a)—*Continued*

Wavelength (Å)	Identification	Equivalent width (Åm)				
		ZSM-74	KSM-80	HSM-69	SWSM-75	BSM-80
1-1 band; $f_{1-1} = 1.41 \times 10^{-1}$						
5059.71	$R_1(20)$	101.6	95.9	81.7	86.8	80.7
5071.16	$R_2(18)$	103.5	97.9	82.9	88.5	88.2
5100.27	$Q_3(25)$	108.8	104.3	87.3	93.3	86.9
5109.03	$Q_1(23)$	109.8	105.4	88.1	94.2	87.7
5120.12	$Q_2(20)$	112.5	108.4	90.5	97.0	90.4
5130.18	$Q_2(17)$	113.6	109.7	91.4	98.1	91.5
5132.87	$R_1(6)$	100.0	93.3	79.5	84.5	78.2
5141.08	$R_1(4)$	96.0	88.8	76.7	80.6	74.6
5144 04	$Q_1(12)$	113.6	109.5	91.2	98.0	91.3
2-2 band; $f_{2-2} = 1.24 \times 10^{-1}$						
5049.25	$R_2(18)$	92.4	85.8	75.6	78.1	72.7
5102.28	$Q_2(18)$	103.2	97.8	82.7	87.9	81.7
5102.67	$Q_1(18)$	102.9	97.5	82.5	87.5	81.4
5103.26	$R_2(7)$	88.5	81.5	72.2	73.9	68.6
5105.75	$Q_1(17)$	103.3	97.9	82.8	87.9	81.7
5107.13	$R_2(6)$	86.8	79.8	70.9	72.2	67.0
5108.09	$R_1(6)$	88.0	81.0	71.8	73.3	68.1
5112.12	$R_1(5)$	86.1	79.2	70.4	71.5	66.4
5115.99	$Q_2(13)$	103.3	97.6	82.5	87.8	81.6
5147.00	$P_1(6)$	80.9	74.6	66.2	66.5	61.7
5152.95	$P_2(12)$	88.9	82.0	72.3	73.8	68.5
Scale factor		1.9 ± 0.2	1.8 ± 0.2	1.5 ± 0.2	1.6 ± 0.2	1.5 ± 0.2

Table 2(b). Calculated intensities of MgH lines in the spectrum of sunspots ($\Delta v = -1$ band sequences)

Wavelength (Å)	Identification	Equivalent width (mÅ)				
		ZSM-74	KSM-80	HSM-69	SWSM-75	BSM-80
1-2 band: $f_{1-2} = 1.59 \times 10^{-2}$						
5488.75	$Q_1(19)$	66.1	62.6	54.7	52.3	49.0
5523.03	$R_2(5)$	40 9	36.6	37.6	34.1	31.9
5524.79	$Q_1(12)$	67.3	63.2	55.0	52.9	49.4
5531.71	$Q_2(10)$	64.4	60.3	53.0	50.7	47.3
5533.59	$P_1(24)$	42.5	39.7	39.7	35.5	33.7
5534.15	$R_1(3)$	35.6	31.5	33.8	30.3	28.4
5541.21	$Q_1(7)$	60.7	56.6	50.5	48.0	44.8
5545.59	$Q_1(5)$	54.8	50.6	46.7	43.7	40.9
5554.06	$P_1(19)$	47.6	44.3	42.7	38.8	36.7
5556.51	$P_2(18)$	48.4	44.9	43.1	39.3	37.1
5563.38	$P_2(15)$	48.4	44.7	42.9	39.2	37.0
5563.99	$P_1(15)$	48.9	45.2	43.3	39.6	37.3
0-1 band; $f_{0-1} = 8.61 \times 10^{-3}$						
5520.23	$R_1(13)$	51.1	46.6	44.2	41.2	38.5
5527.40	$R_2(12)$	50.7	46.1	43.9	40.8	38.2
5539.07	$Q_1(19)$	64.1	60.1	52.8	50.4	47.1
5544.82	$Q_2(18)$	65.4	61.2	53.5	51.3	47.9
5548.90	$R_2(9)$	48.0	43.2	42.0	38.8	36.2
5550.68	$Q_2(17)$	65.9	61.5	53.7	51.6	48.3
5551.10	$Q_1(17)$	65.5	61.2	53.6	51.3	48.0
5555.52	$R_2(8)$	46.5	41.6	40.9	37.7	35.3
5566.43	$Q_2(14)$	66.1	61.5	53.7	51.7	48.2
5566.92	$Q_1(14)$	66.3	61.7	53.8	51.8	48.4

Continued

Table 2(b)—*Continued*

Wavelength (Å)	Identification	Equivalent width (mÅ)				
		ZSM-74	KSM-80	HSM-69	SWSM-75	BSM-80
5571.54	$Q_1(13)$	66.2	61.5	53.7	51.7	48.2
5583.57	$Q_1(10)$	64.3	59.5	52.3	50.2	46.7
5586.31	$Q_2(\ 9)$	61.4	56.5	50.3	48.0	44.7
5596.76	$P_1(22)$	42.5	38.9	39.0	35.0	33.0
5603.94	$P_2(20)$	45.2	41.3	40.6	36.8	34.6
5616.92	$P_2(14)$	46.2	41.8	40.8	37.3	34.9
5617.52	$P_1(15)$	46.9	42.7	41.4	37.9	35.5
Scale factor		3.0 ± 0.6	2.8 ± 2.6	2.6 ± 0.7	2.5 ± 0.6	2.3 ± 0.5
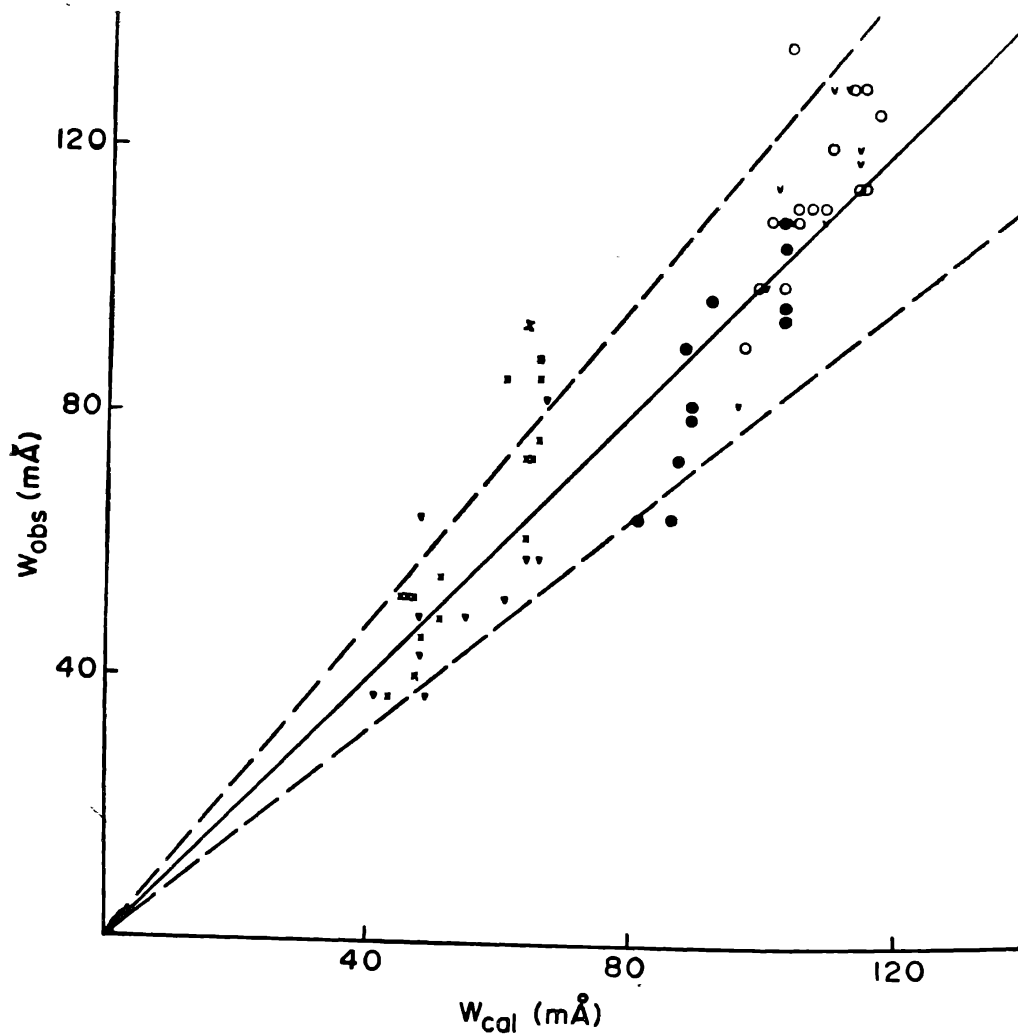
Figure 1. A plot of the scaled observations of MgH equivalent widths against the ZSM-74 based results (*cf.* section 3). The open circles are used for the (0-0) band, v's for the (1-1) band, filled circles for the (2-2) band, crosses for the (0-1) band and the filled inverted triangles for the (1-2) band.

The higher scale factors for the $\Delta v \neq 0$ (compare tables 2a and 2b) sequence might indicate the possibility of uncertainties in the theoretical values of the oscillator strengths used here for the weaker bands. This point was further investigated by
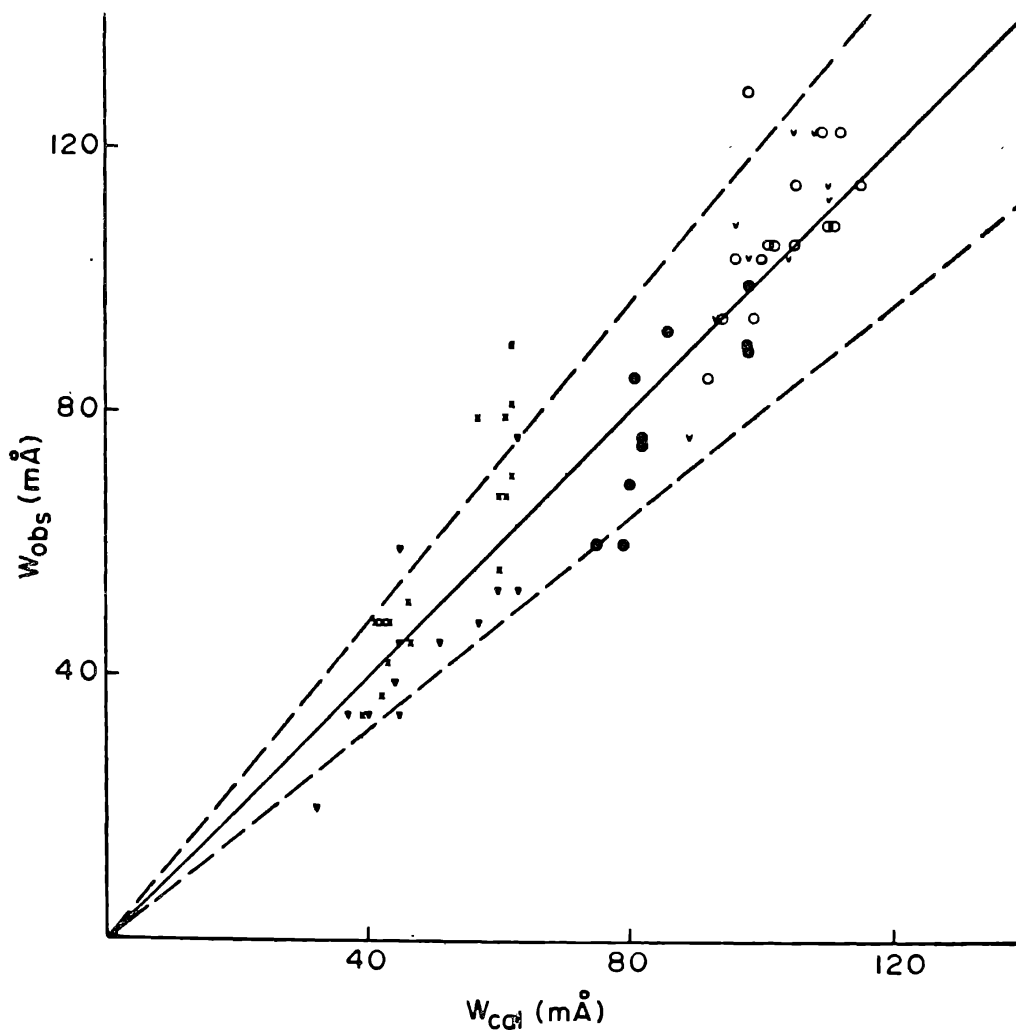
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Figure 2. Same as in figure 1 but for the model KSM-80.

recalculating the equivalent widths of the lines of the (0–1) band for which Tomkin & Lambert (1980) show that the oscillator strength due to Kirby *et al.* (1979) is exaggerated by a factor 3 and that the real value is $f_{0-1} = 0.0029$. The results for $f_{0-1} = 0.0029$ are given in figure 6 and table 3. In figure 6 it can be seen that with an exception of only one or two points, all points lie within dotted lines. Also the scale factors in table 3 are now in conformity with the results arrived at in table 2a. Therefore, it is felt that a laboratory investigation in which the purity of the spectrum is better ensured is needed to assess the oscillator strengths of the $\Delta \upsilon \neq 0$ band sequences.

From the foregoing it is clear that the calculated line intensities for the green band of the MgH molecules are considerably larger than those reported by Sotirovski (1971). The reason for such a systematic discrepancy in equivalent widths might be an underestimation of the dilution of the observed umbral spectrum by stray light. Sotirovski (1971) assumed the photospheric light to be the only source of stray light whereas Lambert *et al.* (1971) have stressed upon the assessment of contribution from umbral dots also and Stellmacher & Wiehr (1981) have estimated
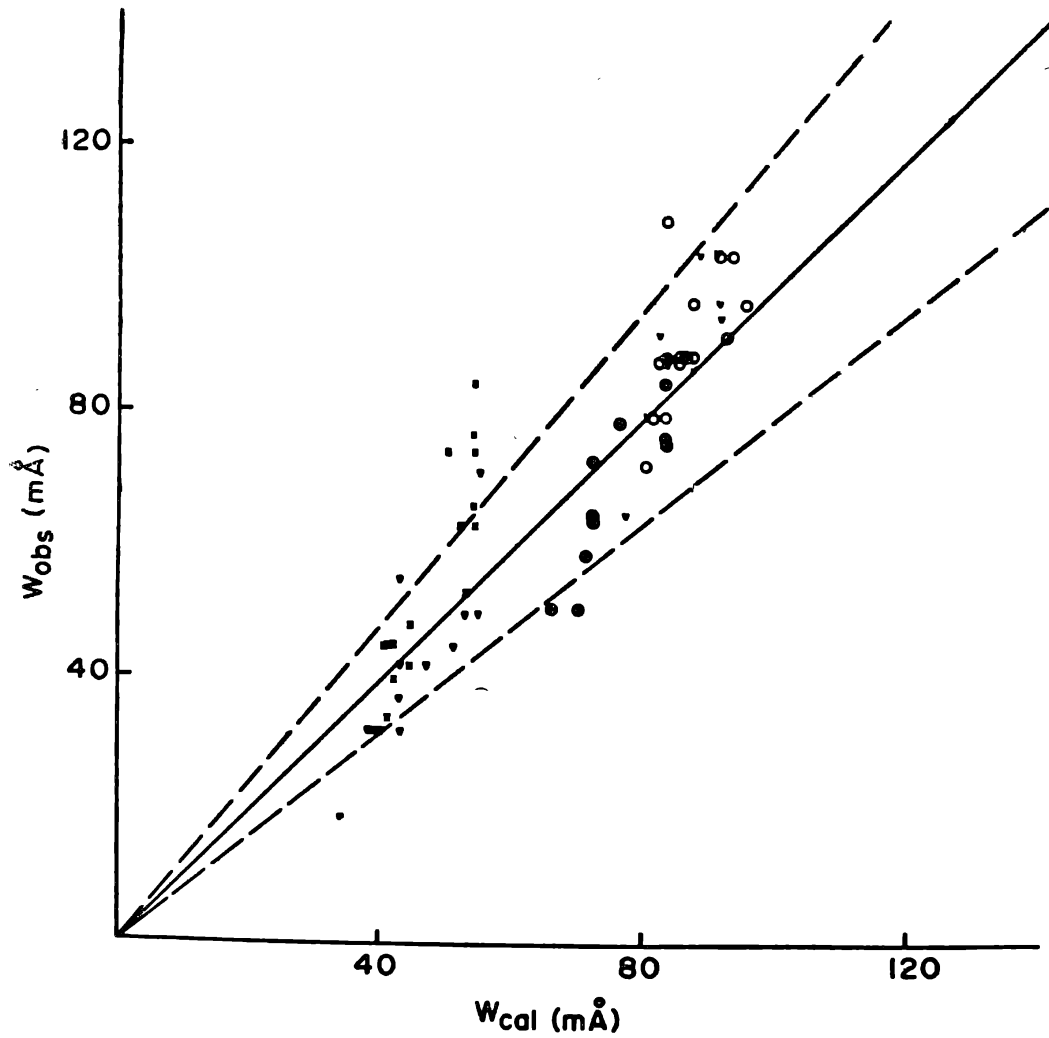
Figure 3. Same as in figure 1 but for the model HSM-69.

Table 3. (0–1) band intensities in five sunspot models with $f_{0-1} = 0.0029$

| Wavelength (Å)	Identification	Equivalent width (mÅ)				
		ZSM-74	KSM-80	HSM-69	SWSM-75	BSM-80
5520.23	$R_1(13)$	26.1	22.5	26.2	23.2	21.6
5527.40	$R_2(12)$	25.8	22.1	25.8	22.9	21.3
5539.07	$Q_1(19)$	37.4	33.5	35.3	31.6	29.7
5544.82	$Q_2(18)$	38.7	33.6	36.1	32.4	30.4
5548.90	$R_2(9)$	23.7	20.1	23.9	21.2	19.6
5550.68	$Q_2(17)$	39.1	34.9	36.3	32.7	30.6
5551.10	$Q_1(17)$	38.7	34.6	36.1	32.4	30.4
5555.52	$R_2(8)$	22.6	19.1	22.9	20.3	18.7
5566.43	$Q_2(14)$	39.2	34.8	36.2	32.6	30.6
5566.92	$Q_1(14)$	39.4	35.1	36.4	32.8	30.7
5571.54	$Q_1(13)$	39.2	34.9	36 2	32.6	30.6
5583.57	$Q_1(10)$	37.3	32.9	34.7	31.2	29.1
5586.31	$Q_2(9)$	34.6	30.2	32.6	29.2	27.2
5596.76	$P_1(22)$	20.0	17.5	21.3	18.4	17.2
5603.94	$P_2(20)$	21.8	19.0	22.7	19.8	18.5
5616 92	$P_2(14)$	22.4	19.2	22.9	20.1	18.6
5617.52	$P_1(15)$	23.0	19.8	23.5	20.6	19.1
Scale factor		1.5 ± 0.2	1.3 ± 0.2	1.5 ± 0.2	1.3 ± 0.2	1.2 ± 0.2
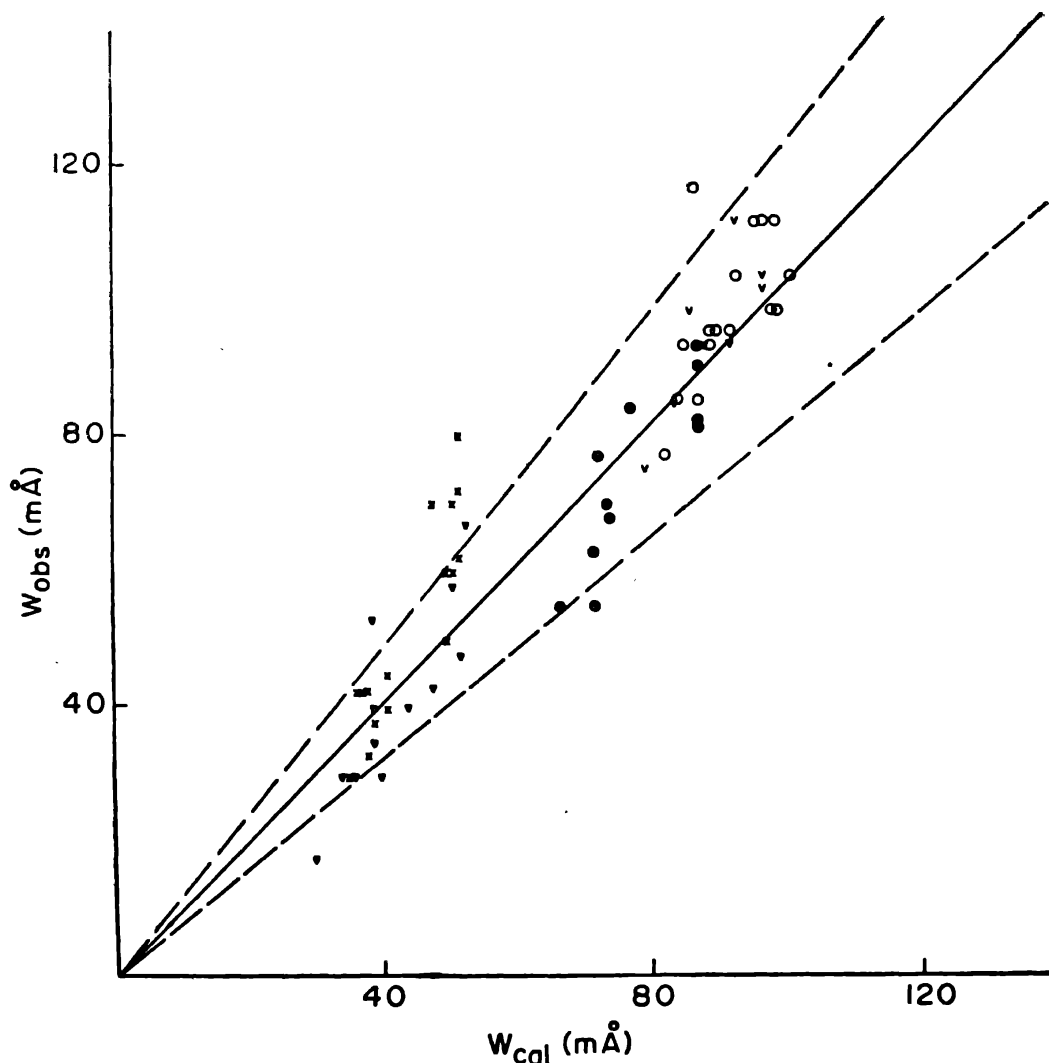
Figure 4. Same as in figure 1 but for the model SWSM-75.

similar contributions from penumbral blurring. It appears to us that the range 5–10 per cent given by Stellmacher & Wiehr (1981) for the stray light includes the contribution from umbral dots. If we accept 2 per cent contribution from photosphere, the total amount of stray light to dilute the umbral spectrum could be as high as 7–12 per cent. Further, using $(1 + a/i) = 1.33$ for $\lambda = 5000$ Å (Sotirovski 1972), we calculated the amount of scattered light needed to give the scale factors given in table 2a for the different photosphere-to-sunspot contrast values. The contrast was calculated by utilizing the photospheric model of Vernazza *et al.* (1976) and the five sunspot models discussed above. It is found that only 8 to 14 per cent of stray light is sufficient to explain the scale factors in table 2a.

The other possible causes for the inequality $W_{cal} > W_{obs}$ could be (i) a lower value of microturbulence velocity; (ii) the neglect of formation of molecules like MgS, MgOH and MgH_2 in the calculation of $p(Mg)$ *i.e.*, the partial pressure of Mg and (iii) some uncertainties in the magnesium abundance.
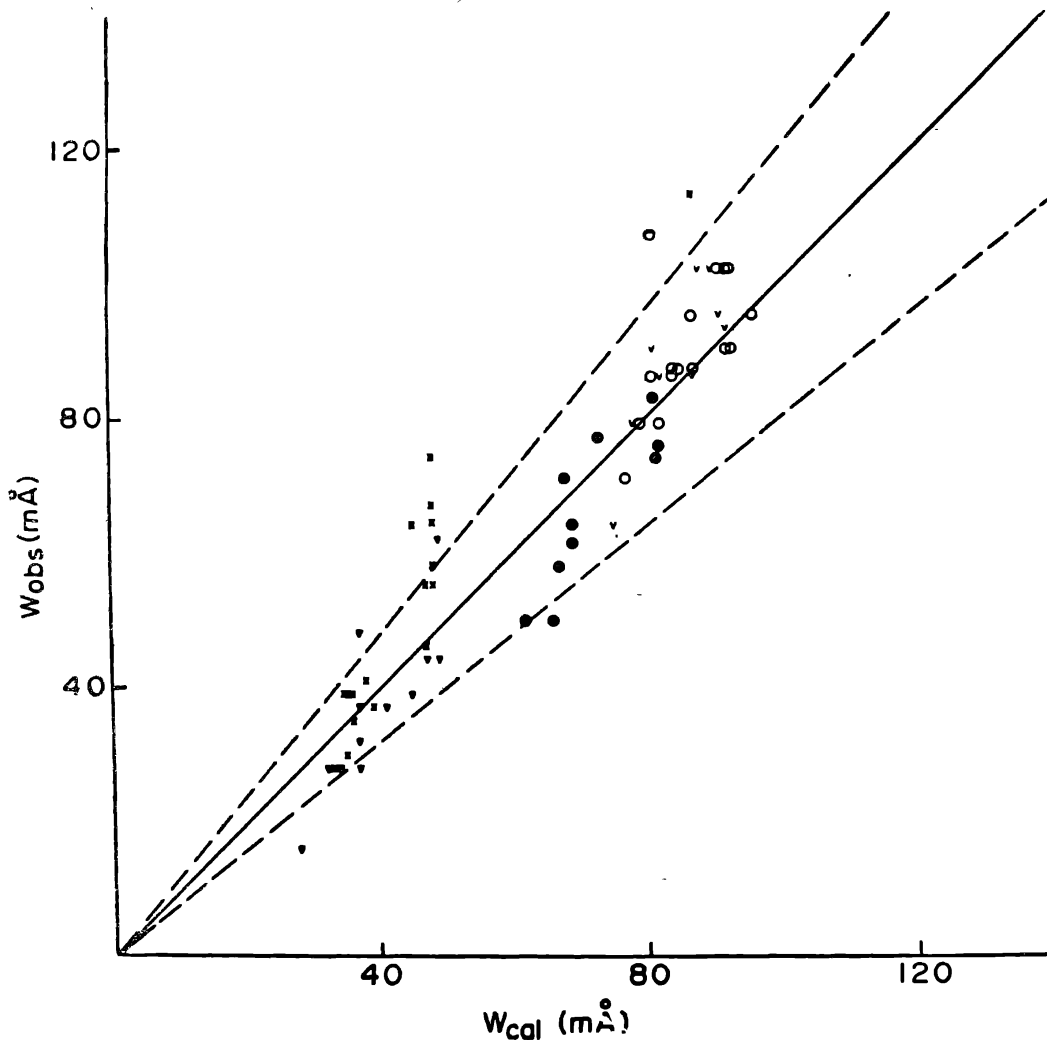
Figure 5. Same as in figure 1 but for the model BSM-80.

Using 0.5 km s^{-1} as the other value of microturbulence (Boyer 1980), the results of calculation for the (0–0) band are presented in table 4 for the model ZSM-74 with $f_{0-0} = 0.161$. It is inferred that the reduction in the value of microturbulence is not enough to explain the stated discrepancy.

A reconsideration by us on the basis of the dissociation constants provided by Tsuji (1973) for MgS and MgOH indicated that because of low concentrations, these molecules can be neglected in the calculation of $p(\text{Mg})$. For MgH_2 dissociation constants are not available. It may, however be noted that the atoms Be, Ca, Cd, Mg and Zn have completely filled outermost sub-shells and also the dissociation energies of the hydrides of these atoms are low and about the same as that of MgH (Huber & Herzberg 1979). On the basis of this analogy, if we assume the dissociation energies of BeH_2 and MgH_2 to be almost equal then it may be expected that $n(\text{BeH})/n(\text{BeH}_2)$ is the same as $n(\text{MgH})/n(\text{MgH}_2)$, where n denotes the molecular concentration. We have compared the concentrations of BeH and BeH_2 following Tsuji (1973) and concluded that at sunspot temperatures BeH_2 is much less abundant then BeH. Therefore, we are inclined to believe that the molecular concentration of MgH_2 too should be less

than that of MgH under the physical conditions prevalent in sunspots. A lowering of magnesium abundance in sunspots would be in clear contrast to the well established photospheric abundances (Lambert & Luck 1978, Hauge & Engvold 1977). Also the model atmospheres chosen here present a wide range in the sunspot models and a change in their structure could be too drastic.
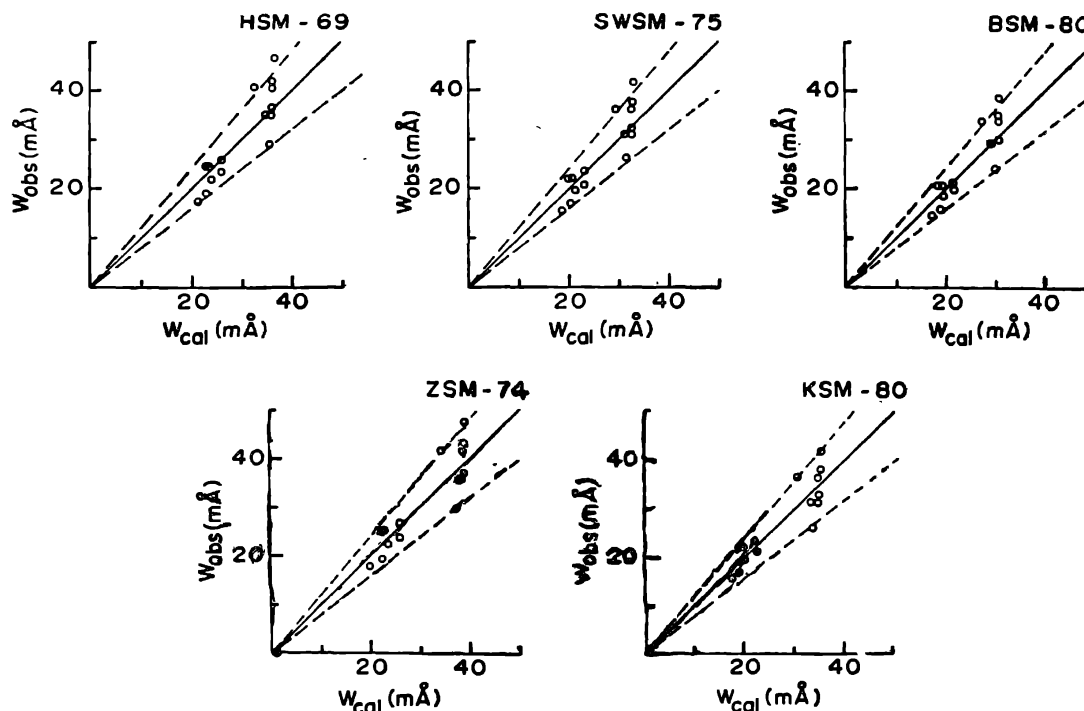

Figure 6. Plots of the scaled observations of the (0-1) band of MgH against different model based results. Here $f_{0-1} = 0.0029$ was used.

Table 4. Comparison of equivalent widths of the (0-0) band of MgH obtained with different values of microturbulence velocity

Wavelength (Å)	Identification	Equivalent widths (mÅ)	
		$\zeta = 1$ km s^{-1}	$\zeta = 0.5$ km s^{-1}
5055.40	$Q_2(38)$	99.2	89.7
5055.77	$Q_1(38)$	97.3	87.9
5061.54	$Q_2(37)$	101.2	91.4
5073.38	$Q_2(35)$	105.0	94.6
5073.75	$Q_1(35)$	103.2	93.1
5079.51	$Q_1(34)$	105.0	94.7
5085.18	$Q_1(33)$	106.8	96.2
5095.34	$R_1(18)$	113.3	101.6
5101.06	$Q_2(30)$	112.7	101.3
5106.21	$Q_2(29)$	114.0	102.3
5106.85	$R_2(16)$	114.5	102.6
5111.26	$Q_2(28)$	115.2	103.3
5125.82	$Q_1(25)$	117.3	105.1
5134.20	$Q_2(33)$	109.0	98.1
5190.56	$P_2(29)$	103.7	93.5
5207.78	$P_2(10)$	110.3	99.1
Scale factor		1.8 ± 0.1	1.6 ± 0.1

In brief it appears that the equivalent widths of MgH lines are stronger than reported by Sotirovski (1971). A similar conclusion is reached by Wiehr (1981, personal communication). A good quality sunspot spectrum in which the stray light is properly accounted for is needed to give the true intensities of MgH lines.

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Note added in proof : Gustaffson (1982, personal communication) has pointed out the possibility of an error in the K_p values given by Tripathi & Gaur (1979). The corrections needed for the results on equivalent width calculation are negligibly small. They shall, however, be important while calculating the partial pressure of MgH. Correct coefficients of $\log K_p$(MgH) from equation (1) are being published elsewhere.