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Behaviour of some neutral molecular absorption lines in facula models

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Abstract. The equivalent widths of some selected absorption lines of C_2, CH, MgH, NH, OH and SH molecules in five facula and two photospheric models have been calculated under the assumption of LTE. The calculations reveal that the lines belonging to C_2 can be used for refining spatially limited models. Molecules MgH and SH are good candidates for homogeneous facula models, but the lines would be extremely weak or absent in spatially limited models. Molecules CH, NH and OH seem to be good candidates both for the homogeneous and the spatially limited facular models.

Key words : neutral molecules—absorption lines—equivalent width—facula models

1. Introduction

The presence of the molecules C_2, CH, MgH, NH & OH in the solar photospheric spectrum is well established. The problems in their identifications in photosphere have been discussed in detail (Grevesse & Sauval 1973; Lambert 1978). The presence of the (0, 0) band of the transition $A^2\Sigma - X^2\Pi_i$ of the molecule SH in the solar photospheric spectrum has been theoretically investigated by Sinha *et al.* (1977). Sauval *et al.* (1977) are of the opinion that the SH lines are very probably present in the solar disk spectrum.

The behaviour of absorption lines in facula has been studied in far less detail (Badalyan 1980). This prompted us to theoretically investigate for five facular models as to how sensitive the lines belonging to the above molecules are to the physical conditions. Two photospheric models have also been selected. The facular models are Chapman (1979, 7B14), Schmahl (1967, SF), Shine & Linsky (1974, SLF), Stellmacher & Wiehr (1973, SWF) and Stenflo (1975, StF). The two photospheric models are Holweger & Müller (1974, HM) and Vernazza *et al.* (1976, VAL).

2. Equivalent width calculations

The equivalent widths in each case have been calculated under the assumption of LTE. The procedure is as described by Sinha (1978). References for the elemental

Table 1. Molecular data used in the present work

Molecule	Electronic transition	No. of lines included	Oscillator strength f_{00}	Dissociation energy D_0^0
C_2	$d^3\Pi_g - a^3\Pi_u$	13	2.39×10^{-2} (Curtis *et al.* 1976)	6.21
CH	$A^2\Delta - X^2\Pi$	10	4.93×10^{-3} (Lambert 1978)	3.46
MgH	$A^2\Pi - X^2\Sigma$	15	0.25 (Henneker & Popkie 1971)	1.27
NH	$A^3\Pi - X^3\Sigma$	13	8.24×10^{-3} (Lambert 1978)	3.47
OH	$A^2\Sigma - X^2\Pi$	8	9.4×10^{-4} (Lambert 1978)	4.39
SH	$A^2\Sigma - X^2\Pi$	11	1.63×10^{-3} (Henneker & Popkie 1971)	3.55

abundances, the atomic partition functions for the constituent elements, the spectroscopic constants and dissociation energies used are the same as in Tripathi *et al.* (1981). The dissociation energy for MgH is however from Balfour & Lindgren (1978) and has been discussed by Tripathi & Gaur (1979). The chosen electronic transitions, oscillator strengths and the dissociation energies used are given in table 1. Lines of the (0, 0) band have been selected in all cases.

3. Discussions and conclusions

Molecular line intensities included in this study still lack observations in facular atmosphere. Photospheric line intensities have, however, been measured by different authors (Moore *et al.* 1966; Grevesse & Sauval 1973). The computations of equivalent widths of the lines have therefore been done in two representative photospheric models (*viz.* HM & VAL) also so that they could be compared with the observed photospheric values. An inspection showed that the photospheric model equivalent widths turned out to be higher than the observed photospheric values in the cases of C_2, CH, NH and OH. This could be attributed to the different values of abundance, D_0^0 and f_{00} values used by us. So a scale factor was determined which could bring the calculated equivalent widths in photosphere close to those of the observed ones in photosphere. The factors so determined are 1.96, 1.40, 2.11 and 2.11 for C_2, CH, NH and OH respectively. All the facular model-based results for C_2, CH, NH and OH have been scaled down by the corresponding factors. In cases where many lines are coincident with other lines of the same molecule having different J-values, the equivalent width of individual lines has been calculated and the observed equivalent width of the individual line determined as in Sinha *et al.* (1979).

For C_2 lines (*cf.* table 2) we find that it gets weakened when subjected to various facular model atmospheres. The minimum weakening being in SF and the maximum weakening in the 7B14 model. It appears that the equivalent widths of the C_2 lines should be better used for refining spatially limited models. For CH lines (*cf.* table 3)

Table 2. Equivalent widths of C_2 lines (in mÅ) in different models

Wavelength	Line	Models							Observations in photosphere	
		SF	SWF	SLF	StF	7B14	HM	VAL	MMH	GS
5149.210	$P_3(35)$	6.8	4.5	5.7	3.9	1.4	6.8	6.9	—	—
5148.325	$R_2(8)$	2.9	1.9	2.4	1.6	0.6	2.9	3.0	—	—
5147.816	$P_3(36)$	6.7	4.5	5.7	3.9	1.1	6.8	6.9	—	—
5146.212	$P_3(37)$	6.7	4.4	5.6	3.8	1.4	6.7	6.8	—	—
5144.924	$R_1(11)$	3.9	2.5	3.2	1.9	0.7	3.8	3.9	6.5	3.0
5109.301	$R_1(26)$	6.7	4.4	5.5	3.7	1.3	6.6	6.8	4.5	5.4
5103.750	$R_2(29)$	5.8	4.6	5.7	3.9	1.4	6.8	7.0	} 11.0	13.0
5103.731	$R_1(30)$	6.9	4.6	5.7	3.9	1.4	6.8	7.0		
5102.528	$P_3(57)$	4.4	3.0	3.8	2.6	1.0	4.5	4.4	4.4	4.9
5098.142	$R_2(31)$	6.9	4.7	5.7	3.9	1.4	6.9	7.1	8.9	10.7
5043.368	$P_3(75)$	1.9	1.4	1.7	1.2	0.5	2.1	2.0	3.3	1.8
5037.708	$R_1(50)$	5.3	3.6	4.5	3.1	1.2	5.5	5.4	} 20.0	12.2
5037.708	$R_2(49)$	5.4	3.7	4.6	3.2	1.2	5.6	5.6		

MMH : Moore, Minnaert and Houtgast (1966)
GS : Grevesse and Sauval (1973)

Table 3. Equivalent widths of CH lines (in mÅ) in different models

Wavelength	Line	Models							Observations in photosphere		
		SF	SWF	SLF	StF	7B14	HM	VAL	MMH	W	GS
4192.568	$R_{1dd}+R_{2dd}(19)$	92.8	70.7	87.8	37.4	31.3	80.0	76.2	66.0	69.3	78.0
4210.997	$R_{1dd}+R_{2dd}(16)$	121.9	91.5	112.3	48.4	39.5	103.2	99.4	100.0	103.8	100.0
4248.945	$R_{1dd}(10)$	84.4	62.1	75.6	34.5	25.8	69.7	68.6	70.0	63.0	70.0
4255.252	$R_{1dd}(9)$	85.6	62.9	76.3	34.9	26.0	70.6	69.6	69.0	61.3	76.0
4328.829	$P_{2dd}(3)$	6.9	5.0	6.1	3.0	2.0	5.6	5.6	9.0	—	5.0
4328.915	$P_{2cc}(3)$	6.9	5.0	6.1	3.0	2.0	5.6	5.6	5.5	—	5.0
4328.336	$P_{1cc}(7)$	66.1	48.3	59.0	28.7	19.8	53.8	53.6	50.2	46.2	49.0
4356.375	$P_{2cc}(9)$	76.0	55.7	68.2	33.2	23.0	62.2	61.4	55.0	—	55.0
4387.084	$P_{1dd}+P_{2dd}(20)$	63.9	48.6	61.5	29.0	21.7	54.4	53.1	59.0	57.2	68.0
4388.894	$P_{1dd}+P_{2dd}(21)$	58.3	44.4	56.5	26.5	20.0	49.7	52.1	47.0	51.8	57.0

MMH : Moore, Minnaert and Houtgast (1966).
W : Withbroe (1967, 1968).
GS : Grevesse and Sauval (1973).

Table 4. Equivalent widths of NH lines (in mÅ) in different models

Wavelength	Line	Models							Observations in photosphere	
		SF	SWF	SEF	StF	7B14	HM	VAL	MMH	GS
3338.116	$R_1(5)$	70.4	47.9	58.0	25.4	19.7	40.4	45.8	31.0	36.0
3340.690	$R_2(4)$	48.1	32.6	39.5	17.3	13.3	27.5	31.3	29.0	35.0
3344.182	$R_2(3)$	38.8	26.3	31.7	13.9	10.7	22.2	25.2	29.0	30.0
3347.625	$R_2(2)$	27.7	18.7	22.6	9.9	7.6	15.8	18.0	14.0	24.0
3365.196	$Q_3(24)$	36.2	27.2	35.8	14.5	13.0	23.1	24.2	16.0	20.0
3377.277	$P_2(5)$	29.7	20.2	24.7	10.7	8.3	17.1	19.4	17.0	14.0
3391.596	$P_3(9)$	48.5	33.4	41.1	17.6	14.0	28.2	31.7	40.0	33.0
3395 759	$P_2(10)$	54.4	37.6	46.5	19.9	15.8	31.8	35.6	40.0	36.0
3399.800	$P_1(11)$	61.0	42.3	52.5	22.4	18.0	35 8	39.9	38.0	39.0
3413.664	$P_1(15)$	52.6	37.3	47.2	19.6	16.3	31.6	34.6	53.0	43.0
3420.100	$P_3(17)$	40.4	29.0	37.0	15.3	13.0	24.6	26.6	18.0	24.0
3420.286	$P_2(17)$	42.4	30.4	39.9	16.0	13.6	25.8	28.0	23.0	35.0
3430.288	$P_3(20)$	30.0	21.9	28.5	11.6	10.1	18.6	19.9	19.0	17.0

MMH : Moore, Minnaert and Houtgast (1966)
GS : Grevesse and Sauval (1973)

Table 5. Equivalent widths of OH lines (in mÅ) in different models

Wavelength	Line	Models							Observations in photosphere	
		SF	SWF	SLF	StF	7B14	HM	VAL	MMH	GS
3069.177	$R_2(7)$	130.9	88.3	97.3	48.8	32.1	73.4	85.2	69.0	68.0
3066.913	$R_1(15)$	123.8	86.3	97.5	47.7	33.2	71.8	80.5	66.0	62.0
3080.231	$R_2(2)$	71.4	47.3	51.8	26.1	16.9	39.3	46.1	37.0	37.0
3384.894	$R_2(19)$	76.5	54.7	63.1	30.3	22.2	45.6	50.0	69.0	52.0
3086.226	$R_1(20)$	69.4	50.0	58.0	27.7	20.6	41.7	45.4	75.0	57.0
3136.888	$P_1(11)+R_2(7)$	136.2	93.0	104.8	51.3	35.1	77.7	88.7	84.0	78.0
3167.168	$Q_2(22)$	105.0	77.3	94.8	42.5	33.1	64.8	69.4	72.0	59.0
3172.997	$Q_1(23)$	93.0	69.0	92.3	38.0	30.0	57.9	61.6	58.0	58.0

MMH : Moore, Minnaert and Houtgast (1966).
GS : Grevesse and Sauval (1973).

Table 6. Equivalent widths of SH lines (in mÅ) in different models

Wavelength	Line	Models							
		SF	SWF	SLF	StF	7B14	HM	VAL	SJP
3280.314	$Q_2(1.5)$	1.4	0.9	1.1	0.4	0.4	0.8	0.9	0.8
3280.201	$Q_2(2.5)$	2.1	1.4	1.6	0.6	0.5	1.2	1.3	1.2
3280 356	$Q_2(3.5)$	2.8	1.9	2.2	0.8	0.7	1.6	1.8	1.6
3280.849	$Q_2(4.5)$	3.5	2.3	2.8	1.1	0.9	2.0	2.3	2.1
3281.636	$Q_2(5.5)$	4.3	2.8	3.3	1.3	1.1	2.4	2.8	2.5
3282.742	$Q_2(6.5)$	5.0	3.3	3.9	1.5	1.3	2.8	3.2	2.8
3284.153	$Q_2(7.5)$	5.6	3.7	4.4	1.7	1.5	3.2	3.6	3.3
3285.891	$Q_2(8.5)$	6.2	4.2	4.9	1.8	1.6	3.5	4.0	3.6
3287.941	$Q_2(9.5)$	6.8	4.5	5.3	2.0	1.8	3.8	4.4	4.0
3290.315	$Q_2(10.5)$	7.2	4.8	5.7	2.2	1.9	4.1	4.7	4.2
2293.020	$Q_2(11.5)$	7.6	5.1	6.1	2.3	2.0	4.3	4.9	4.4

SJP : Sinha, Joshi and Pande (1977) calculated in HSRA.

the models SF and SLF show strengthening of the lines whereas SWF, StF and 7B14 show weakening against the photospheric models. This shows that more molecules form in SF while the formation in 7B14 is the least. Models StF and 7B14 appear to be similar and show diminution in equivalent widths when compared against the photospheric models. The calculations tell us that the three homogeneous facula models show appreciable equivalent width variations. The facula models SF, SWF and SLF show strengthening of the lines whereas StF & 7B14 show weakening in respect of NH, OH and SH lines (*cf.* tables 4, 5 & 6).

The molecule MgH has a low dissociation energy and Mg has a low ionization potential; its presence in photosphere is not doubted (*cf.* Schadee 1964; Lambert *et al.* 1971). The value of D_0^0 used by us is in close agreement with the value derived from the Birge-Sponer extrapolation and is also comparable with the theoretical estimate of D_0^0 (1.25 $\pm$ 0.05 eV) given by Meyer & Rosmus (1975). The value of f_{00} used is in excellent agreement with the recent experimental results of Balfour & Cartwright (1976). Our values for the epuivalent widths would go down by a factor of 1.5 if the theoretical estimate of Kirby *et al.* (1979) ($f_{00} \simeq 0.161$) is to be used (*cf.* Sinha 1981). The equivalent width calculations tell us (*cf.* table 7) that the models SF and SLF show strengthening of MgH lines against the HM model. SWF, however, does not reflect much change compared against the photospheric values. Models StF and 7B14 show much weakening of the lines and show that

Table 7. Equivalent widths of MgH lines (in mÅ) in different models

Wavelength	Line	Models							Observations in photosphere		
		SF	SWF	SLF	StF	7B14	HM	VAL	MMH	Schadee	GS
5178.464	$Q_2(8)$	9.0	4.6	5.4	0.4	1.1	4.7	6.1	5.5	—	4.6
5180.573	$Q_1(7)$	9.2	4.7	5.5	0.4	1.2	4.8	6.3	4.5	4.5	3.9
5185.725	$Q_1(2)$	3.5	1.8	2.1	0.1	0.4	1.8	2.4	1.5	1.5	0.9
5177.811	$P_1(33)$	3.7	2.1	2.5	0.2	0.6	2.1	2.5	—	1.5	—
5180,874	$P_2(32)$	3.8	2.2	2.6	0.2	0.6	2.2	2.6	2.5	2.0	—
5181.956	$Q_1(6)$	8.2	4.2	4.9	0.3	0.6	4.3	5.6	3.5	4 0	—
5106.877	$R_2(16)$	7.0	3.7	4.3	0.3	0.9	3.8	4.8	4.5	3.5	—
5106.237	$Q_2(29)$	9.3	5.2	6.2	0.4	1.4	5.2	6.4	—	3.5	—
5111.257	$Q_2(28)$	9.8	5.5	6.5	0.4	1.4	5.5	6.7	—	4.0	—
5112.648	$R_2(15)$	6.9	3.6	4.3	0.3	0.9	3.7	4.8	3.0	3.5	—
5116.190	$Q_2(27)$	10.2	5.7	6.8	0.5	1.5	5.8	7.0	—	5.0	—
5061.516	$Q_2(37)$	5.5	3.3	3.9	0.3	0.9	3.2	3 8	3.5	2.5	—
5063.508	$R_1(23)$	6.5	3.5	4.2	0.3	0.9	3.6	4.5	3.0	3.0	2.3
5055.426	$Q_2(38)$	5.0	3.1	3.6	0.2	0.8	3.0	3.5	1.5	1.5	—
5069.625	$R_2(22)$	6.4	3.5	4.1	0.3	0.9	3.5	4.4	—	2.5	—

these lines are only close to the limit of detectability, if they do not disappear at all.

In brief, molecule C_2 can be used for refining spatially-limited models, whereas MgH and SH are good candidates for homogeneous facula models. Molecule CH seems to be a better candidate for testing both the homogeneous and the spatially-limited facular models. Both NH and OH seem to be good molecules for refinement of facula models because they show appreciable variation in equivalent widths for both the homogeneous and spatially-limited models and these variations should be easily detectable because the lines are fairly strong. However, in all the cases it would be extremely important to secure low noise high resolution spectra with corrections applied carefully for scattered photospheric light in order to achieve a refinement over the existing facula models.

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