Vibration-rotation bands of SiH and MgH in sunspot spectra

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Abstract. We have calculated the equivalent widths of the vibration-rotation bands of SiH and MgH molecules for a possible detection in the sunspot spectrum. Five different models were utilized and the results obtained with and without using the line haze opacity discussed by Joshi $et\ al.$ (1979). It is found that the P_1 and the P_2 branches of SiH and the R branch of MgH lie in a region less dominated by the line haze opacity and consequently can be detected.

Key words: SiH molecules—MgH molecules—sunspot spectrum

1. Introduction

The (2-0) overtone band of CO is observed in the umbral spectrum with an equivalent width $\simeq 250$ mÅ (Hall 1970). Much higher intensities for the (1-0) band can be expected for which the oscillator strength is greater by about two orders of magnitudes (Kirby & Liu 1978). Further, the vibration-rotation bands of the molecules CH, CN, HCl, HF, NH, OH and SiO are either already observed or predicted to be observable in the spectrum of a sunspot (Hall 1970). It is of interest to find out which other molecules can be detected in the infrared region of the sunspot spectrum. The molecules SiH and MgH are of special interest because of low dissociation energies— D_0^o (SiH)=3.06 eV and D_0^o (MgH)=1.27 eV. These molecules are already detected in the sunspot spectrum through their electronic transitions in the visible range (Lambert & Mallia 1970; Sinha 1982).

2. Formulations and calculations

The method of equivalent width calculation and the reason for selecting the five sunspot models due to Henoux (1969), Zwaan (1974), Stellmacher & Wiehr (1975), Boyer (1980) and Kollatschny *et al.* (1980) is the same as mentioned already by Sinha (1982). Hereinafter these models are referred to as HSM-69, ZSM-74, SWSM-75, BSM-80 and KSM-80 respectively. The saturation of the lines was accounted for and the microturbulence velocity was assumed to be 1 km s⁻¹ (Sotirovski 1971). The elemental abundance was taken to be N(Si) = 7.63 and N(Mg) = 7.62 (Lambert & Luck 1978).

Singh & Vanlandingham (1978) give the oscillator strength for SiH as $f_{1-0} = 4.658 \times 10^{-5}$ and Kirby et al. (1979) for MgH as $f_{1-0} = 4.76 \times 10^{-5}$. Hönl-London factors are available from Carpenter & Franzosa (1965) and Herzberg (1953). Expressions are given by Tsuji (1973) for computing the molecular dissociation constants including those of SiH. The molecular constants are taken from Huber & Herzberg (1979) except the dissociation energy of MgH which is from Balfour & Lindgren (1978). It may be noted here that the S_J factors given by Carpenter & Franzosa (1965) are to be divided by 2 so that the summation over S_J yields (2J + I). Tripathi & Gaur (1979) utilized Gibbs free energy functions from the JANAF Thermochemical Tables (Stull et al. 1970) for Mg and H atoms while calculating the dissociation constants, K_p , for MgH. The reference temperature in JANAF Tables is 298 K and not 0 K. A correction for this difference in reference temperatures leads to different dissociation constants. The following relationship gives K_p values accurate up to 2.5 per cent in the temperature range 2000 < T < 6000

$$\log K_p \text{ (MgH)} = 6.89229714 \times 10^{-2} \theta^2 - 1.70936016 \theta + 10.7293372. ...(1)$$

Here $\theta = 5040/T$ with T as temperature. The correct Gibbs energy functions for Mg and H atoms are taken from Glushko et al. (1962).

3. Results and discussions

Since the line intensities are directly proportional to the partial pressures which depend upon the dissociation energy and the abundance of the atoms constituting it, we compare in figure 1 the partial pressures of MgH and SiH with those of HF and HCl in two sunspot models, *i.e.* ZSM-74 and HSM-69. The vibration-rotation lines of the molecules HF and HCl have already been detected in the infrared region of the umbral spectrum (Hall & Noyes 1969, 1970).

Compared to the molecules HF and HCl in the model HSM-69 (figure 1) the molecule SiH is more abundant, because of a larger abundance of Si in the solar atmosphere (N(Si) = 7.63, N(F) = 4.56 and N(Cl) = 5.65 on the relative logarithmic scale of N(H) = 12.00). However, in the cooler atmosphere of ZSM-74, because of a larger association of Si atoms in SiO formation (D_0^0 (SiO) = 8.26 eV), the partial pressure of SiH is adversely affected in the upper layers of the model and its partial pressure becomes lower than that of HF and HCl. The curves for MgH for both the models lie lower than that of SiH. This is so because of a lower dissociation energy for MgH (D_0^0 (MgH)=1.27 eV, D_0^0 (SiH)=3.06 eV). Thus on a qualitative basis alone one can expect observable lines of SiH in the infrared part of the umbral spectrum. The MgH lines should be weaker than the SiH lines though they may still be detectable. Gains in partial pressure calculations may be offset due to decrease in oscilator strengths. The oscillator strength for the R(13.5) line of SiH is 1.288 × 10⁻⁶ while that of R(12) line of MgH is 2.29×10^{-5} . Also while assessing the individual line strengths due attention is to be paid to the opacity changes with wavelength.

In table 1 we present the results of equivalent width calculations for the MgH and SiH lines originating from a rotational level J which is most populated in the umbral atmosphere at an average temperature T = 3000 K. The following relationship due to Schadee (1964) is used to calculate J_{max} i.e., the most populated J level,

$$J_{\text{max}} = 0.59 \left(\frac{T}{B_{\text{v}}}\right)^{1/2} - 0.5$$
 ...(2)

where B_{v} is the rotational constant of the vibrational level v of the lower electronic state. The method of equivalent width calculations accounts for differences in oscillator-strength, abundances, opacities, dissociation energies and the like.

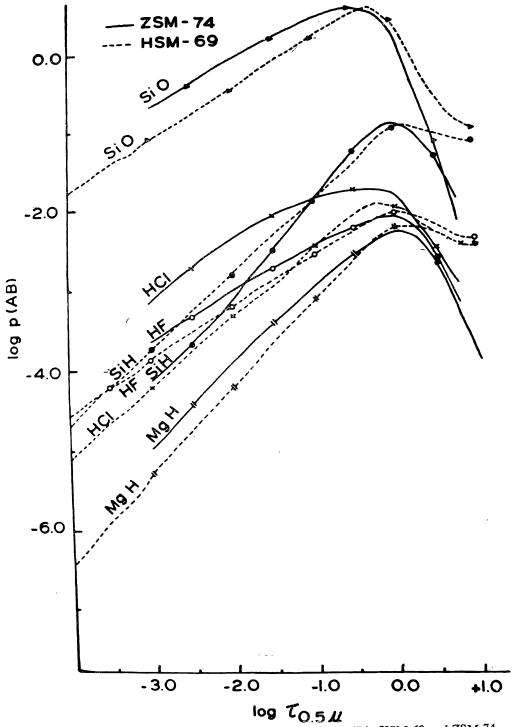


Figure 1. Partial pressures of SiO, HF, HCl, SiH and MgH in HSM-69 and ZSM-74.

| Table | 1. | Equivalent widths | (mĂ` | and the central | depth ra | for the molecules SiH and | MoH |
|-------|----|-------------------|-----------|-------------------|----------|----------------------------------|---------|
| Labic | т. | Edanation Migning | (***** * | , and the contrar | achm 10 | o tot tile illotecules bitt alle | IVIGIL. |

| √ Warelengt | h | | SiH | | MgH | | |
|--------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|----------------------|--------------------|--|
| Model (μm) | 4.6960 R ₁ (13.5) | 4.6809 R ₂ (13.5) | 5.7233 P ₁ (13.5) | 5.7755 P ₂ (13.5) | 6.4706 R(12) | 7.6762 P(10) | |
| | • () | | -1() | 4 () | () | _ (, | |
| HSM-69 | *237(27%) 13.7(2%) | 237(27 %) 28(5 %) | 251(24%) 186(18%) | 260(24 %) 199(20 %) | 86(11 %) 78(10 %) | 74(8 %) 19(2 %) | |
| | $13.7(2/_{0})$ | 20(3/0) | 100(10 /0) | 199(20/0) | 70(10/0) | 19(2/0) | |
| ZSM-74 | 272(34%) | 272(35%) | 276(29%) | 276(29%) | 102(13%) | 94(10%) | |
| _21,1 | 2.5(0.5%) | 10.5(2%) | 69(8%) | 80(9 %) | 67(9%) | 8 (1 %) | |
| SWSM-75 | 196(24%) | 196(24%) | 187(19%) | 187(19%) | 54(7%) | 45(5%) | |
| BW SINI 13 | 4.5(1%) | 11.6(2%) | 124(13%) | 132(14%) | 47(6%) | 10(1%) | |
| BSM-80 | 193(23%) | 192(23%) | 199(20%) | 199(20%) | 56(7%) | 45(5%) | |
| DSWI 00 | 6.4(1%) | 14(2%) | 153(15%) | 144(15%) | 51(6%) | 12(1%) | |
| KSM-80 | 423(47%) | 423(47%) | 456(42%) | 459(42%) | 147(19%) | 151(16%) | |
| 1221.1 00 | 15(3%) | 32(5%) | 340(32%) | 359(34%) | 135(17%) | 36(4%) | |

^{*}First entry is equivalent width without line haze opacity and the second entry is the same quantity with line haze opacity. The quantity in brackets is the central depth.

Now a days considerable attention is paid to the lowering of the continuum due to unresolved atomic and molecular lines in a sunspot spectrum (Kollatschny et al. 1980, Zwaan 1974). Joshi et al. (1979) have discussed this aspect due to molecular line haze in the infrared. The same approach as outlined by Joshi et al. (1979) in the calculation of line haze opacity was used in the present calculations. An inspection of table 3 shows that the P_1 and the P_2 branches of SiH and the R branch of MgH remain sufficiently intense to be observed easily. The intensities of the R_1 and the R_2 branches of SiH is very much reduced because of the veil produced by the CO lines whereas the P branch of MgH is rendered weaker because of the SiO and H_2 O molecules.

In brief an effort in the infrared region of the umbral spectrum should help in the identification of the bands discussed above. Also it will help in assessing the accuracy with which Singh & Vanlandingham (1978) and Kirby et al. (1978) have given estimates of oscillator strengths. An elaborate set of infrared wavenumbers of MgH and SiH is available in the papers by Singh & Vanlandingham (1978) and Maciel & Singh (1977).

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