

# SOLAR PHOTOSPHERIC MODELS AND THE ROTATIONAL TEMPERATURES OF THE C<sub>2</sub> AND MgH MOLECULES

K. Sinha, D.S. Shukla and B.M. Tripathi

U.P. State Observatory, Manora Peak, Naini Tal 263129

(Received March 20, 1979; revised June 14, 1979)

## Abstract

Four photospheric models have been utilized to derive model based rotational temperatures of the (0-0) band of the Swan system of C<sub>2</sub> and that of the green system of the MgH molecules. The dissociation energies were varied within reasonable limits to assess their influence on the derived temperatures. It is found that observations are not consistent with the model based results. The need for more refined photospheric models is emphasized.

## 1. INTRODUCTION

Currently two categories of photospheric models are available. The first category belongs to models that are based largely upon continuum observations (cf., Gingerich *et al.* 1971; Vernazza *et al.* 1976) and the second category belongs to those that attempt to explain the line intensities (cf., Altrock and Cannon 1972; Holweger and Müller 1974; Ayers and Linsky 1975). The two types of models are quite different from each other, particularly in the upper photospheric layers. In fact, Zachary *et al.* (1977) have noted, "In order to match the observed Si I continuum with continuum model, the minimum temperature must be less than 4200 K, but in order to match the Ca II and Mg II H and K lines the minimum value must be about 4400 K." So the need to construct a unified photospheric model which may explain the continuum as well as the line opacities is obvious.

Since molecular line intensities are known to be sensitive to the physical conditions of a model atmosphere, they can be used to test a photospheric model and to improve it in the region of line formation. Considerable interest in such studies have been aroused by Mount *et al.* (1973) and by Mount and Linsky (1974a, 1974b, 1975).

Here, the results of our investigations for the photospheric C<sub>2</sub> and the MgH molecules are reported with a view to test the model atmospheres. This is based upon a comparison of the observed and the model based rotational temperatures, i.e., T<sub>O</sub>(rot) and T<sub>m</sub>(rot) respectively. The models due to Gingerich *et al.* (1971), Altrock and Cannon (1972), Holweger and Müller (1974) and Vernazza *et al.* (1976) were used and they are hereinafter referred to as HSRA-71, AC-72, HM-74 and VAL-76 respectively. It may be mentioned that the line model AC-72 explained the centre to limb spectra of CN and CH lines best (Mount and Linsky 1975). Also, the line model HM-74 explains similar observations of the continuum (Lambert 1978). Tsuji (1977) utilized the VAL-76 model to obtain an agreement between the

model based excitation temperature and that obtained from observations for the vibration-rotation bands of the CO molecule.

The reasons for the selection of C<sub>2</sub> and MgH molecules are two fold. Hinkle and Lambert (1975) have shown that for the calculation of equivalent widths at the centre of the solar disk one need not include the effects of departures from LTE for these molecules. The Sun being an oxygen rich star (compared to the carbon abundance) the formation of C<sub>2</sub> molecules is adversely affected by slight changes in the temperature structure of a model atmosphere. A lowering of model temperatures increases CO formation and reduces C<sub>2</sub> abundance. Similarly, having a low ionisation potential, Mg will be affected by such changes and the effects should be noticeable in the observations of MgH lines.

Our observations for the considered molecular transitions were obtained at a dispersion of 0.24 Å/mm for the centre of the solar disk. The single pass spectrograph, attached to the Horizontal Solar Telescope of the Uttar Pradesh State Observatory was used for the purpose. A description of the instrument is given by Pande (1969). The spectra were recorded using a 1P21 photomultiplier, thermoelectrically cooled to -20°C. Each selected line was traced more than five times for averaged equivalent width evaluation.

## 2. FORMULATIONS AND CALCULATIONS

The weighting function method used by Sinha (1977) for the determination of T<sub>m</sub>(rot) in the case of umbral TiO molecules, provided the basis for the present calculations. The molecular constants were taken from Rosen (1970) and the rotational intensity factors from Schadee (1964).

For the C<sub>2</sub> molecules, Tatum (1966) used D<sub>0</sub><sup>0</sup>(C<sub>2</sub>) = 6.25 eV while JANAF tables (Stull *et al.* 1971) use a slightly lower value D<sub>0</sub><sup>0</sup>(C<sub>2</sub>) = 6.11 eV. Similarly for the

MgH molecules, the JANAF tables use a  $D_0^{\circ}(\text{MgH}) = 2.0$  eV, Balfour and Cartwright (1976) use a  $D_0^{\circ}(\text{MgH}) = 1.33$  eV and more recently Balfour and Lindgren (1978) have reported a  $D_0^{\circ}(\text{MgH}) = 1.27$  eV. The use of different dissociation energies, lowers or raises the molecule forming layers, affecting the depth of line formation. In view of this, we investigated the influence of various dissociation energies upon  $T_m(\text{rot})$ , i.e., the model based estimates of rotational temperature of the molecules  $\text{C}_2$  and MgH.

The partition functions were obtained by utilizing the polynoms given by Glushko *et al.* (1962) for the hydrogen and carbon atoms. For the magnesium atoms we used the algorithms given by Bolton (1970). The effect of the use of different molecular dissociation energies in the calculation of atomic partial pressures is negligible, because in the photosphere, relatively few atoms are locked in molecule formation as compared to the number of atoms available as free atoms and to those participating in ionisation.

The MgH rotational temperatures were estimated from the well known relation (cf., Schadee 1964),  
 $\log(W_N/f_v', v'' S_N) = \text{constant} - 0.62473 B_v N(N+1)/T_0(\text{rot})$  (2.1)

This formula cannot, however, be used for the  $\text{C}_2$  molecules. Many  $\text{C}_2$  lines are coincident with other lines of the same molecule having different J but the same N values (Sinha 1979). Since the equivalent width, W, of a molecular line is directly proportional to the rotational intensity factor S, for three such lines one can write

$$W_1 : W_2 : W_3 :: S_1 : S_2 : S_3.$$

The equivalent width of each line can therefore be obtained from the relation

$$W_i = WS_i / \sum_{i=1}^3 S_i \quad (2.2)$$

where W is the combined equivalent width of the lines and i can take values from 1 to 3. Thus, having resolved each coincident line into individual equivalent widths, one can use the following formula

$$\log(W_J/S) = \text{constant} - 0.62473 F_J''/T_0(\text{rot}) \quad (2.3)$$

for estimating  $T_0(\text{rot})$ . Here one may neglect the higher order terms in the rotational energy. Using the expressions quoted by Ballik and Ramsay (1963) we have verified that such an approximation does not lead to any significant change in the  $T_0(\text{rot})$  values.

### 3. RESULTS AND DISCUSSIONS

**3.1 The rotational temperature of  $\text{C}_2$ :** The  $\text{C}_2$  lines  $P_3(35)$ ,  $P_3(36)$ ,  $P_3(37)$ ,  $P_3(75)$ ,  $R_1(5)$ ,  $R_1(11)$ ,  $R_1(51)$ ,  $R_2(8)$ ,  $R_2(29)$ ,  $R_2(31)$ ,  $R_2(49)$ ,  $R_2(50)$ ,  $R_3(26)$  and  $R_3(49)$  were used for  $T_m(\text{rot})$  calculation. It allowed us a wide coverage of lines in J values which are shown in brackets. Our model based results are presented in Table 1 along with the observational estimates of  $T_0(\text{rot})$  due to various authors. It can be inferred from this table that the considered photospheric models are unable to reproduce the observed molecular rotational temperatures for  $\text{C}_2$ . The merits and the demerits of various investigations are discussed below.

Schadee (1964) has summarised and clarified various confusions and obscurities in the line identifications of the earlier works due to Hunnaerts (1947) and Laborde (1961). So, they are not included in Table 1. However, as Greene (1969) has stated, still there are a few uncertainties of  $\pm 1$  in the J values for the P and R branches. But there are only two such lines at wavelengths 5111.743 Å and 5111.880 Å in Schadee's (1964) investigation that were apparently not included in the  $T_0(\text{rot})$  estimate. Therefore the rotational temperature determination carried out by Schadee (1964) is free of such uncertainties.

Considering that different authors have given different equivalent widths for the same  $\text{C}_2$  line, Lambert (1968) borrowed Mallia's observations and derived a  $T_0(\text{rot})$  value in agreement with Schadee (1964).

TABLE 1  
The rotational temperatures of the (0-0) band of the Swan system of the  $\text{C}_2$  molecules

Model based rotational temperatures (Present investigations)			Observational estimates of rotational temperature	
Model	$T_m(\text{rot})$		$T_0(\text{rot})$	References
	$D_0^{\circ} = 6.25$ eV	$D_0^{\circ} = 6.11$ eV		
HSRÅ-71	$5030 \pm 20$	$5040 \pm 20$	4650	Schadee (1964)
AC-72	$5070 \pm 20$	$5080 \pm 20$	4620	Lambert (1968)
HM-74	$5150 \pm 20$	$5160 \pm 20$	$4780 \pm 135^*$	Grevesse and Sauval (1973)
VAL-76	$5010 \pm 20$	$5020 \pm 20$	$4450 \pm 305$ $4330 \pm 430$	Persi (1975) This study

\* Based on the data on equivalent widths given by the authors. High order terms were included in the expression for rotational energy.

Grevesse and Sauval (1973) have given equivalent widths of a number of photospheric  $C_2$  lines which we utilized to derive a rotational temperature. The rotationally dependent Franck-Condon factors calculated by Dwivedi *et al.* (1978) were included in equation (2.3) to assess the effect of the vibration-rotation interaction on  $T_0(\text{rot})$  determinations (Sinha 1979). The result is presented in Table 1. We found that the vibration-rotation interaction modifies the  $T_0(\text{rot})$  values very slightly and for all practical purposes one may ignore it for the (0,0), band of the Swan system.

To ensure the choice of unsaturated lines, Persi (1975) utilized very weak lines of the Swan band ( $W < 10 \text{ m}\text{\AA}$ ). He derived  $T_0(\text{rot}) = 4450 \pm 305 \text{ K}$ . He also obtained an HSRA-71 based temperature, significantly higher than his observations.

The results of our observations for the  $C_2$  Swan bands have been presented in Figure 1 and Table 2 which are consistent with other observations (cf., Table 2).

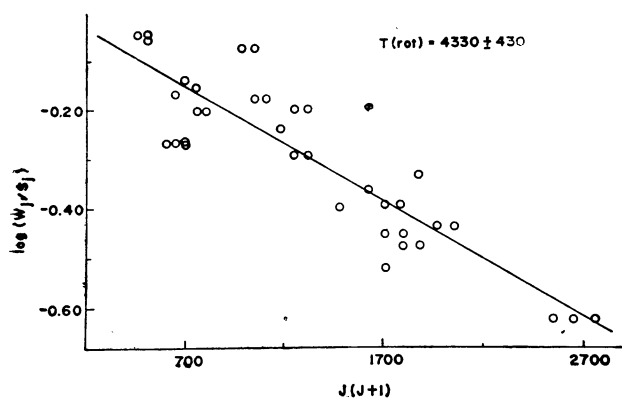


Fig. 1: Our observations for  $T_0(\text{rot})$  of the (0-0) band of the Swan system of the  $C_2$  molecules.

Thus we find that for  $C_2$ , various investigators have tried to remove the different causes of uncertainty to obtain a reasonable estimate of rotational temperature under the hypothesis of LTE and now fairly dependable estimates of  $T_0(\text{rot})$  are available which, however, are not consistent with our model based results.

**3.2 The rotational temperature of MgH:** The molecule MgH has not been as extensively studied as the other photospheric molecules. So only a few  $T_0(\text{rot})$  estimates are available and they are listed in Table 3. We note that Mallia's (1968) estimate is the highest and that it appears consistent with our model based calculations. The consistency should, however, be treated as fortuitous only, because of the following reasons. Mallia's (1968) estimate is based upon only 9 lines, whereas those of Schadee (1964) and Lambert *et al.* (1971) are based upon 46 and 66 lines respectively. The importance of a large data in such estimates is long realised (Schadee 1966; Wöhl 1970; Webber 1971) and in the case of such weak lines as those due to MgH ( $W < 5 \text{ m}\text{\AA}$ ), reliance on too few data might lead to erroneous results. It may be remarked here that in Schadee's (1964) investigation only pure MgH lines were used. Further, a use of pure MgH lines alone in Lambert *et al.*'s (1971) investigation, does not significantly change

TABLE 2

Equivalent widths and line identifications for the  $C_2$  molecule utilized in our observations

Branch (J)	Wavelength ( $\text{\AA}$ )	Equivalent width ( $\text{m}\text{\AA}$ )
R <sub>1</sub> (43)	5063.164	4.88
R <sub>2</sub> (42)	5063.164	4.76
R <sub>3</sub> (41)	5063.290	4.20
R <sub>1</sub> (42)	5066.723	5.02
R <sub>2</sub> (41)	5066.723	4.90
R <sub>3</sub> (40)	5066.845	8.60
R <sub>3</sub> (38)	5073.583	5.15
R <sub>1</sub> (36)	5086.234	6.26
R <sub>2</sub> (35)	5086.234	6.09
R <sub>3</sub> (34)	5086.386	6.68
R <sub>1</sub> (33)	5095.147	7.50
R <sub>2</sub> (32)	5095.192	7.27
R <sub>1</sub> (32)	5098.132	9.22
R <sub>2</sub> (31)	5098.142	8.94
R <sub>3</sub> (26)	5109.301	4.80
R <sub>3</sub> (22)	5119.364	6.70
P <sub>1</sub> (52)	5120.617	4.10
P <sub>2</sub> (51)	5120.617	4.03
P <sub>3</sub> (50)	5120.707	3.68
P <sub>3</sub> (43)	5135.693	6.63
P <sub>1</sub> (45)	5135.586	5.46
P <sub>2</sub> (44)	5135.586	5.34
P <sub>1</sub> (42)	5141.206	5.64
P <sub>2</sub> (41)	5141.206	5.50
P <sub>3</sub> (40)	5141.318	5.74
P <sub>1</sub> (36)	5150.558	7.56
P <sub>2</sub> (35)	5150.558	7.34
P <sub>3</sub> (27)	5158.654	6.29
P <sub>1</sub> (28)	5159.453	5.83
P <sub>2</sub> (27)	5159.470	5.62
P <sub>3</sub> (26)	5159.600	6.25
P <sub>3</sub> (25)	5160.385	5.66
P <sub>1</sub> (26)	5161.037	4.67
P <sub>2</sub> (25)	5161.054	4.49
P <sub>3</sub> (24)	5161.054	4.31
P <sub>1</sub> (22)	5163.420	6.56
P <sub>2</sub> (21)	5163.420	6.26

the results (see below). Schadee (1964) has expressed doubts regarding the reliability of some of the equivalent widths reported by Laborde (1961). So one wonders how on the basis of corrections for the line strengths only, Mallia (1968) could get such a good agreement with Laborde's (1961) measurements, which gave  $T_0(\text{rot}) = 5190 \pm 300 \text{ K}$ .

However, the importance of the contribution of the isotopic MgH lines should be realized in the equivalent width measurements as pointed out by Mallia (1968). Since the isotopic abundances of  $Mg^{24}$ ,  $Mg^{25}$  and  $Mg^{26}$  are in the ratio 80 : 10 : 10 (Boyer *et al.* 1971), such contri-

TABLE 3

The rotational temperatures of the (0—0) band of the green bands of the MgH molecules

Model based rotational temperatures (Present investigation)			Observational estimates of rotational temperature	
Model	$T_m$ (rot)		$T_o$ (rot)	Reference
	$D_o^\circ = 2.00$ eV	$D_o^\circ = 1.33$ eV		
HSRA—71	$5090 \pm 20$	$5140 \pm 20$	4700	Schadee (1964)
AC—72	$5090 \pm 20$	$5140 \pm 20$	$5132 \pm 200$	Mallia (1968)
HM—74	$5220 \pm 20$	$5270 \pm 20$	$4770 \pm 260^*$	Lambert et al. (1971)
VAL—76	$4960 \pm 20$	$5020 \pm 20$		

\* Based on the  $\log (W_J / S_J)$  values given by the authors.

butions may produce large scatters in observations. So in all equivalent width measurements due corrections must be applied or else one should choose only those lines that are free of such uncertainties. From the investigations by Lambert *et al.* (1971) if one uses the lines not blended with  $Mg^{25}H$  or  $Mg^{26}H$  and marked  $P_3$  in quality i.e., "clearly present, essentially unblended and with continuum nearby",  $T_o(\text{rot})=4700$  K is obtained.

The good agreement between the photographic estimates of Schadee (1964) and the high quality photoelectric estimates of Lambert *et al.* (1971) gives the impression that for the MgH molecules, perhaps with the exception of the VAL-76 model, photospheric models have failed to yield  $T_m(\text{rot})$  values consistent with observations (cf., Table 3). It may be pointed out that if the most recent value  $D_o^\circ(\text{MgH})=1.27$  eV is used, a slightly higher value of  $T_m(\text{rot})$  than the VAL-76 result i.e.,  $5020 \pm 20$  K is expected. Reliable data on vibration-rotation interaction are not available for MgH. Considering Morse Oscillator for their study, Bell *et al.* (1976) concluded that for a large range of J values "all bands except the (0, 0) and (1, 1) show a vibration-rotation effect greater than 25%". However, the dissociation energy,  $D_o^\circ(\text{MgH})=2.49$  eV, used by them is not correct in view of the recent findings by Balfour and Cartwright (1976) and by Balfour and Lindgren (1978). Further, one may like to revise Bell *et al.*'s (1976) investigations by using perturbed Morse Oscillator method for better results (Dwivedi *et al.* 1978). So we are unable to give enough weight to our results for MgH.

Results from our observations are presented in Table 4. Since the lines are intrinsically very weak ( $W < 5$  mÅ), considerable scatter in a  $\log (W_N/S_N)$  versus  $N(N+1)$  plot was found. However, a comparison with

TABLE 4

Equivalent widths and line identifications for the MgH molecules utilized in our observations

Wavelength (Å)	Branch (N)	Equivalent width (mÅ)
5061.516	$Q_2$ (37)	4.48
5090.397	$Q_2$ (32)	2.90
5106.877	$R_2$ (16)	4.50
5121.220	$Q_1$ (25)	3.27
5134.210	$Q_2$ (23)	4.60
5153.650	$Q_1$ (17)	8.45
5159.777	$Q_2$ (16)	4.56
5165.964	$Q_1$ (13)	4.83
5178.464	$Q_2$ ( 8)	5.24
5180.573	$Q_1$ ( 6)	4.31

Withbroe's (1968) and Grevesse and Sauval's (1973) data gave equal scatter and a large probable error in  $T_o(\text{rot})$  estimates. The results based on less extensive data are not given in Table 3.

For the model based calculations of  $T_m(\text{rot})$  of MgH molecules, we utilized  $P_1(33)$ ,  $P_2(32)$ ,  $Q_1(2)$ ,  $Q_1(6)$ ,  $Q_2(27)$ ,  $Q_2(28)$ ,  $Q_2(29)$ ,  $Q_2(37)$ ,  $R_1(23)$ ,  $R_2(15)$ ,  $R_2(16)$  and  $R_2(22)$  lines of the MgH molecule.

#### 4. CONCLUDING REMARKS

A comparison of the  $T_m(\text{rot})$  and  $T_o(\text{rot})$  values for the photospheric  $C_2$  molecules in Table 1 gives an impres-

sion that the recently proposed photospheric models need some improvements in the region of line formation. Prior to any definite conclusion regarding the rotational temperature of the MgH molecules, one would like to have dependable estimates of vibration-rotation interaction.

For refinements in the photospheric models high quality centre to limb spectra of a large number of molecules and some judicious improvements in the method of  $T_{\text{O}}(\text{rot})$  calculation might become necessary (Sinha 1979). The results obtained here might be indicative of temperature inhomogeneities in the upper layers of the photosphere and consequently one would probably need a multicomponent photospheric model

#### ACKNOWLEDGEMENTS

We express our indebtedness to Dr. M. C. Pande for critically going through the manuscript and for several valuable suggestions. We are thankful to the National Aeronautics and Space Administration, U.S.A. for assistance with some of the accessorial instruments used in our observations. We feel grateful to the referee for useful comments.

#### References :

- Altrock, R.C. and Cannon, C.J. 1972, *Sol. Phys.*, **26**, 21.  
 Ayers, T.R. and Linsky, J.L. 1975, *Astrophys. J.*, **205**, 874.  
 Balfour, W.J. and Cartwright, H.M. 1976, *Astr. Astrophys. Suppl.*, **26**, 389.  
 Balfour, W.J. and Lindgren, B. 1978, *Can. J. Phys.*, **56**, 767.  
 Ballik, E.A. and Ramsay, D.A. 1963, *Astrophys. J.*, **137**, 61.  
 Bell, R.A., Branch, D. and Upson II, W.L. 1976, *J. quantit. spectrosc. radiat. Transfer*, **16**, 177.  
 Bolton, G.T. 1970, *Astrophys. J.*, **161**, 1187.  
 Boyer, R., Henoux, J.C. and Sotirovski, P. 1971, *Sol. Phys.*, **19**, 330.  
 Dwivedi, P.H., Branch, D., Huffaker, J.N. and Bell R.A. 1978, *Astrophys. J. Suppl. Ser.*, **36**, 573.  
 Gingerich, O., Noyes, R.W., Kelkofen, W. and Guny, Y. 1971, *Sol. Phys.*, **18**, 347.  
 Glushko, V.P., Gurevich, L.V., Khachkuruzov, G.A., Veits, I.V. and Medvedyev, V.A. 1962, *Termodinamicheskie Svoistva Individual'nykh Veshchestv* (Izd. Akad. Nauk, SSSR, Moskva).  
 Greene, T.F. 1969, *Astrophys. J.*, **157**, 737.  
 Grevesse, N. and Sauval, A.J. 1973, *Astr. Astrophys.*, **27**, 29.  
 Hinkle, K.H. and Lambert, D.L. 1975, *Mon. Not. R. astr. Soc.*, **170**, 447.  
 Holweger, H. and Müller, E.A. 1974, *Sol. Phys.*, **39**, 19.  
 Hunnaerts, J. 1947, *Ann. Astrophys.*, **10**, 237.  
 Laborde, G. 1961, *Ann. Astrophys.*, **24**, 89.  
 Lambert, D.L. 1968, *Mon. Not. R. astr. Soc.*, **138**, 143.  
 Lambert, D.L., Mallia, E.A. and Petford, A.D. 1971, *Mon. Not. R. astr. Soc.*, **154**, 265.  
 Lambert, D.L. 1978, *Mon. Not. R. astr. Soc.*, **182**, 249.  
 Mallia, E.A. 1968, *Sol. Phys.*, **5**, 281.  
 Mount, G.H., Linsky, J.L. and Shine, R.A. 1973, *Sol. Phys.*, **32**, 13.  
 Mount, G.H. and Linsky, J.L. 1974a, *Sol. Phys.*, **35**, 259.  
 Mount, G.H. and Linsky, J.L. 1974b, *Sol. Phys.*, **36**, 287.  
 Mount, G.H. and Linsky, J.L. 1975, *Sol. Phys.*, **41**, 17.  
 Persi, P. 1975, *Sol. Phys.*, **43**, 39.  
 Pande, M.C. 1969, Proc. of the Seminar on "Optical Astronomy with Moderate Size Telescopes", p. 14., CASA, Hyderabad, India.  
 Rosen, B. 1970, *Selected constants, Spectroscopic Data Relative to Diatomic Molecules*, Pergamon Press, London.  
 Schadee, A. 1964, *Bull. astr. Inst. Netberl.*, **17**, 311.  
 Schadee, A. 1966, *Astrophys. J.*, **145**, 348.  
 Sinha, K. 1977, *Bull. astr. Soc. India*, **5**, 49.  
 Sinha, K. 1979, *Bull. astr. Soc. India*, **7**, 17.  
 Stull, D.R. et al. 1971, *JANAF Thermochemical Tables*, 2nd edition, Nat. Stand. Ref. Data Ser., Nat. Bur. Stand., U.S.A.  
 Tatum, J.B. 1966, *Publ. Dom. Astrophys. Obs. Victoria*, **13**, 1.  
 Tsuji, T. 1977, *Publ. astr. Soc. Japan*, **29**, 497..  
 Vernazza, J.E., Avrett, E.H. and Loeser, R. 1976, *Astrophys. J. Suppl. Ser.*, **30**, 1.  
 Waddell, J.H. 1958, *Astrophys. J.*, **127**, 284.  
 Webber, J.C. 1971, *Sol. Phys.*, **16**, 340.  
 Wohl, H. 1970, *Sol. Phys.*, **15**, 342.  
 Zachary, A.L., Avrett, E.H., Kurucz, R.L., Loeser, R.K. and Vernazza, J.E. 1977, *Bull. American, astr. Soc.*, **9**, 568.