

Centre-to-limb behaviour of molecular rotational temperatures III

K. Sinha *Uttar Pradesh State Observatory, Manora Peak, Naini Tal 263 129*

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Abstract. Utilizing the KPNO atlas (Brault & Testerman 1972) for the (0-0) band of the Swan system of the C_2 molecules, we determine rotational temperatures T_{rot} , for $\mu = 1.0$ and $\mu = 0.2$. When saturation in the observed equivalent widths is accounted for, the model-based result for T_{rot} comes out slightly lower than observations at a near limb position ($\mu = 0.2$). There is no evidence for an increase in temperature towards the solar limb discussed earlier (Sinha 1979a, b).

Key words : solar spectrum— C_2 molecules—rotational temperature—model atmospheres

1. Introduction

As the molecular lines are considered useful probes for standard model atmospheres (Boyer 1980; Tsuji 1977) a systematic program was undertaken to study the C_2 and the MgH molecules observed in the photospheric spectrum (Sinha 1979a, b; Sinha *et al.* 1979).

The calculation of T_{rot} has certain advantages. In an observational estimate for weak lines, a fairly large number of pure and unblended lines, spanning a large wavelength range, can be used to determine it accurately. Further, considering the scatter in observations, the model-based theoretical results are practically independent of the uncertainties in the dissociation energies, band oscillator strengths and the atomic abundances.

In our previous efforts (Sinha 1979a, b), observed equivalent widths were taken from Withbroe (1968) and it was found that the rotational temperature increases towards the solar limb, contrary to the model-based expectations. Considering the implications of these results and particularly because the rotational temperatures are now being determined for stars also (Fernandez-Figueroa *et al.* 1982; Yerle 1979), we decided to examine the situation in detail with the help of the low noise KPNO atlas (Brault & Testerman 1972). Thanks to the laboratory efforts, fairly reliable molecular parameters are now available for the molecule C_2 (*cf.* Lambert 1978). However, this is not so in the case of the MgH molecules. So we restrict ourselves only to the study of the Swan bands of C_2 molecules.

2. Formulation and calculations

For the unsaturated molecular lines, T_{rot} is determined from (Schadee 1964)

$$\log (W/S_J) = \text{const} - 0.62473 B_{\nu} J(J+1)/T_{\text{rot}}. \quad \dots(1)$$

For the weak molecular lines effects of saturation are small and hence the use of equation (1) is justified (see section 3). It has been pointed out by Wöhl (1970) that uncertainties, if any, in the theoretically available parameter S_J might lead to erroneous results. So, in order to assess the increase or decrease in T_{rot} values towards the limb, we write the above equation for the same line at the centre of the solar disc and at the limb and subtract. In case of Hund's coupling case (b) the quantum number J is replaced by N and thus we get,

$$\log (W_L/W_C) = \text{const} - 0.62473 B_{\nu} \left(\frac{1}{T_L} - \frac{1}{T_C} \right) N(N+1). \quad \dots(2)$$

The slope of the line represented by this equation is positive if and only if $T_L > T_C$. The subscripts L and C represent the near limb position and the centre of the disc ($\mu = 1.0$) respectively.

The equivalent widths at $\mu = 1.0$ and $\mu = 0.2$ for a fairly large number of lines (=67) of the (0-0) band of the Swan system of the C_2 molecules were measured from the KPNO atlas. The Liege atlas (Delbouille & Roland 1963) helped in checking for the blends *etc.* Assuming symmetry in the profiles, only such lines were chosen whose at least one wing, free from blends, could be traced to the nearby continuum. The area under the profile was evaluated by counting the square millimetres of a transparent graph paper placed on it. Finally such lines which are good at $\mu = 1.0$ but deteriorate in quality at $\mu = 0.2$ are dropped, because we are also interested in the quantity W_L/W_C .

To effect a further check upon the reliability of the equivalent widths obtained above and also to evaluate a model-based rotational temperature, equivalent widths were calculated utilizing two model atmospheres *viz.*, HM (Holweger & Müller 1974) and VAL (Vernazza *et al.* 1976). The calculated and the observed results are compared in figure 1. A few lines showing discrepancies more than 30% were eliminated from the list. It left us with only 51 good-quality lines, which are listed in table 1. The wavelengths for line identifications are from Phillips & Davis (1968) which are in excellent agreement with an FTS study by Amiot (1983). We chose the above mentioned models because they are extreme representations of the temperature structure of the solar photosphere. The HM model explains the centre-to-limb observations of the continuum fluxes best and hence the line forming region. We retain the VAL model to compare the results with the HM-based study.

The method for molecular equivalent width calculations is outlined by Gaur *et al.* (1971) on the basis of the method discussed by Waddell (1958) for atomic lines. It may, however, be noted that if we use the expression for the dissociation constant from Tatum (1966), the calculation of a term p (molecule)/ Q_{int} (molecule) in the equation for selective line opacity (Gaur *et al.* 1971) becomes easier as the term Q_{int} (molecule) gets cancelled and one is left with terms corresponding to the atomic partition functions and the dissociation energy. Since the observed equivalent

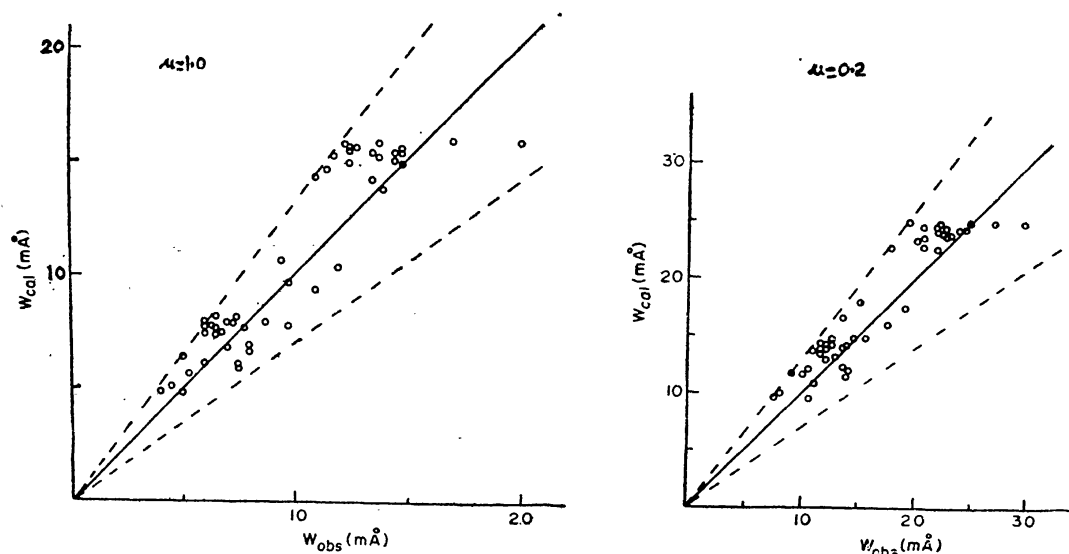


Figure 1. The calculated equivalent widths, W_{cal} , for the model HM is plotted against the corresponding observed values for $\mu = 1.0$ and $\mu = 0.2$. The dotted line represents 30% scatter in observations. The average values of W_{cal}/W_{obs} are $1.07 (\pm 0.15)$ and $1.08 (\pm 0.13)$ respectively for the centre of the solar disc, and the near limb position. The quantities within brackets are the standard deviations.

Table 1. Equivalent widths of the (0-0) band of the Swan system of the C_2 lines in the solar spectrum

Line designation Branch (J)	Wavelength (Å)	Equivalent width (mÅ)			
		$\mu = 1.0$			$\mu = 0.2$
		MMH	GS	Present study	Present study
$P_1(22) + P_3(21)$	5163.420	14	11.0	14.03	21.80
$P_2(25) + P_3(2)$	5161.054	} 16	} 13.0	} 14.79	} 22.55
$P_1(26)$	5161.037				
$P_3(25)$	5160.385				
$P_3(26)$	5159.600	6	6.6	6.52	11.53
$P_3(27)$	5159.470	6	9.4	9.77	13.78
$P_2(28)$	5159.453	} 12	} 13.2	} 13.78	} 21.80
$P_1(28)$	5159.453				
$P_3(27)$	5158.654				
$P_2(28)$	5158.562	6	} 22.5	} 7.27	} 12.03
$P_2(28)$	5158.562				
$P_1(29)$	5158.490				
$P_3(28)$	5157.758	11	} 23.1	} 14.79	} 24.3
$P_2(29)$	5157.643				
$P_1(30)$	5157.605				
$P_2(31)$	5155.524	12	} 23.1	} 12.53	} 22.55
$P_1(32)$	5155.516				
$P_1(32)$	5155.516				
$P_1(36) + P_2(35)$	5150.558	14	—	} 12.78	} 21.8
$P_3(35)$	5149.210				
$P_1(37) + P_2(36)$	5149.088	13	14.1	12.53	20.55
$P_1(38) + P_2(37)$	5147.691	9	} 23.0	—	—
$R_1(11)$	5144.924				
$P_1(40) + P_2(39)$	5144.575	18	—	14.79	24.81
$R_2(11)$	5143.599	18	—	13.53	23.81
$P_3(40)$	5141.318	6.5	3.0	4.01	7.52
$P_1(42) + P_2(41)$	5141.206	12	—	11.78	22.30
$R_3(12)$	5140.381	8.5	5.4	5.01	10.53
$R_1(15)$	5138.112	7.5	} 19.8	6.27	12.03
$R_3(14)$	5136.660				
$R_2(15)$	5136.440	13	—	12.5	20.55
		5.5	5.7	4.51	8.02
		7.5	—	6.01	10.02
		5.5	4.4	5.26	11.03
		8	7.0	7.52	13.78

(Continued)

Table 1. (Continued)

Line designation Branch (J)	Wavelength (Å)	Equivalent width (mÅ)			$\mu = 0.2$ Present study
		$\mu = 1.0$		Present study	
		MMH	GS		
P ₃ (43)	5135.693	6.5	18.0	6.01	11.53
P ₁ (45) + P ₂ (44)	5135.586	10		11.03	17.79
R ₁ (18)	5132.360	7.5	7.0	8.02	12.03
P ₃ (49)	5122.884	—	—	8.02	10.53
P ₃ (50)	5120.710	3.5	14.0	5.01	9.02
P ₁ (52) + P ₂ (51)	5120.637	8.5	—	—	—
R ₃ (22)	5119.377	7	—	6.76	10.78
R ₃ (23)	5116.893	6.5	—	7.77	13.53
R ₃ (25)	5111.844	8	—	8.77	12.53
R ₃ (26)	5109.301	4.5	5.4	7.02	12.53
P ₁ (58) + P ₂ (57)	5105.362	7.5	—	9.52	15.04
R ₂ (29)	5103.750	11	13.0	12.28	19.30
R ₁ (30)	5103.731				
P ₁ (59) + P ₂ (58)	5102.446	12	15.0	12.03	19.05
R ₂ (31)	5098.142	16	21.7	20.05	27.06
R ₁ (32)	5098.132				
P ₁ (62) + P ₂ (61)	5094.018	8.5	14.3	11.03	17.54
R ₃ (32)	5092.453	8	25.8	7.52	14.53
R ₃ (33)	5092.309	14		17.04	29.57
R ₁ (34)	5092.292				
R ₃ (33)	5089.354	7	—	7.52	15.54
R ₃ (34)	5086.395	6.5	—	6.52	12.53
R ₂ (35)	5086.251	12	15.8	13.78	22.05
R ₁ (36)	5086.234				
P ₁ (66) + P ₂ (65)	5081.756	4	—	7.52	11.53
R ₃ (38)	5073.583	4.5	7.0	6.01	11.53
R ₁ (40) + R ₂ (39)	5073.461	9.5	—	14.53	22.55
R ₃ (40)	5066.848	7.5	—	6.01	12.53
R ₁ (42) + R ₂ (41)	5066.730	10	—	14.53	23.06
R ₁ (44) + R ₂ (43)	5059.779	12	—	11.53	20.05
R ₁ (46) + R ₂ (45)	5052.638	11	12.8	13.53	20.55
R ₁ (61) + R ₂ (60)	4992.305	6	8.0	9.77	15.54
R ₁ (68) + R ₂ (67)	4960.863	7	—	6.52	12.78
R ₁ (70) + R ₂ (69)	4951.425	4.5	4.7	7.02	13.53
R ₁ (73) + R ₂ (72)	4936.672	3	—	7.52	14.03

MMH : Moore *et al.* (1966).

GS : Grevesse & Sauval (1973).

widths might be a result of saturation, we chose to compute equivalent widths both with saturation ($\psi \neq 1$) and without saturation ($\psi = 1$). A depth-independent microturbulence velocity ($\xi = 0.85 \text{ km s}^{-1}$) from Brault *et al.* (1982) was used. A slightly different value for microturbulence, say 1.0 km s^{-1} or 1.2 km s^{-1} leads to inappreciable changes in the results of this study. The dissociation energy used here is $D_0^{\circ}(\text{C}_2) = 6.11 \text{ eV}$ which differs insignificantly from $D_0^{\circ}(\text{C}_2) = 6.16 \text{ eV}$ used by Brault *et al.* (1982). The carbon abundance $N(\text{C}) = 8.67$ and the oscillator strength $f_{0-0} = 0.0239$ are the same as in Lambert (1978). This value of oscillator strength is in excellent agreement with $f_{0-0} = 0.0250$ given by Goebel *et al.* (1981). The rotational intensity factors are from Schadee (1964). Since different authors use different normalisations (Schadee 1967) due care should be observed while accounting for them in the evaluation of the line opacity. The molecular constants were taken from Huber & Herzberg (1979).

3. Results and discussions

The calculation of the rotational temperature involves a few simplifying assumptions. The main assumption that the lines of a molecular band originate from a thin isothermal layer of the atmosphere is shown to be close to reality (*cf.* Schadee 1964). A comparison between the observed $T_{0,\text{rot}}$ and the calculated $T_{\text{m,rot}}$ for $\mu = 1.0$ and $\mu = 0.2$ is expected to throw some light on the reliability of the chosen model atmosphere and this will also tell us if the temperature rises towards the limb (Sinha 1979a, b).

Utilizing equation (2) Adam (1938) first reported an increase in T_{rot} towards the limb. She obtained a positive slope, $m = + (0.0334 \pm 0.0691)$. We reviewed the situation with the help of the limited data available in Withbroe's (1968) work, confirming the existence of a positive slope (Sinha 1979b). As pointed out in section 2, we here use the better results obtainable from the KPNO atlas and it can be concluded from figure 2 that because of a large scatter in observations an increase towards limb cannot be inferred. Further, the model-based broken line with a negative slope is also a good fit through observations.

In figures 3a and b we present the results of T_{rot} calculations for $\mu = 1.0$ and $\mu = 0.2$ respectively. The temperatures are $T_{0,\text{rot}} = 5420^{+230}_{-210}$ at $\mu = 1.0$ and $T_{0,\text{rot}} = 5430^{+240}_{-220}$ at $\mu = 0.2$. From these figures it can be seen that a satisfactory agreement with similar model-based results is obtained. The scatter in a model-based estimate is larger at limb because of the saturation effects. The vibration-rotation interaction for the (0-0) band of the Swan bands is small. The use of J-dependent Franck-Condon factors given by Dwivedi *et al.* (1978) affects the $T_{0,\text{rot}}$ values only slightly.

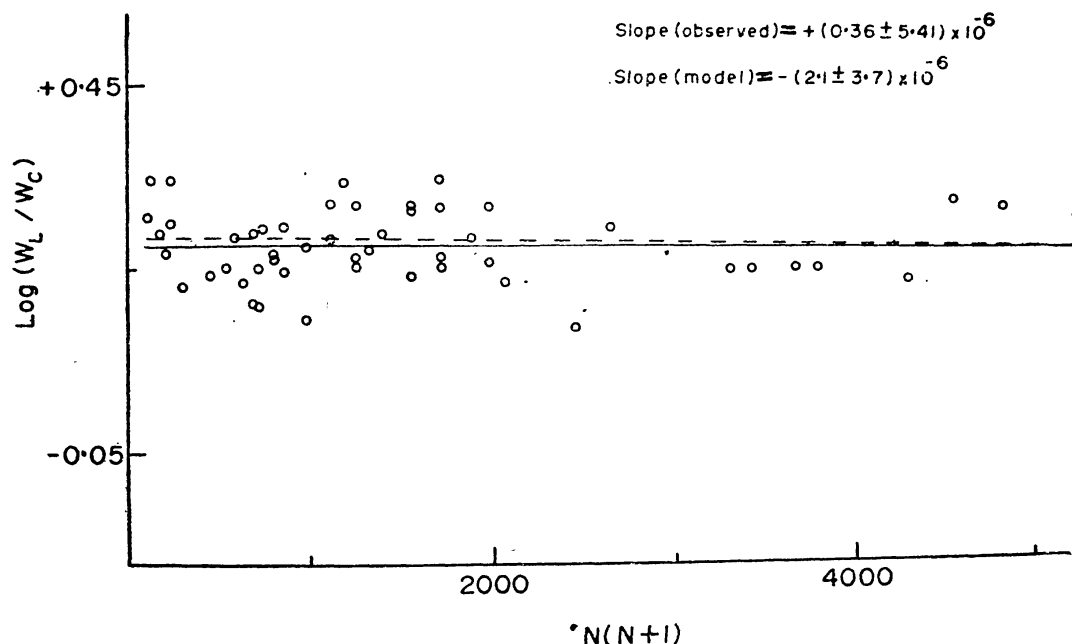


Figure 2. $\text{Log}(W_L/W_C)$ plotted against $N(N+1)$. The VAL result is slope (model) = $-(2.2 \pm 4.0) \times 10^{-6}$ (*cf.* equation (2.2)).

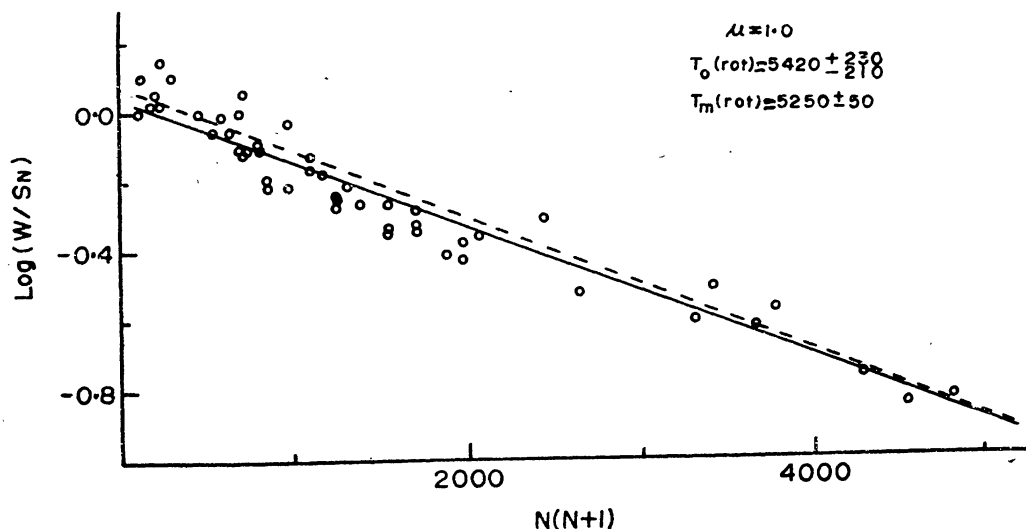


Figure 3a. Determination of $T(\text{rot})$ at $\mu = 1.0$ for the (0-0) band of the Swan system of C_2 molecules. The solid line is the least squares fit through the observed points while the broken line is the HM result. The VAL result for the temperature is $T_m(\text{rot}) = 5140 \pm 55$.

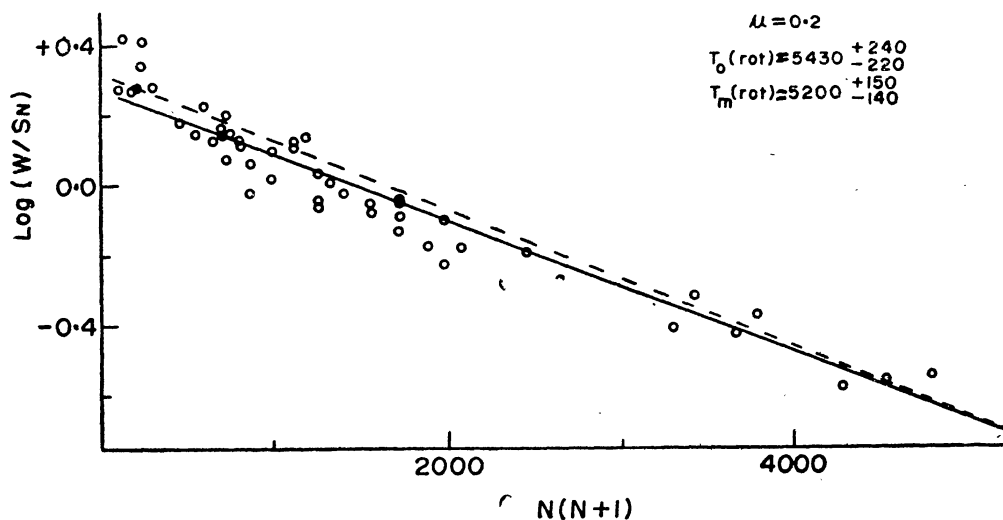


Figure 3b. Same as in figure 3a but for $\mu = 0.2$. The VAL result is $T_m(\text{rot}) = 5080 \begin{smallmatrix} +160 \\ -150 \end{smallmatrix}$.

Analysing photospheric CO lines Sarychev (1978) too found spurious results regarding an increase in temperature towards the limb. This he could correct by properly accounting for saturation in the lines. In the case of the C_2 molecules also this could be an important factor because the lines are expected to strengthen in intensity by a factor of about two towards the limb. The saturated lines produce deviations from a straight line in a $\log(W/S_N)$ versus $N(N+1)$ curve. In order to assess the role of saturation, we corrected the observed values of equivalent widths. To do this the model-based equivalent widths with saturation ($\psi \neq 1$) were plotted against similar quantities with no saturation ($\psi = 1$) for $\mu = 1.0$ and 0.2 (cf. figures 4a, b). The following curve valid for an interpolation only gives a good relationship between the quantities in question :

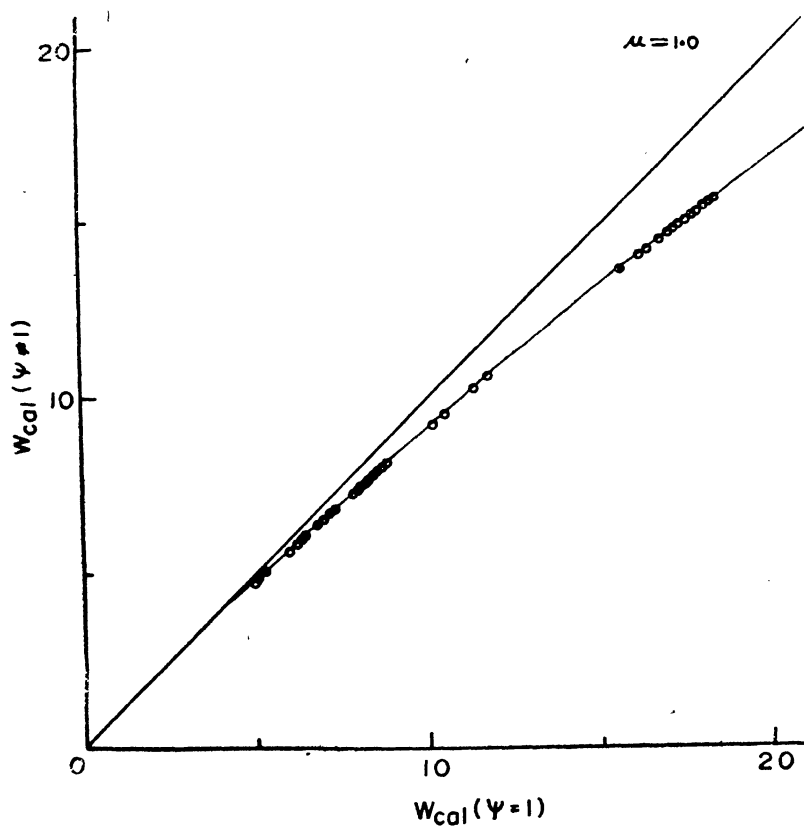


Figure 4a. The calculated equivalent widths for the HM model are plotted to assess the role of saturation in reducing the equivalent widths for the centre of the solar disc.

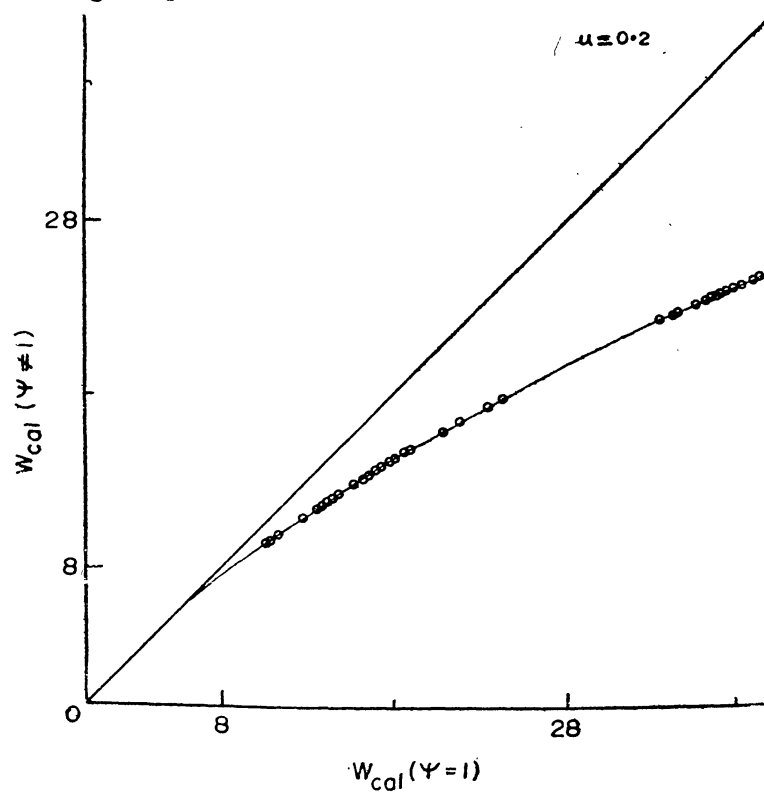


Figure 4b. Same as in figure 4a but for $\mu = 0.2$.

$$W(\psi \neq 1) = a W^2(\psi = 1) + bW(\psi = 1) + c. \quad \dots(3)$$

The values of the coefficients a , b and c given in table 2 for the models HM and VAL were obtained through a least squares solution and reproduce $W(\psi \neq 1)$ values

Table 2. The coefficients a , b and c used in equation (3)

a	b	c	Remarks
$-6.36843889 \times 10^{-3}$	$9.75092041 \times 10^{-1}$	$9.63284363 \times 10^{-2}$	for HM model & $\mu = 1.0$
$-5.17395224 \times 10^{-3}$	$7.96671421 \times 10^{-1}$	1.53843335	for HM model & $\mu = 0.2$
$-5.86587430 \times 10^{-3}$	$9.66809428 \times 10^{-1}$	$1.52722072 \times 10^{-1}$	for VAL model & $\mu = 1.0$
$-3.93578255 \times 10^{-3}$	$7.57823323 \times 10^{-1}$	2.40922726	for VAL model & $\mu = 0.2$

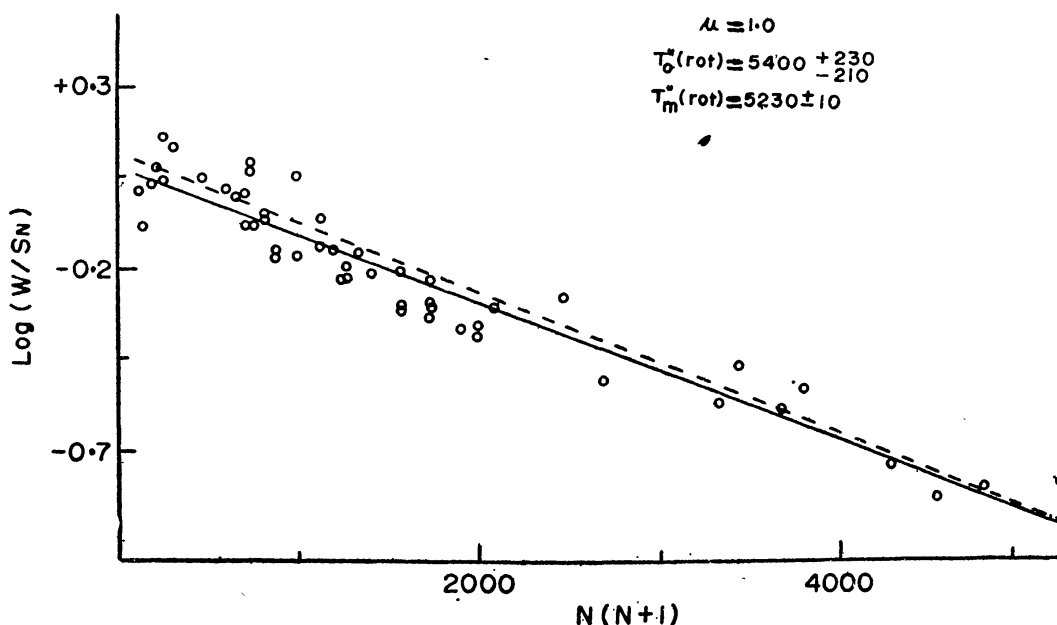


Figure 5a. Determination of T_{rot} after correcting the observed equivalent widths for saturation according to the HM model for $\mu = 1.0$. The VAL result is $T_m^*(rot) = 5100 \pm 10$.

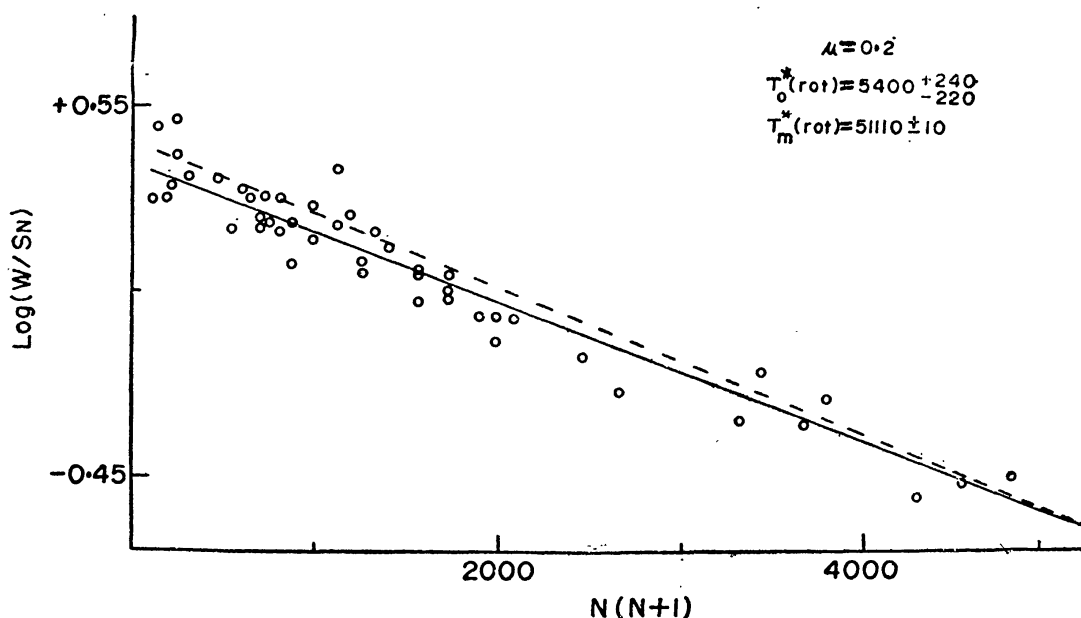


Figure 5b. Same as in figure 5 a but for $\mu = 0.2$. The VAL result is $T_m^*(rot) = 4950 \pm 10$.

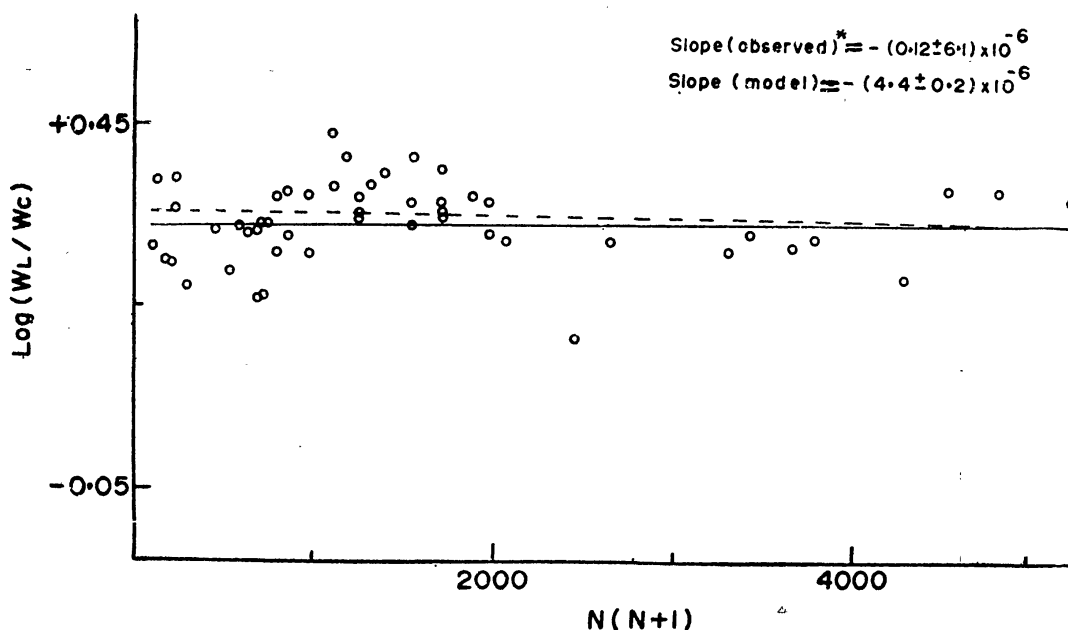


Figure 6. Observed equivalent widths are corrected for saturation utilizing the HM model and then an estimate is made of the slope of the line in a $\log (W_L/W_C)$ versus $N(N+1)$ plot (cf. equation (2.2)). The VAL result is slope (model) = $-(5.8 \pm 0.3) \times 10^{-6}$.

with an uncertainty less than 1%. The T_{rot} values for the corrected equivalent widths are presented in figures 5a and 5b. It can now be clearly seen that the cooler model VAL does not fit in and also that the HM result is lower than observations at $\mu = 0.2$, though it is in good agreement at $\mu = 1.0$. This could be a pointer for slight improvements in the upper layers of the HM model. An increase in the model temperature should be such that it still retains the good match between the observed and the calculated temperatures for $\mu = 1.0$. This could also imply a slight increase in the carbon abundance chosen here. Alternatively temperature inhomogeneities could play a crucial role in near limb observations.

In figure 6 we again find that there is no evidence for an increase in temperature towards limb. Here also the corrected equivalent widths have been used.

In brief, we have obtained rotational temperatures consistent with model-based predictions for $\mu = 1.0$. There is no evidence for an increase in rotational temperature towards the limb. The HM model might need slight changes in the upper layers.

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