EQUIVALENT WIDTH OF MOLECULAR LINES IN STARS

I: *Lyman and Werner Bands of H_2 in the Solar Atmosphere*

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Abstract. The expected equivalent widths of the individual rotational lines of the Lyman and Werner bands of the hydrogen molecule from the solar atmosphere have been calculated. These results are used to predict what one expects to observe with a specified wavelength bandpass. These are compared with the observation of Dupree and Reeves.

1. Introduction

There have been a large number of studies on the various aspects of molecules in the solar atmosphere. One interesting aspect is the study of the lines arising out of the electronic transitions from the molecules. These lines usually lie in the ultraviolet region of the spectrum (Goldberg *et al.*, 1965). This field of investigation has become important in recent years because of the successful use of rockets and satellites. The present work has been started with the idea of calculating the equivalent width of some of those molecular lines. Molecular equilibrium calculations indicate that molecular hydrogen can exist in appreciable amounts in the solar atmosphere. Therefore, it is of interest to see whether the Lyman and Werner bands of the molecular hydrogen can be detected in the solar spectrum. In fact, a careful observation of H_2 would be of importance, as it will give us information about the region of solar temperature minimum This study is of further interest as the absorption coefficient due to $(B-X)$ and $(C-X)$ bands of the hydrogen molecule are appreciable in the solar atmosphere (Tarafdar and Vardya, 1972). Therefore, we would like to calculate the expected equivalent width of individual rotational lines of Lyman and Werner bands of hydrogen molecule from the solar atmosphere. This is then used to calculate the expected equivalent width for a given bandpass for comparing with observations.

2. Method of Calculation

We are interested in the calculation of the equivalent width of an individual rotational molecular line arising from a given initial electronic (n), vibrational (v) and rotational (J) state. It is given for the linear and flat portions of the curve of growth as (Spitzer,

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1968)

$$W_J = 2b\,F(C), \tag{1}$$

where b is the Doppler width of the line given by

$$b = \frac{\lambda}{c}\left(\frac{2k\,T}{M_{\mathrm{mol}}}\right)^{1/2}. \tag{2}$$

Here T and M_{mol} represent the temperature and the mass of the molecule respectively. In Equation (1), $F(C)$ is a complicated function whose values have been tabulated as a function of C (see Spitzer, 1968) where C is the optical depth at the line center and is given by

$$C = \frac{\pi^{1/2}}{m_e b}\,e^2\,\frac{\lambda^2}{c^2}\,N_{nvJ} f. \tag{3}$$

Here N_{nvJ} represent the number of molecules per cm^3 in the state of interest. f is the total oscillator strength and the other quantities have their usual meanings.

The total equivalent width of a molecular line integrated over the whole atmosphere is therefore given by (Schadee, 1964, 1968)

$$W_J = 2\int_0^\infty \frac{bF(C)}{K_\lambda}\,G(\tau,\mu)\,\mathrm{d}\tau, \tag{4}$$

where $G(\tau, \mu)$ is the weighting factor, K_λ is the absorption coefficient per cm^3 and τ is the optical depth at the wavelength under consideration. For the equivalent width calculation of any line, we have to know the number of molecules in the level under consideration and the total oscillator strength of the transition. The number of molecules in the level of interest is essentially given by (Schadee, 1964)

$$N_{nvJ} = g_{el} g_v g_r \exp(-Ehc/kT)\,\Psi_{\alpha\beta}\Phi_\alpha\Phi_\beta\varepsilon_\alpha\varepsilon_\beta\,\frac{P_F^2}{(1+B)^2\,kT}, \tag{5}$$

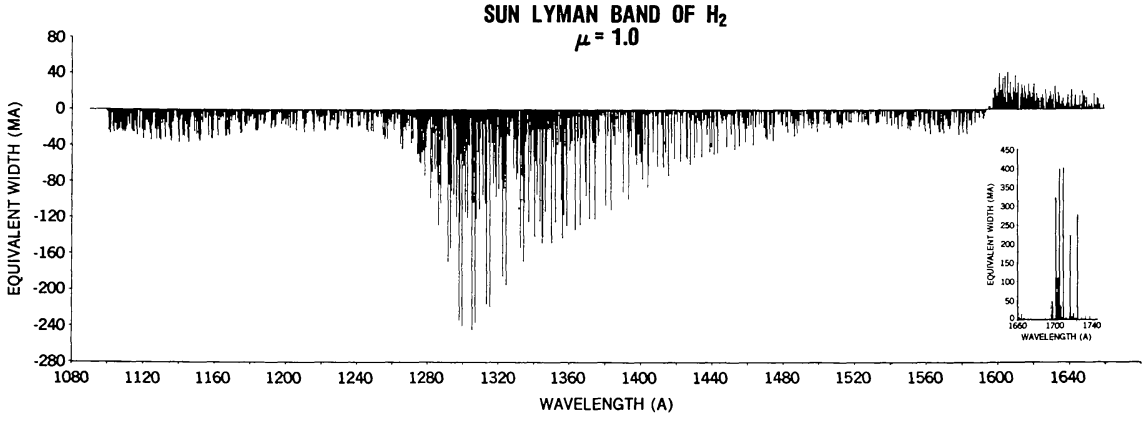

Fig. 1. Equivalent widths for the Lyman band of H_2, are plotted as a function of wavelength for μ=1.0.

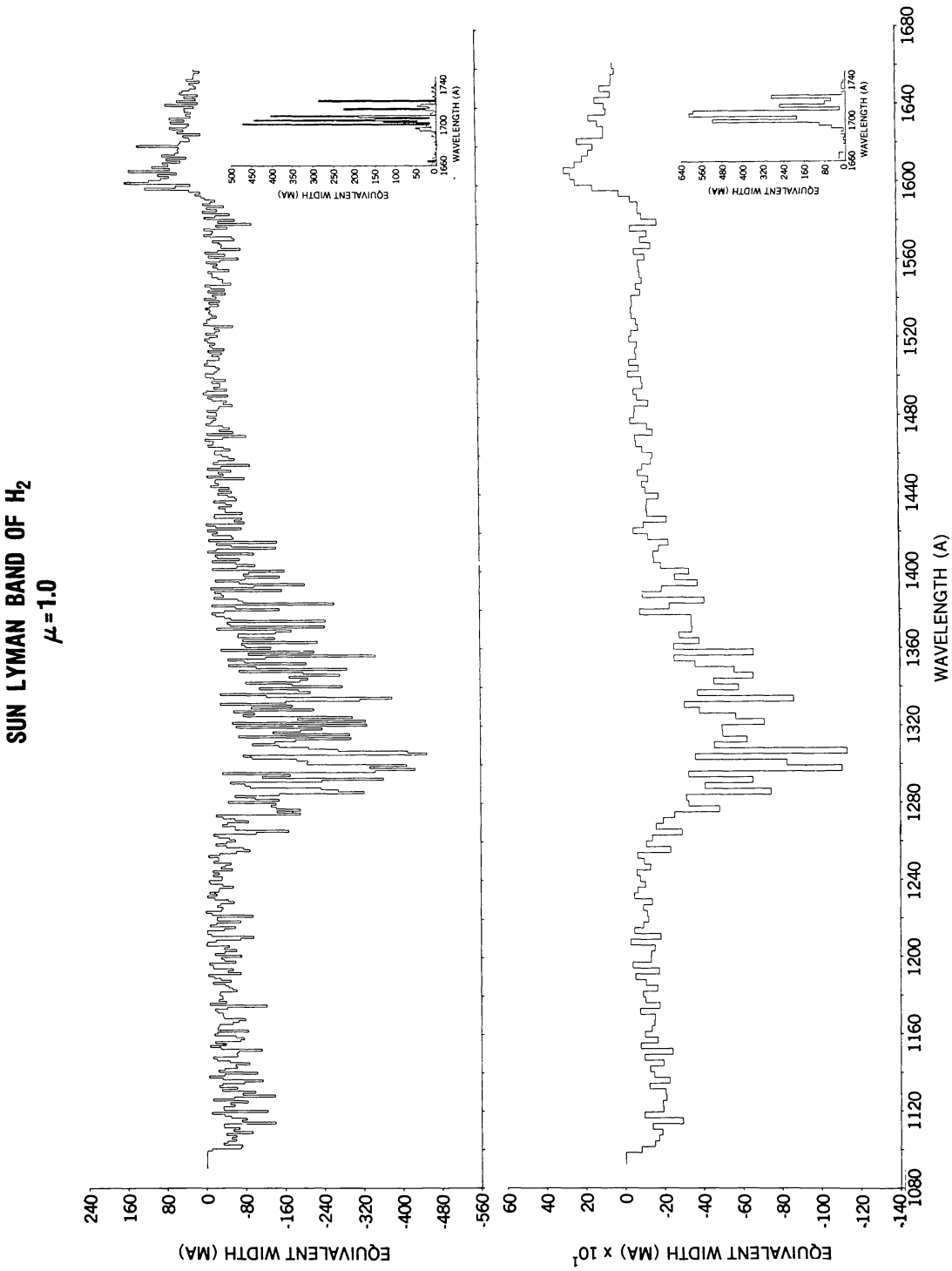

Fig. 2. Total equivalent width within $\Delta\lambda = 1.0$ (upper curve) and 3.0 Å (lower curve) are plotted as a function of wavelength for $\mu = 1.0$.

where $E=T(n'')+G(v'')+F(J'')$. Here T, G, and F are the electronic, vibrational and rotational term values of the lower state of the transition. ε_α and ε_β represent the relative number of the two species α and β with respect to hydrogen and Φ's the ratio of the partial atomic pressure to the total pressure of the element. $\Psi_{\alpha\beta}$ is the dissociation function of the molecule and $P_F=P_g+P_{H_2}$. g_{el}, g_v, and g_r represent the electronic, vibrational and rotational statistical weights respectively. B is the ratio of helium to hydrogen by number.

The total oscillator strength for any specific transition can be writtten as

$$f=f_{el}f_v f_r \tag{6}$$

the product of the electronic, vibrational oscillator strengths and the rotational line strength factor.

3. Results of Calculations

The oscillator strengths for different lines of Lyman and Werner bands of the hydrogen molecule are taken from the work of Allison and Dalgarno (1970). The rotational strength factors, called Hönl-London factors, are given by Schadee (1964). For the variation of physical parameters as a function of optical depth, the model solar atmosphere of Gingerich *et al.* (1971) has been used. This is one of the best solar models available which resulted in a detailed comparison between calculations and various observations. For elemental abundances, the tabulated values of Withbroe (1971) are used. For helium abundance, we use a value of $B=0.1$. The partial pressures of the various constituents in the model solar atmosphere are calculated from the molecular equilibrium program of Dr Vardya. For the integration of Equation (4), we have to know K_λ and τ_λ in the far ultraviolet region. These quantities are a bit uncertain at the present time because of the incomplete knowledge of opacity in these wavelength regions. However, in the present work, we have included the absorptions due to H, H^-, He^-, He I, Si II, Mg I, C I, Fe I, Al I and scattering of H, H_2 and e. It may be noted that the absorption due to the above metals are the ones which are important in the region of our interest (Matsushima, 1968). For some of the absorption calculations,

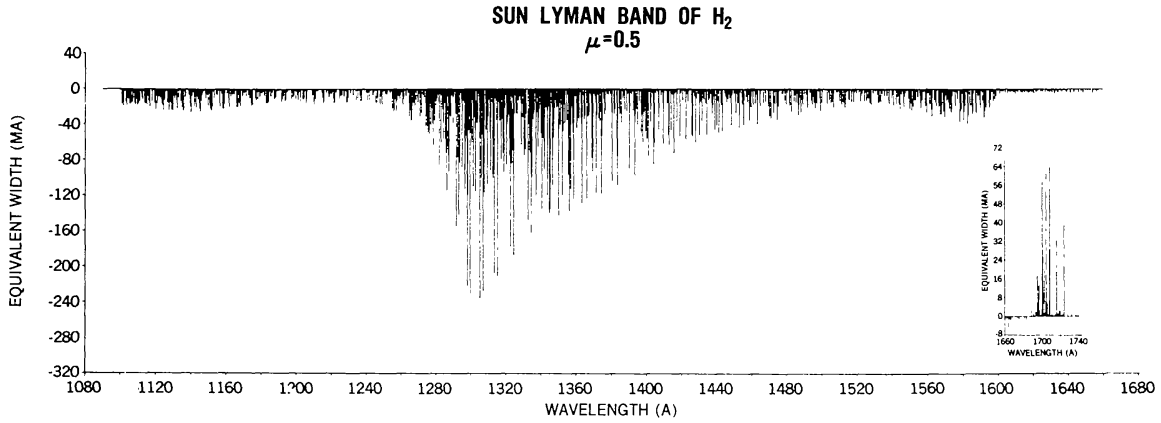

Fig. 3. Same as Figure 1, except $\mu=0.5$.

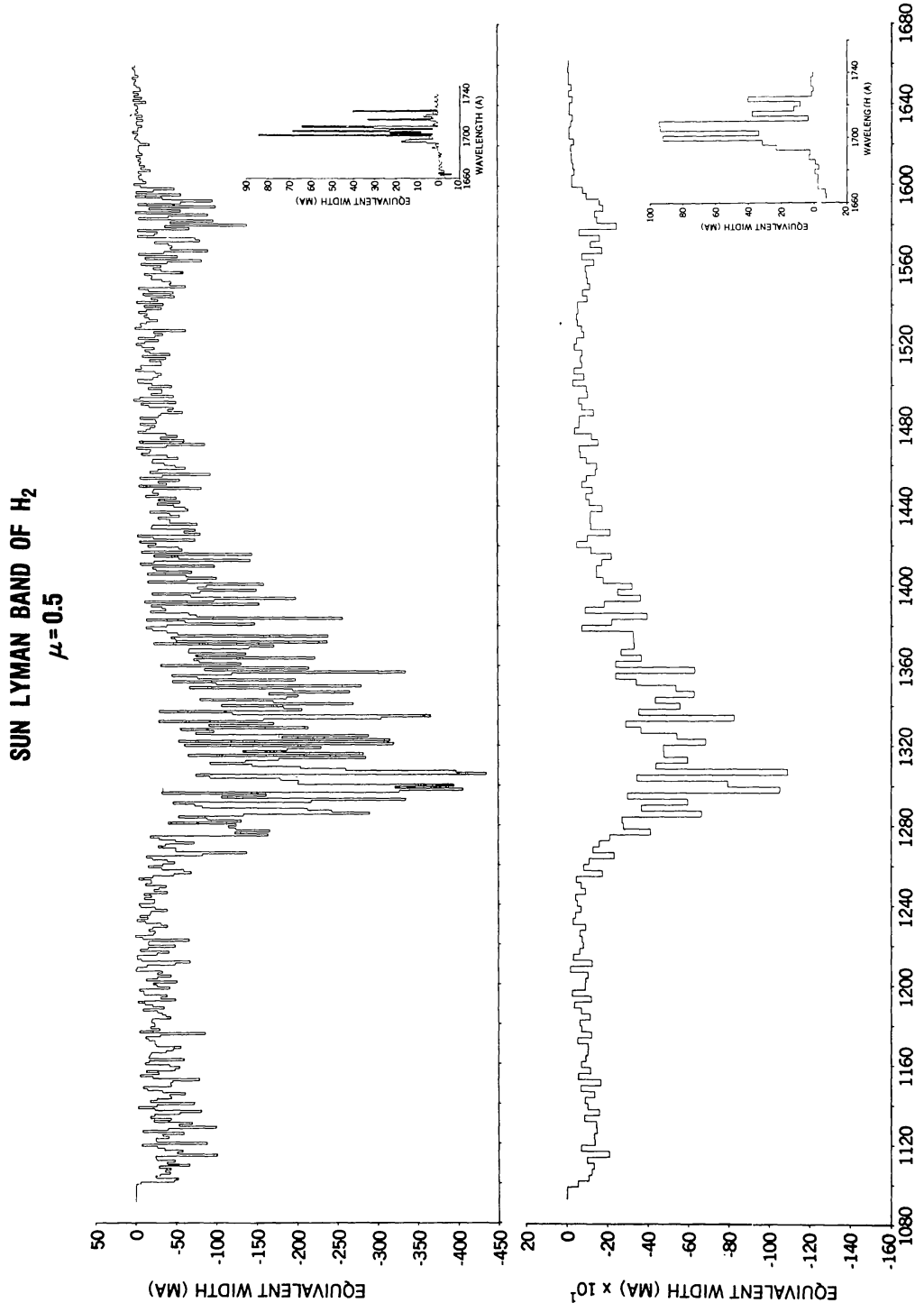

Fig. 4. Same as Figure 2, except $\mu = 0.5$.

we have made use of the sub-routines of Carbon and Gingerich (1969) and Gingerich *et al.* (1971). For Al I, we have used the absorption cros-ssections of Travis and Matsushima (1968). The monochromatic optical depth at any wavelength for the solar model atmosphere of Gingerich *et al.* (1971) can then be calculated. From a knowledge of the monochromatic optical depths, the weighting factor $G(\tau, \mu)$ van be calculated (see Böhm, 1960). The wavelength of each vibrational-rotational transition for the Lyman band has been calculated using the measured values of the energies for the various vibrational and rotational levels (Herzberg and Howe, 1959). For the Werner band, wavelengths have been calculated using spectroscopic data of Herzberg and Howe (1959), Namioka (1965), Rosen (1970), and Dieke (1968). For the two bands of interest, we have considered various transitions arising from $v''=0$ to 14, $v'=0$ to 13 and $J''=0$ to 29, with appropriate energy cut-off.

The expected equivalent widths of the rotational lines of the Lyman and Werner bands of the hydrogen molecule are shown in Figures 1 to 8. These are due to the

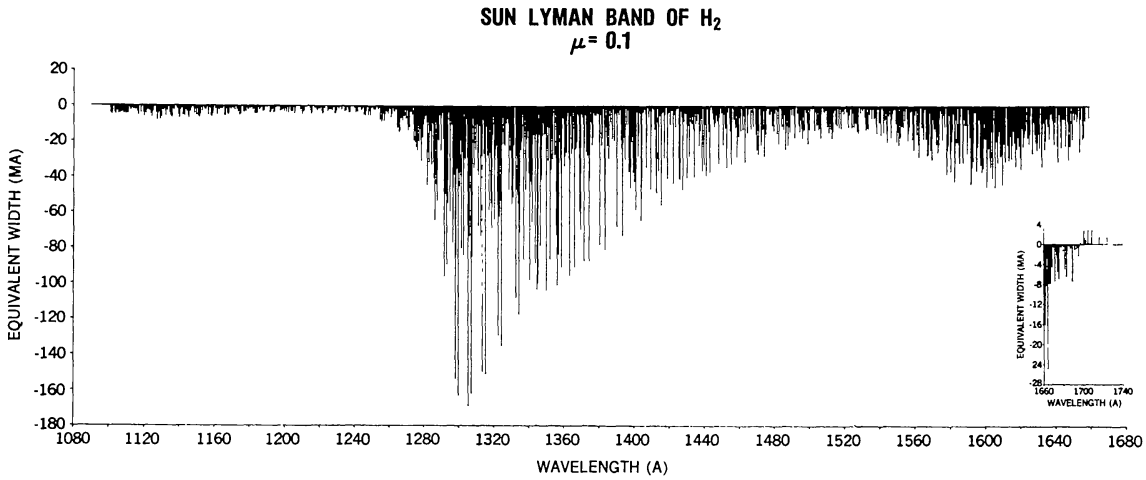

Fig. 5. Same as Figure 1, except $\mu=0.1$.

superposition of numerous lines arising out of the various transitions. The calculations for the Lyman band are done for $\mu=1.0$, 0.5 and 0.1. For Werner band, results are shown for $\mu=1.0$. The negative and positive numbers in these figures mean that the lines should be in emission and absorption respectively. It may be noted from these figures that the calculated equivalent widths are of measurable amounts. However, at the present time the resolution in the ultraviolet region of the spectrum is not good enough to resolve each individual rotational line, although such resolution is likely to become available in the next few years. Until this time, in order to compare with the observations, we have to calculate the total equivalent width of all the lines for a given wavelength resolution of the instrument. With this in mind, we have given in Figure 2, 4, 6 and 8 the expected total equivalent width for two bandpasses, namely $\Delta\lambda=1.0$ and 3.0 Å.

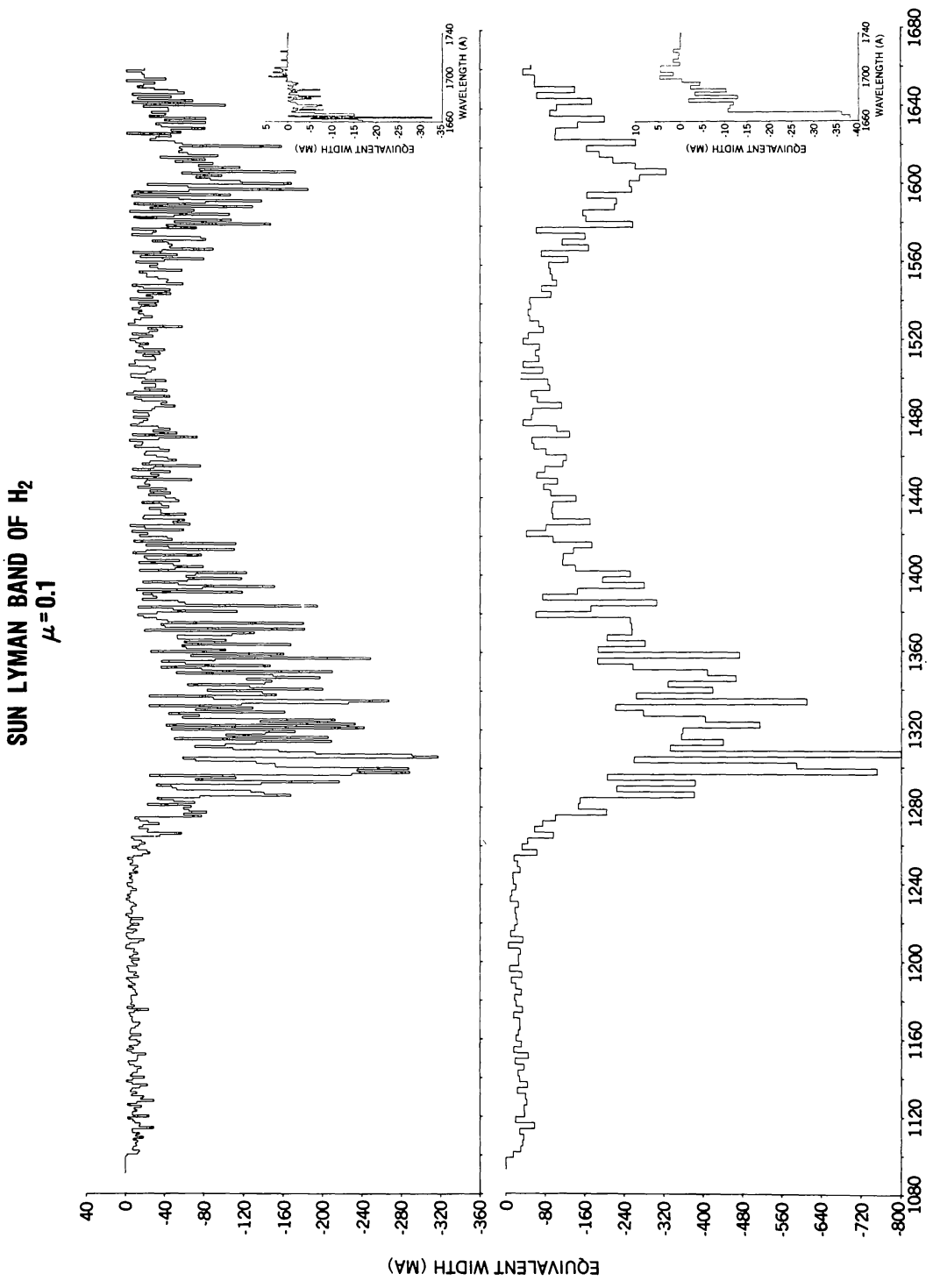

Fig. 6. Same as Figure 2, except μ=0.1.

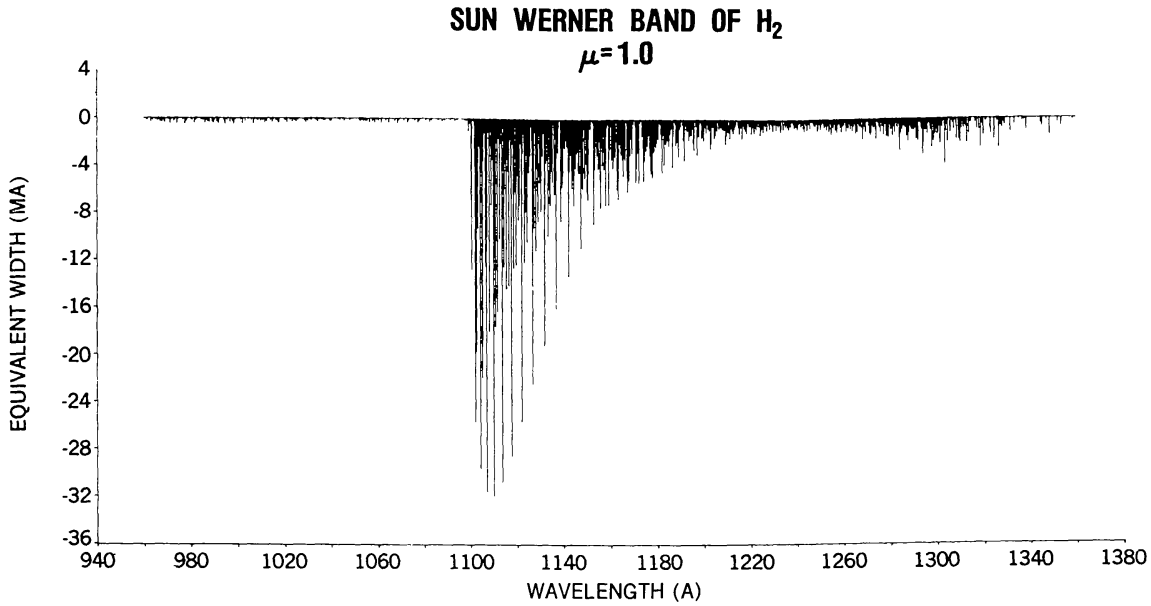

Fig. 7. Equivalent widths for the Werner band of H_2 are plotted as a function of wavelength for $\mu=1.0$.

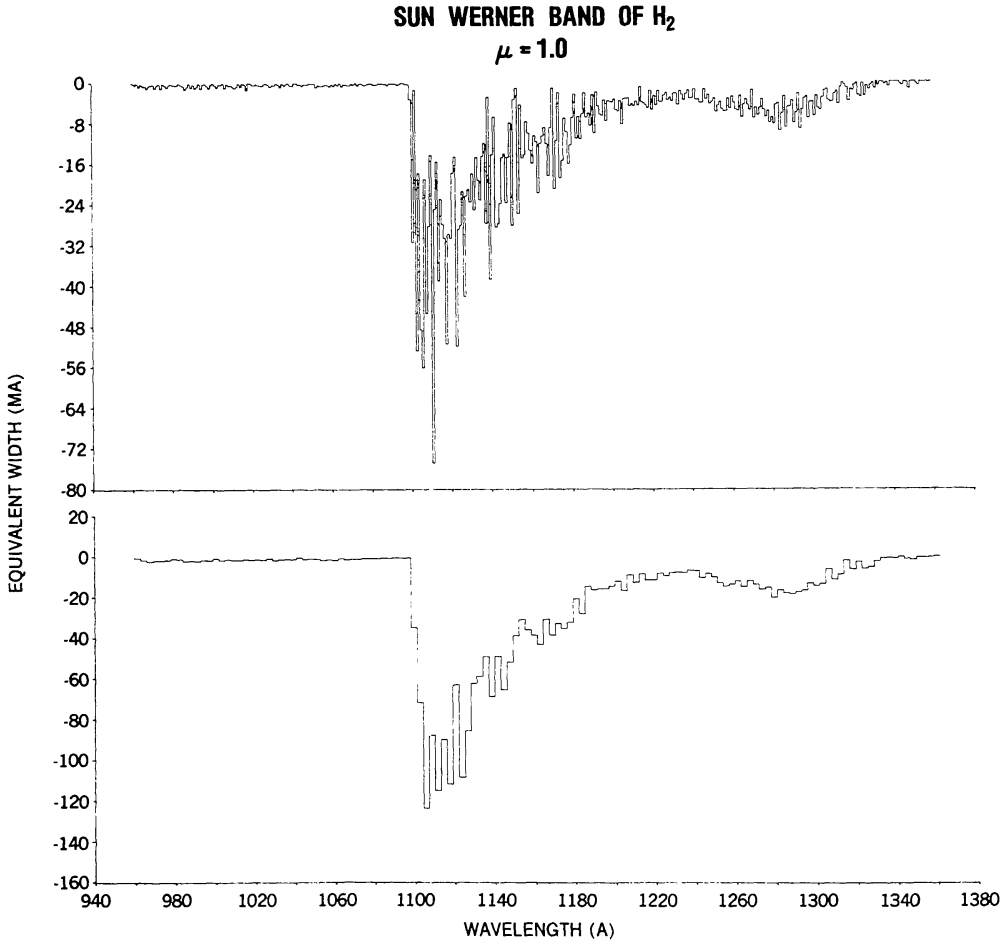

Fig. 8. Total equivalent width within $\Delta\lambda=1.0$ and 3.0 Å are plotted as a function of wavelength for $\mu=1.0$.

4. Discussion

We may see from Figure 1, that there is a transition around $\lambda \sim 1600$ Å, above which the lines should be in absorption and below which it should be in emission. To understand this, as a typical case, we have shown in Figure 9, the value of the integrand of

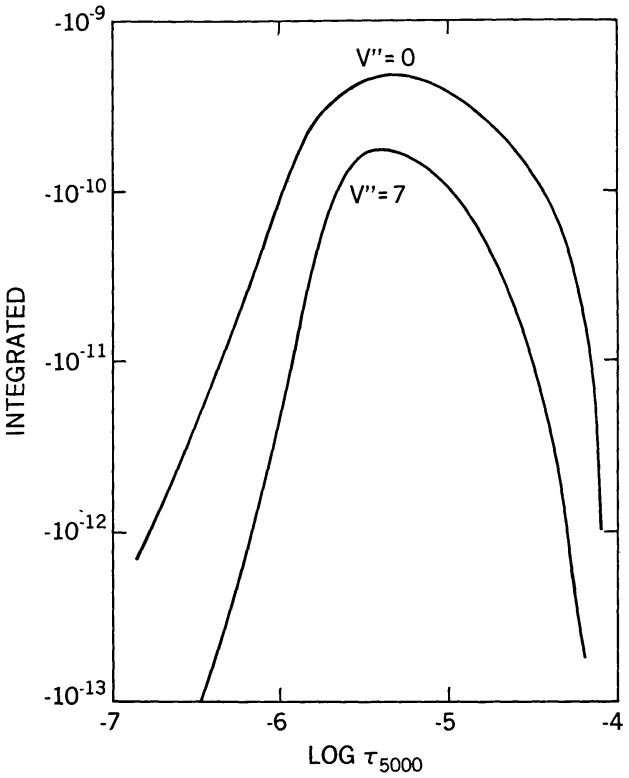

Fig. 9. Plot of the integrand of Equation (4), for $R(0)$ line of Lyman band for $v'=0$ and for different v'', as a function of optical depth. The ordinate scale is arbitrary. Curves are for $\mu=1.0$.

Equation (4) as a function of the optical depth for $R(0)$ line of the Lyman band for $v'=0$ and for two values of v''. One may see that the contribution to the total integral comes essentially from optical depths between 10^{-7} and 10^{-4}. This is the region where the temperature increases outward and so the contribution to the total equivalent width comes mainly from the emission component. As we go to larger wavelengths the contribution from the deeper regions of the atmosphere also becomes important. Since the temperature minimum in the solar atmosphere occurs around the optical depth 10^{-4}, there is an appreciable contribution from the absorption component for these wavelengths. This can be seen from Figure 10. Therefore, for most of the lines shown in Figures 1 to 8 there is a sort of cancelling effect due to the emission and absorption components. Finally for very large wavelengths, contribution from the absorption component dominates over the emission component and so the resultant line should be in absorption. In Figure 10, we have also shown the value of the integrand arising out of the same transition for $\mu=1.0$ and 0.1. It may be seen that the

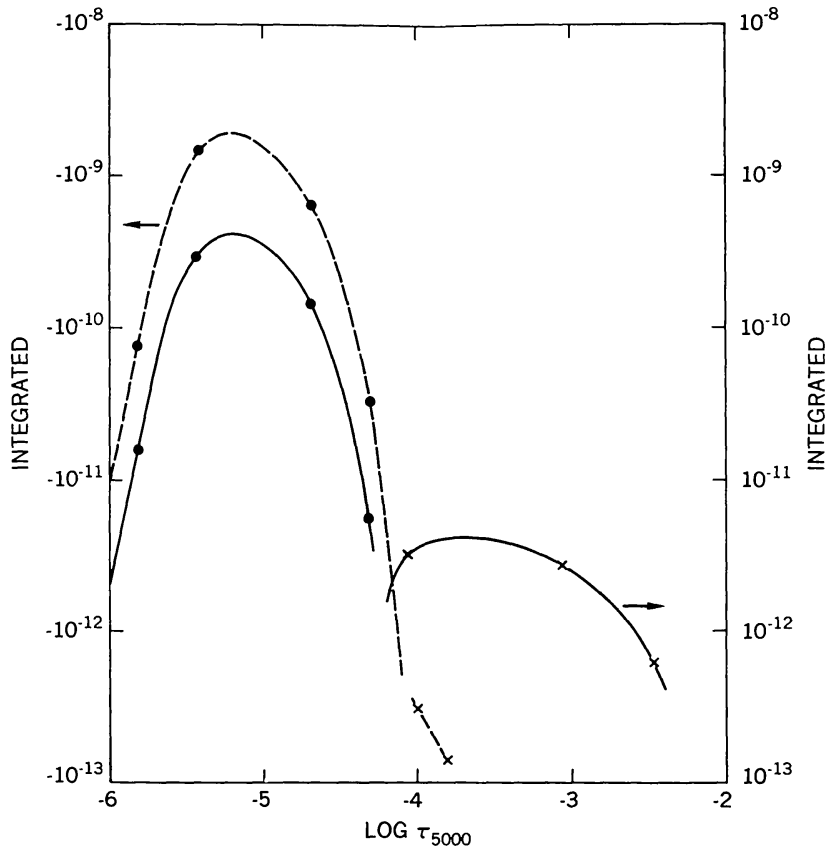

Fig. 10. Plot of the integrand of Equation (4), for the $R(0)$ line of Lyman band for $v'=0$ and $v''=9$, as function of optical depth. Continuous and dashed curves refer to $\mu=1.0$ and 0.1 respectively. The curves with dots and crosses refer to emission and absorption contributions respectively.

contribution to the integral from deeper layers for the case $\mu=1.0$ is appreciable compared to the case of $\mu=0.1$. As a result, most of the lines for $\mu=0.1$ should be in emission compared to that of $\mu=1.0$.

From Figures 1 to 8, we can see that the lines of Lyman and Werner bands of the hydrogen molecule should be observable mostly in emission in the far ultraviolet region of the solar spectrum. In fact, Dupree and Reeves (1971) have obtained the solar disk spectrum from an orbiting solar observatory (OSO-IV) in the spectral region 304 to 1394 Å with a resolution of about 3.2 Å. It may be noted that for most of the strong features of the Lyman band as shown in Figure 2, in the region 1250 to 1400 Å, there is a corresponding emission feature in the observations of Dupree and Reeves (Figure 11). This tempts one to identify some of these observed emission features as due to the lines of the Lyman bands of the hydrogen molecule. However, better observations of the solar ultraviolet spectrum and a careful search for H_2 lines will help one to understand better the temperature minimum region of the solar atmosphere. One may also note that the lines of the Lyman band of the hydrogen molecule should be observable in absorption in the wavelength region around 1700 Å (Figures 1–6). However, the absorption due to $(A-X)$ band of CO in this wavelength

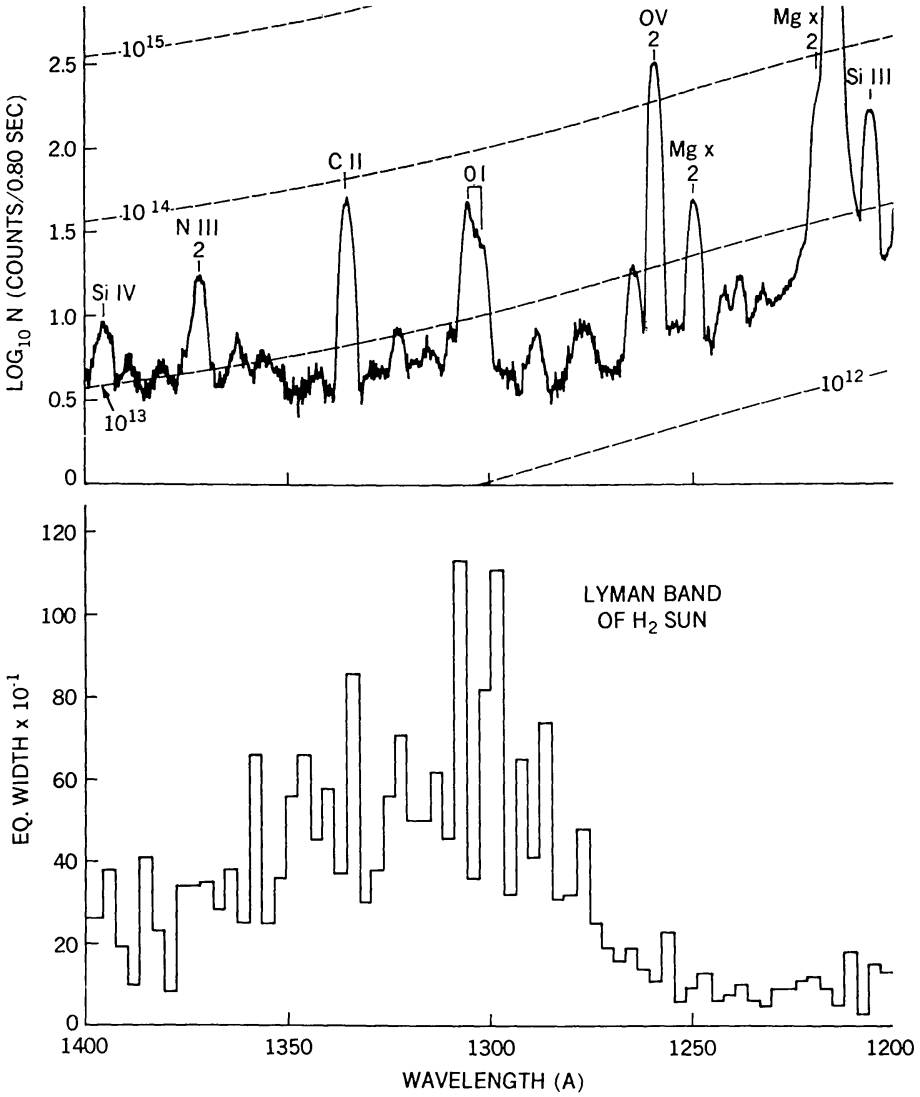

Fig. 11. Comparison of the calculated features of Lyman band with the observations of Dupree and Reeves.

region is very strong and so it is not clear whether one will be able to observe the lines of molecular hydrogen.

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