

THE ASTROPHYSICAL SIGNIFICANCE OF THE CONTINUOUS SPECTRUM OF THE HYDROGEN QUASI-MOLECULE

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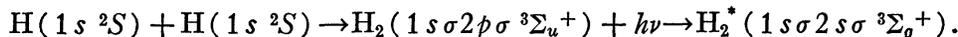
ABSTRACT

The importance of quasi-molecular hydrogen as a source of continuous absorption in stellar atmospheres is re-examined as a result of a recently revised calculation of this absorption coefficient that included the explicit dependence on the rotational state of the nuclei. At stellar temperatures, the detailed summation of the absorption coefficient over rotational states increases the strength by about a factor of 2 at short wavelengths. It is found that quasi-molecular hydrogen absorption is of maximum importance relative to other sources of opacity in dwarf stars along the main sequence at about solar temperature.

In the solar case, it exceeds 1 per cent of the total known opacity at wavelengths less than 3000 Å and generally contributes more than Rayleigh scattering and the negative hydrogen ion below about 2000 Å. The inclusion of quasi-molecular hydrogen absorption substantially reduces the disagreement between observed and calculated fluxes between 2000 and 1700 Å in the solar spectrum, and it contributes some opacity down to 1525 Å, a region that may include observable effects of the temperature minimum in the solar atmosphere.

I. INTRODUCTION

Many authors have reported calculations of the strength of the continuous spectrum of the hydrogen quasi-molecule (Coolidge, James, and Present 1936; James and Coolidge 1939; Grandsire 1954; Varsavsky 1957; Erkovich 1960; Solomon 1964; Soshnikov 1964; Doyle 1968*a*). This spectrum corresponds in absorption to transitions to the lowest bound triplet state $a\ ^3\Sigma_g^+$ of the hydrogen molecule from the repulsive unbound state $b\ ^3\Sigma_u^+$ formed from two normal hydrogen atoms in parallel spin states,



The great strength and extent of the continuum (1600–5000 Å) have inspired others to suggest, independently, that it might be significant in various astrophysical applications (Wildt 1947 [cited in Varsavsky 1966], 1949; Swings 1951 [cited in Hynek 1951]; Herzberg 1954; Varsavsky 1957). Applications of the calculations to astrophysical problems have been made by Zwaan (1962), Stecher (1962), Meinel (1962), and Solomon (1964).

In § II we discuss the important aspects of past calculations and applications and describe the essential differences between the absorption coefficient used in this paper and the 1964 calculations of Solomon. In § III we survey the importance of quasi-molecular hydrogen absorption in stellar atmospheres, and in § IV we make a detailed analysis of its contribution to the solar ultraviolet spectrum.

II. CALCULATIONS AND APPLICATIONS

The original calculations by Coolidge *et al.* (1936) provided only the relative wavelength dependence of the emission intensity from the first four vibrational states. In 1939, James and Coolidge made the first calculation using a variable electronic dipole moment. They reported the mean lifetimes of the first four vibrational states, which are equivalent to the absolute strength of the transitions, but they did not publish, explicitly, absolute absorption or emission coefficients.

Varsavsky (1957) reported that he had made quantitative calculations of the strength of this absorption and its wavelength dependence. Although he did not publish his values, he did state that the process provides a major source of opacity in the Sun between 1600 and 2600 Å.

Erkovich (1960) published quantitative calculations of the absorption into the first four vibrational states (intrinsically the same information as in the James and Coolidge calculations). However, he made an error in estimating the appropriate cross-section for the number of collisions between ground-state hydrogen atoms in the $b\ ^3\Sigma_u^+$ state (the number of quasi-molecules). The wavelength dependence of his result was correct, but the absolute strength of his calculation was too large by about 2 orders of magnitude, as was noted by Solomon (1964) and by Soshnikov (1964).

Zwaan (1962) pointed out that at the high temperatures of stellar atmospheres the contribution from higher vibrational states becomes important, and he extended Erkovich's erroneous calculation to include two more vibrational states, through $v' = 5$. He applied his results to the ultraviolet solar spectrum, and concluded that quasi-molecular hydrogen absorption, together with the continuous absorption from certain metallic ionization continua, could quantitatively account for the anomalous absorption in the Sun from about 4800 Å to shorter wavelengths (Barbier 1946; Chalonge, Divan, and Kourganoff 1950; Michard 1953; Pierce and Waddell 1961). Stecher (1962) independently suggested that the Erkovich value of the quasi-molecular hydrogen absorption was itself sufficient to explain the anomalous absorption.

Meinel (1962) noted a striking similarity between a relative maximum in the rocket ultraviolet intensity distribution in B stars (Kupperian, Boggess, and Milligan 1958; Stecher and Milligan 1962) and the emission intensity of this continuum as produced in the laboratory under conditions of selective excitation by Coolidge (1944). Although the wavelength dependence of the emission continuum in thermodynamic equilibrium is somewhat different from that used by Meinel, this possible identification of the hydrogen molecule in stellar atmospheres is no longer relevant, since subsequent observations of several early-type stars have failed to reproduce the original intensity anomaly (see Field, Somerville, and Dressler 1966, p. 223).

Solomon (1964) published new calculations in which he extended the vibrational sum through $v' = 7$. His results had a slightly different frequency dependence from those of Erkovich, and were about 1 per cent of the strength of the latter. Soshnikov (1964) published similar results, but he did not describe his calculation in detail. Solomon concluded not only that quasi-molecular hydrogen absorption was not the anomalous solar absorption but also that its contribution to the total opacity was negligible for all frequencies in all types of stellar atmospheres.

Varsavsky (1966) noted in a recent review that while he believed Solomon had now shown quasi-molecular hydrogen to be definitely not the strong unknown absorber below 4800 Å,¹ it still might play a role in the continuous opacity of subdwarfs. The low metallic abundance of the subdwarfs lowers the electron pressure, which reduces continuous absorption by the negative hydrogen ion and enhances the relative importance of the quasi-molecular hydrogen absorption.

In a recent study, Doyle (1968*a*) showed that the matrix element of the electronic dipole moment for this transition is not independent of the rotational state of the nuclei (the angular momentum of the colliding atoms). The detailed summation of the absorption coefficient over all rotational states, for temperatures at which several states are populated, differs significantly from the absorption calculated with a constant rotation-independent matrix element. The explicit variation of the matrix element with rotational quantum number is reported in Doyle (1968*b*).

¹ A recent study of the remaining discrepancy between observed and theoretical fluxes in this spectral region has been made by Carbon, Gingerich, and Kurucz (1968).

The full expression for the absorption coefficient, including rotational dependence, is

$$k_{\nu}^{b \rightarrow a} = \frac{8\pi^3\nu}{3hc} \frac{3}{4} n(\text{H})^2 \frac{\hbar^3}{(2\pi\mu kT)^{3/2}} \sum_{\nu} \sum_{J'} \exp\left(-\frac{E_{avJ'} - h\nu}{kT}\right) 2 \left(\frac{2\mu}{E_{avJ'} - h\nu}\right)^{1/2} \\ \times \bar{\omega}_{J'} \{ (J' + 1) [\int \mathfrak{R}_{K, J'+1}^b(R) D_{ba}(R) \mathfrak{R}_{\nu, J'}^a(R) dR]^2 \\ + J' [\int \mathfrak{R}_{K, J'-1}^b(R) D_{ba}(R) \mathfrak{R}_{\nu, J'}^a(R) dR]^2 \}, \quad (1)$$

with

$$K = \left[\frac{2\mu}{\hbar} (E_{avJ'} - h\nu) \right]^{1/2}, \quad \bar{\omega}_{J'} = \frac{1}{4} (J' \text{ even}), \quad \bar{\omega}_{J'} = \frac{3}{4} (J' \text{ odd}).$$

Most of the symbols have the conventional meanings: $n(\text{H})$ is the density of neutral atomic hydrogen; μ is the reduced mass of the hydrogen molecule; $E_{avJ'} - h\nu$ is the energy in the continuous electronic state $b \ ^3\Sigma_u^+$ that is $h\nu$ below a bound vibrational-rotational state $\nu J'$ in the electronic state $a \ ^3\Sigma_g^+$; and $\bar{\omega}_{J'}$ is the nuclear-spin statistical weight. The matrix elements of the electronic dipole moment $D_{ba}(R)$ are evaluated between the radial (R), the internuclear distance, is the radial dimension) parts of the bound-state vibrational-rotational wave functions $\mathfrak{R}_{\nu, J'}^a(R)$ and the continuum wave functions $\mathfrak{R}_{K, J'+1}^b(R)$.

The essential difference between this and past calculations is that the latter implicitly assumed that the summation over rotational states J' could be carried out before the evaluation of the matrix elements, resulting in an expression that is simply the $J' = 0$ contribution, multiplied by a rigid-rotator partition function. This corresponds to the assumption that all collisions are "head-on" or, more specifically, that the contribution to the absorption coefficient from collisions with an arbitrary impact parameter has the same wavelength dependence as the contribution of the head-on collisions. In this " $J' = 0$ approximation," equation (1) becomes

$$k_{\nu}^{b \rightarrow a} = \frac{8\pi^3\nu}{3hc} \frac{3}{4} n(\text{H})^2 \frac{\hbar^3}{(2\pi\mu kT)^{3/2}} \frac{2\mu R_0^2 kT}{\sigma \hbar^2} \\ \times \sum_{\nu} \exp\left(-\frac{E_{av0} - h\nu}{kT}\right) 2 \left(\frac{2\mu}{E_{av0} - h\nu}\right)^{1/2} \\ \times [\int \mathfrak{R}_{K,0}^b(R) D_{ba}(R) \mathfrak{R}_{\nu,0}^a(R) dR]^2, \quad (2)$$

where R_0 is the equilibrium internuclear distance of the bound electronic state $a \ ^3\Sigma_g^+$, and σ is the nuclear symmetry factor, equal to 2 for the hydrogen molecule.

The calculations of Erkovich and Solomon contained one other important approximation,² in which the continuum wave function was replaced by a δ function located at the classical turning point of the motion, R_T , which is a function of the energy in the continuous state. The matrix elements in equation (2) were taken as proportional to

$$\int \mathfrak{R}_{K,0}^b(R) D_{ba}(R) \mathfrak{R}_{\nu,0}^a(R) dR \propto D_{ba}(R_T) \mathfrak{R}_{\nu,0}^a(R_T). \quad (3)$$

At stellar temperatures, the errors introduced into the absorption coefficient by the $J' = 0$ approximation (2) are larger than those from the δ -function approximation (3). For example, at 5000° K the detailed summation over rotational states in equation (1) resulted in an absorption coefficient that is about twice the value of that resulting from

² This is the "reflection" method of Condon (1928), which was first used in a calculation by Winans and Stueckelberg (1928) and modified by James and Coolidge (1939) to include a variable electronic dipole moment

the $J' = 0$ approximation (2) at short wavelengths (1800 Å) and about half the value at long wavelengths (4000 Å). At the same temperature, the errors in the δ -function approximation (3), specifically the difference between equations (2) and (3), are seen to be of the order of 20 per cent or less in Figure 1, where we have plotted the ratio of the $J' = 0$ approximation (2) to the detailed summation (1) and the ratio of Solomon's δ -function calculation (3) to the detailed summation (1).

Because the number of quasi-molecules, or collisions, depends on the square of the density or pressure, it is convenient to define a quantity that is independent of density,

$$k_{\nu}^{b \rightarrow a} \equiv K_{\nu}^{b \rightarrow a} n(\text{H})^2, \quad (4)$$

where $k_{\nu}^{b \rightarrow a}$ has dimensions cm^{-1} and $K_{\nu}^{b \rightarrow a}$ has dimensions cm^5 . It is equivalent to the volume absorption coefficient (in cm^{-1}) of a neutral atomic-hydrogen gas at unit density. Figure 2 shows the wavelength dependence of $K_{\nu}^{b \rightarrow a}$ with temperature as a parameter.

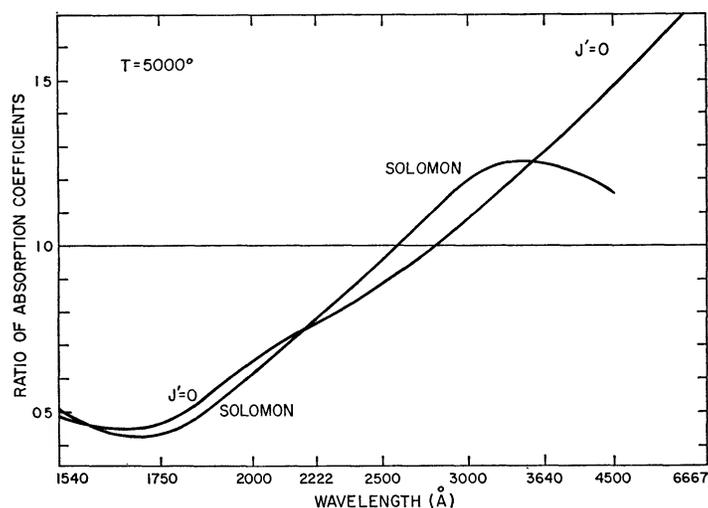


FIG. 1.—Ratio of the $J' = 0$ approximation (eq. [2]) to the detailed summation over rotational states (eq. [1]) and the ratio of Solomon's (1964) calculation using the δ -function approximation (eq. [3]) to the detailed summation.

The extremely strong variation with wavelength and temperature, which is caused primarily by the exponential factor in equation (1), is used in the next section to make a rough estimate of the particular stellar conditions under which quasi-molecular hydrogen is likely to make the largest relative contribution to the total opacity of stellar material. Values of $K_{\nu}^{b \rightarrow a}$ at stellar surface temperatures are tabulated in Table 1.

An analysis of truncation of infinite summations over vibrational and rotational states, the neglect of higher electronic states, and other explicitly estimated errors (Doyle 1965) indicates that the present numerical results are reliable to within 10 per cent below 8000° K and for densities of neutral hydrogen less than 10^{21} cm^{-3} . This error is approximately constant (independent of density and temperature below these critical values), having been caused by the uncertainty in the value of the electronic dipole moment $D_{ba}(R)$. At 8000° K, the higher electronic states that are not included in this calculation contribute an estimated 10 per cent additional absorption of unknown wavelength dependence, and this amount increases with increasing temperature. At the critical density an estimated 10 per cent of the photon absorptions take place while a third atom is within molecular dimensions (less than 5 atomic units). While this does not add to the absorption, the perturbations of the third body at higher densities will affect the wavelength dependence in an undetermined way.

III. IMPORTANCE OF QUASI-MOLECULAR HYDROGEN ABSORPTION IN STELLAR ATMOSPHERES

To determine which types of stars, if any, provide conditions favorable to the continuous absorption coefficient of quasi-molecular hydrogen, we make a preliminary reconnaissance using Aller's (1963) values of mean gas pressure as a function of surface temperature and gravity. This absorption increases strongly with increasing temperature and pressure, but subject to the restriction that the hydrogen remains un-ionized. The strong pressure dependence suggests that we look at dwarf stars (main sequence) rather than giants. Assuming a solar composition of 80 per cent hydrogen (by number), we

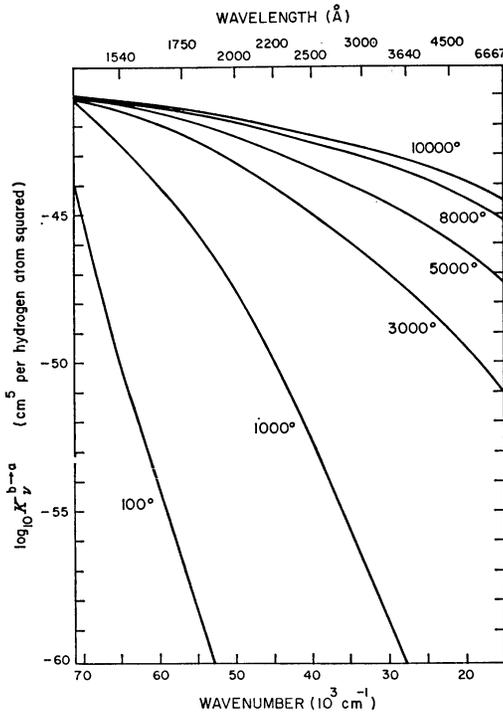


FIG 2

FIG. 2.—Absorption coefficient of the hydrogen quasi-molecule per $n(\text{H})^2$, summed in detail over rotational states (eqs. [1] and [4]).

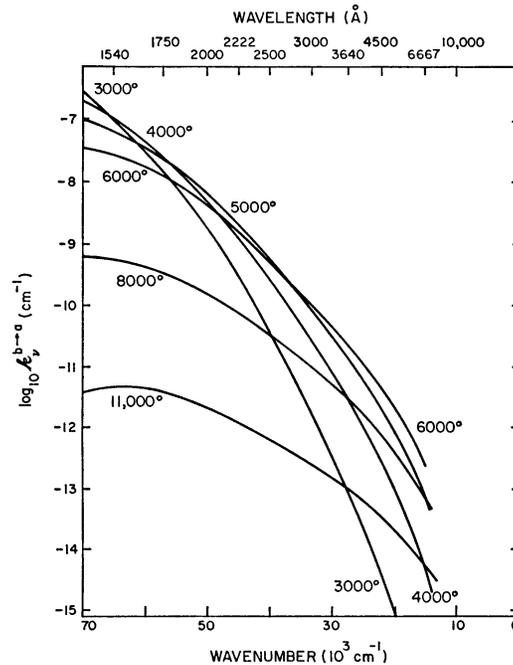


FIG 3

FIG. 3.—Logarithm of the continuous absorption coefficient of quasi-molecular hydrogen at the surface of main-sequence stars with assumed solar compositions, with temperature as a parameter.

compute the quasi-molecular absorption at various wavelengths with temperature along the main sequence as a parameter. The values of the mean gas pressure, or surface gravity, along the main sequence are also from Aller. The results, shown in Figure 3, indicate that quasi-molecular hydrogen absorption is at its greatest strength along the main sequence for stars with surface temperatures between 4000° and 6000° K. Here the absorption is at its greatest absolute strength. For a determination of the relative contribution of the hydrogen quasi-molecule to the total opacity, a detailed comparison should be made with the temperature, pressure, and wavelength dependence of other sources of absorption.

As a first estimate, we can make use of the fact that the variation with temperature along the main sequence of the Rosseland mean absorption coefficient (Böhm-Vitense 1951) for the above mean surface conditions is less than an order of magnitude ($3 \times$

TABLE 1
CONTINUOUS ABSORPTION COEFFICIENT OF THE HYDROGEN QUASI-MOLECULE (in cm^5)^{*}

$\lambda(\text{\AA})$	2500°K	3000°K	4000°K	5000°K	6000°K	8000°K	10000°K
1540	2.60×10^{-42}	3.44×10^{-42}	4.75×10^{-42}	5.63×10^{-42}	6.16×10^{-42}	6.50×10^{-42}	6.49×10^{-42}
1750	3.27×10^{-43}	6.23×10^{-43}	1.388×10^{-42}	2.21×10^{-42}	2.95×10^{-42}	4.05×10^{-42}	4.69×10^{-42}
2000	2.06×10^{-44}	5.93×10^{-44}	2.22×10^{-43}	4.90×10^{-43}	8.19×10^{-43}	1.510×10^{-42}	2.08×10^{-42}
2222	2.25×10^{-45}	9.10×10^{-45}	5.23×10^{-44}	1.490×10^{-43}	2.96×10^{-43}	6.77×10^{-43}	1.066×10^{-42}
2500	1.882×10^{-46}	1.128×10^{-45}	1.055×10^{-44}	4.02×10^{-44}	9.69×10^{-44}	2.83×10^{-43}	5.18×10^{-43}
3000	5.06×10^{-48}	5.50×10^{-47}	1.070×10^{-45}	6.30×10^{-45}	2.04×10^{-44}	8.60×10^{-44}	1.970×10^{-43}
3640	1.500×10^{-49}	2.89×10^{-48}	1.154×10^{-46}	1.041×10^{-45}	4.45×10^{-45}	2.66×10^{-44}	7.52×10^{-44}
4500	3.99×10^{-51}	1.330×10^{-49}	1.061×10^{-47}	1.470×10^{-46}	8.40×10^{-46}	7.24×10^{-45}	2.55×10^{-45}
6667	1.380×10^{-53}	9.79×10^{-52}	2.10×10^{-49}	5.40×10^{-48}	4.71×10^{-47}	7.00×10^{-46}	3.42×10^{-45}

* To get the absorption cross section per H atom, multiply by $n(\text{H})$; to get $\kappa_{\nu}^{b \rightarrow a}$ in cm^{-1} , multiply by $n(\text{H})^2$ (see eq. [4]).

$10^{-8} \text{ cm}^{-1} \lesssim \langle k_\nu \rangle$ [Rosseland] $\lesssim 10^{-7} \text{ cm}^{-1}$). However, as can be seen from Figure 3, quasi-molecular hydrogen absorption at a particular wavelength passes through a maximum as a function of temperature along the main sequence. This occurs for long wavelengths (6667 Å) at about 6000° K and for short wavelengths (1750 Å) at about 4000° K. At higher and lower temperatures, the quasi-molecular absorption decreases by several orders of magnitude. The decrease is caused primarily by the intrinsic decrease in the absorption per quasi-molecule with decreasing temperature and by the decrease in mean gas pressure with increasing temperature. In addition, the reduction of neutral atomic hydrogen below about 3000° K by molecular association and above about 10000° K by ionization reduces the number of quasi-molecules and hence the total quasi-molecular absorption, an effect that has not been included in Figure 3 but only serves to strengthen the above discussion.

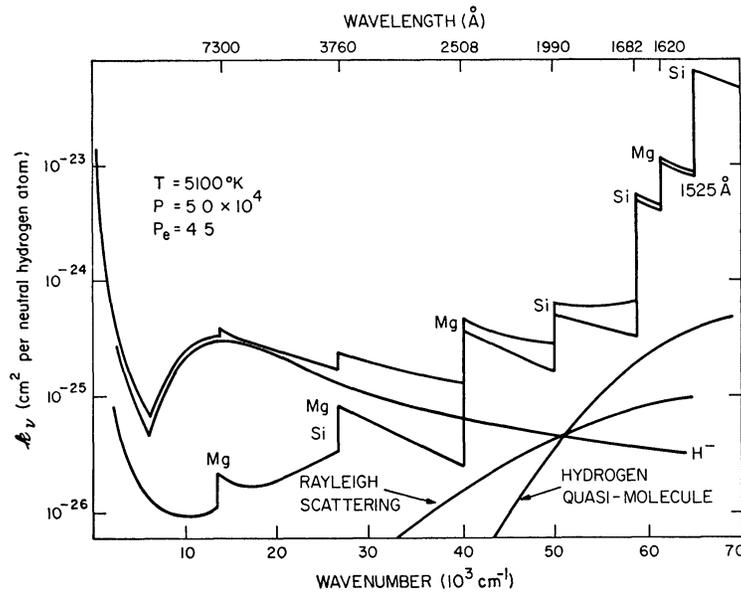


FIG. 4—Known sources of absorption at optical depth $\tau_{5000} \simeq 0.1$ in a solar model. Top line shows the total opacity.

This rough analysis therefore indicates that quasi-molecular hydrogen absorption is at its greatest strength relative to the total opacity (as well as at its greatest absolute strength) for main-sequence stars with temperatures between about 4000° and 6000° K. Since the Sun is included in this range, we investigate in § IV the hydrogen quasi-molecule as a source of continuous absorption in the ultraviolet spectrum of the solar atmosphere. We shall see in retrospect that the wavelength variation of the total opacity, neglected in the rough analysis, is also considerably smaller than the strong variation of the quasi-molecular absorption, the former amounting to about 2 orders of magnitude between 1500 and 10000 Å, as can be seen in Figure 4.

IV. IMPORTANCE OF QUASI-MOLECULAR HYDROGEN ABSORPTION IN THE SOLAR ATMOSPHERE

In order to have an observable effect on the solar spectrum, the absorption of quasi-molecular hydrogen must be an important fraction of the total opacity at a given wavelength λ for the physical conditions that prevail at the height in the atmosphere where the continuum is being formed, that is, where $\tau_\lambda \simeq 1$. Because of the rapid increase in

the quasi-molecular hydrogen absorption with decreasing wavelength, we expect that this is most likely to occur in the ultraviolet, provided that other known sources of opacity do not increase even more rapidly.

Gingerich (1964) and Gingerich and Rich (1968) have published graphs illustrating the sources of opacity for physical conditions at certain optical depths in various stellar models. We adapt one of these graphs for a solar model at optical depth $\tau_{5000} \simeq 0.1$, which is the approximate physical height of $\tau_{2000} \simeq 1$, to illustrate the detailed comparison of the quasi-molecular hydrogen absorption with the other sources of absorption at all wavelengths (Fig. 4). We see that the quasi-molecular absorption rises relative to the other sources with decreasing wavelength, varying from 10 per cent of the total opacity at about 2000 Å to about one-third of the total on the red side of the Si(¹D)

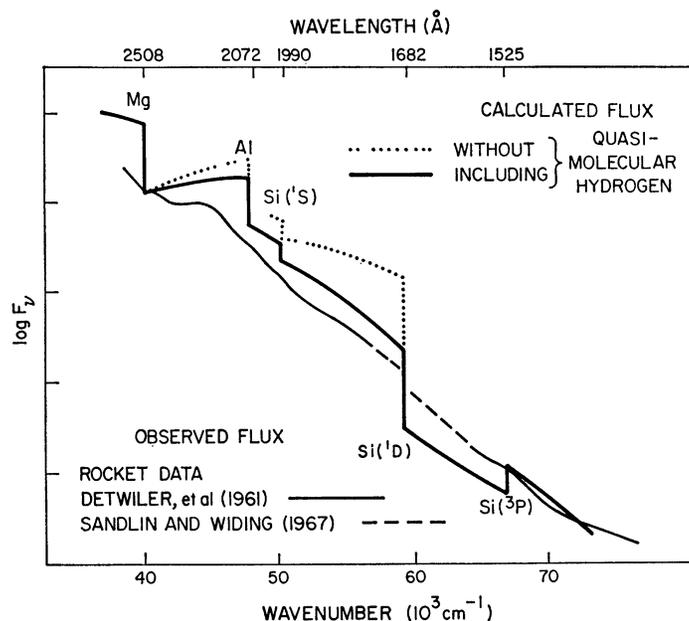


FIG. 5.—Observed and calculated fluxes in the solar ultraviolet spectrum, with and without the absorption of the hydrogen quasi-molecule. The sharp edges are idealizations.

ionization edge at 1682 Å. Below 1682 Å, it is a small fraction of the total. We note that below 2000 Å it exceeds the Rayleigh scattering and is thus the most important continuous absorber after the metallic ionization continua.

To establish whether this additional absorption could have an observable effect on the predicted solar spectrum, O. Gingerich and D. Carbon of the Smithsonian Astrophysical Observatory prepared a polynomial fit to the wavelength and temperature dependence of the quasi-molecular hydrogen absorption. They computed ultraviolet fluxes for the Utrecht reference model of Heintze, Hubenet, and de Jager (1964) with and without the quasi-molecular hydrogen absorption, using the program described by Gingerich (1963). The results are compared with the rocket ultraviolet observations of Detwiler *et al.* (1961; see p. 263) in Figure 5. The sharp discontinuities are caused by the idealized metallic photo-ionization edges. As can be seen, the inclusion of quasi-molecular hydrogen makes a significant improvement in the agreement between observed and theoretical fluxes in the spectral region between 2000 Å and the silicon edge at 1682 Å.

In particular, it reduces the predicted discontinuity at the Si(¹D) edge by about an

order of magnitude. Although this discontinuity is not apparent in the rocket data of Detwiler *et al.* (1961), which have been averaged over 50 Å intervals, it can be seen clearly in the tracing of the 1962 rocket spectrum obtained by Garrett, Purcell, and Tousey (unpublished) and reproduced by Porter, Tilford, and Widing (1967). Sandlin and Widing (1967) have estimated the observed radiation temperatures in this spectral region as 4700° K in the wavelength interval 1760–1700 Å, dropping to a minimum temperature of 4635° K at 1684–1666 Å, and with a rising tendency toward shorter wavelengths, averaging 4650° K, in the interval 1680–1550 Å. The temperature difference across the Si(¹D) edge (65° K) corresponds to a flux difference at 1682 Å of 30 per cent. From these temperatures we deduce the curve shown in Figure 5 for the rocket data in the 1750–1600 Å interval. Additional continuous absorption (not shown in Fig. 5) from blanketing by the stronger lines of silicon, iron, and carbon monoxide (cf. Goldberg, Parkinson, and Reeves 1965; Porter *et al.* 1967) may be able to reduce the remaining discrepancy by half an order of magnitude (Gingerich and Rich 1968). This would make the predicted discontinuity about a factor of 2 in the flux compared with the observed factor of 1.3.

As has been noted by several authors, the solar spectrum changes from a limb-darkened Fraunhofer spectrum to a limb-brightened emission spectrum in the spectral interval between about 1892 Å (the location of the longest-wavelength emission feature; Pottasch 1964) and the photo-ionization continuum of ground-state silicon beginning at 1525 Å. Somewhere in this spectral region the continuum may be formed in the neighborhood of the temperature minimum between the photosphere and the low chromosphere (for a review of this problem see Goldberg 1967). The absorption of the hydrogen quasi-molecule clearly plays a role in shaping the appearance of the solar spectrum in this region.

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