

ON NON-LTE H_2^+ AS MISSING SOLAR OPACITY

S. P. TARAFDAR*

Department of Applied Mathematics and Astronomy, University College, Cardiff, U.K.

AND

M. S. VARDYA

Tata Institute of Fundamental Research, Bombay, India

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ABSTRACT

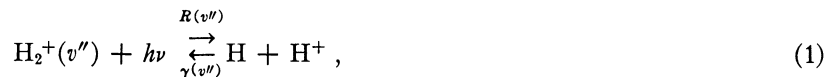
A careful examination has revealed that use of incomplete reaction processes and incorrect rates has lead Krishna Swamy and Stecher to overestimate the H_2^+ opacity by a factor of 10^4 at $\lambda = 2000$ Å. H_2^+ is not a significant source of opacity in the solar atmosphere.

Subject headings: atmospheres, solar — molecules — opacities

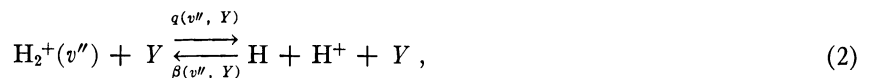
A large discrepancy exists between the observed fluxes and those predicted by the models in the solar ultraviolet (cf. Gingerich *et al.* 1971), which has been attributed to unknown source(s) of opacity. Tarafdar and Vardya (1972*a, b*) found that band absorption by abundant molecules of CO, SiO, OH, and CH may be large enough to account for the missing opacity in the solar ultraviolet spectrum, except in a small interval between 2500 and 3000 Å.

In a recent *Letter*, Krishna Swamy and Stecher (1974) have, however, suggested that the absorption from vibrational levels of H_2^+ having a non-LTE distribution can account for the missing opacity. This is indeed very surprising, as the equilibrium abundance of H_2^+ in the solar photosphere is very small. Therefore, to be significant as a source of opacity, its population has to be highly enhanced by some non-LTE mechanism. As the number density in the photosphere is rather large ($\sim 10^{16}$ cm $^{-3}$), deviations from LTE are unlikely to be very large. This has led us to examine carefully the paper by Krishna Swamy and Stecher (1974) to trace the cause of this inconsistency.

In the steady state, we find by considering the reactions



and



where Y may be hydrogen atom, proton, or electron, that the density $N(v'')$ of H_2^+ in vibrational state v'' is given by

$$N(v'') = \frac{N(\text{H})N(\text{H}^+)[\gamma(v'') + N(\text{H})\beta(v'', \text{H}) + N(\text{H}^+)\beta(v'', \text{H}^+) + N(e)\beta(v'', e)]}{R(v'') + q(v'', \text{H})N(\text{H}) + q(v'', \text{H}^+)N(\text{H}^+) + q(v'', e)N(e)}; \quad (3)$$

in equations (1)–(3), $N(Y)$ is the density of species Y , $R(v'')$ the photodissociation rate in s^{-1} for vibrational level v'' , $\gamma(v'')$ the rate of radiative association for level v'' , $q(v'', Y)$ the collisional dissociation rate of level v'' with species Y , and $\beta(v'', Y)$ is the three-body recombination rate for level v'' in the presence of species Y . Note that equation (3) is the same as the equation (2) of Krishna Swamy and Stecher (1974), except that they did not include the three-body recombination in the presence of a proton or an electron. The inclusion of these reactions is for the sake of completeness and probably has no effect on the result, as the densities of protons and electrons are five and four orders of magnitude smaller than of hydrogen at $\tau_{0.5\mu} = 0.07$. From the principle of detailed balance (cf. Rice 1967; Weston and Schwarz 1972; Solomon and Klemperer 1972)

$$\frac{\gamma(v'')}{R_p(v'')} = \frac{\beta(v'', \text{H})}{q(v'', \text{H})} = \frac{\beta(v'', \text{H}^+)}{q(v'', \text{H}^+)} = \frac{\beta(v'', e)}{q(v'', e)} = \left[\frac{N(v'')}{N(\text{H})N(\text{H}^+)} \right]_{\text{eq}} = \frac{kT}{K(T, v'')}, \quad (4)$$

where $R_p(v'')$ is the photodissociation rate of level v'' in the presence of a radiation field represented by the Planck distribution with temperature T , the kinetic temperature,

$$K(T, v'') = K(T) \exp(+E_{v''}/kT)Q, \quad (5)$$

* On leave from the Tata Institute of Fundamental Research, Bombay 400 005, India.

$K(T)$ is the equilibrium constant of H_2^+ given by (Vardya 1961)

$$\log K(T) = +11.207 - 2.7943 \theta - 0.079197 \theta^2 + 0.024791 \theta^3, \quad (6)$$

$E_{v''}$, the vibrational energy of level v'' , and Q the vibrational partition function. With the help of equation (4), equation (3) can be written as

$$\frac{N(v'')}{N(\text{H})N(\text{H}^+)} = \left[\frac{\gamma(v'')}{X} + \frac{kT}{K(T, v'')} \right] / \left[\frac{R(v'')}{X} + 1 \right], \quad (7)$$

$$= \frac{kT}{K(T, v'')} \frac{1}{\alpha + 1}, \quad (8)$$

where

$$X = N(\text{H})q(v'', \text{H}) + N(\text{H}^+)q(v'', \text{H}^+) + N(e)q(v'', e), \quad (9)$$

and

$$\alpha = \frac{R(v'') - R_p(v'')}{R_p(v'') + X}. \quad (10)$$

Note that Krishna Swamy and Stecher (1974) have not used relation (4), especially for $q(v'', \text{H})$ and $\beta(v'', \text{H})$. They have determined $q(v'', \text{H})$ from the extrapolated cross section of Peek (1965) and used a value $2.5 \times 10^{-33} \text{ cm}^6 \text{ s}^{-1}$ for $\beta(v'', \text{H})$. The extrapolation necessary is rather large; Peek (1965) uses the Born approximation and gives cross sections for energy greater than 1 keV for the $\text{H}_2^+ + \text{H}$ collision; the average thermal energy at $T = 5040 \text{ K}$ is about 0.5 eV.

Equation (8) with (4) shows that the population of H_2^+ is in LTE if $|\alpha| \ll 1$, and non-LTE if $|\alpha| \geq 1$. No attempt has been made here to determine α , as the necessary collisional cross sections are not available at the relevant energies, and extrapolation may not be advisable. The H_2^+ opacity determined using the equilibrium values of $N(v'')$ (eq. [8] with $\alpha = 0$) and the cross sections given by Dunn (1968) has been compared with the other opacities including the H_2^+ non-LTE opacities as given by Krishna Swamy and Stecher (1974) in Figures 1 and 2 for optical depths, $\tau_{0.5\mu} =$

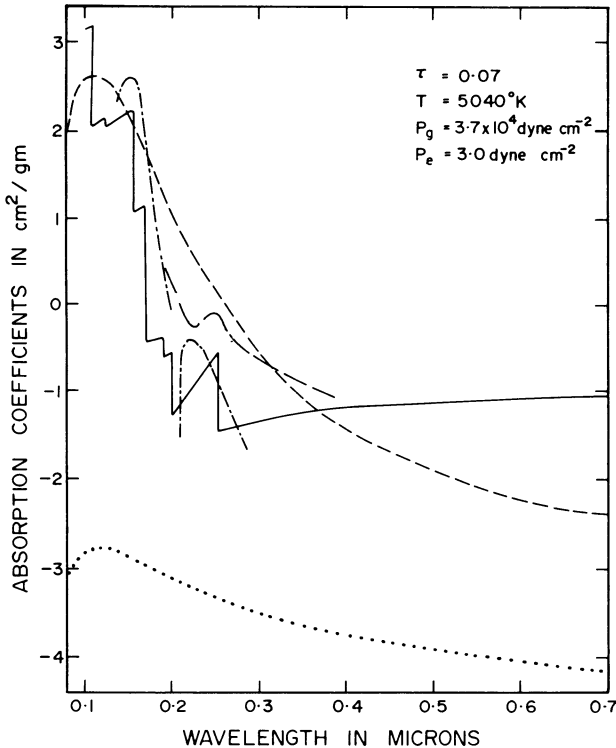


FIG. 1.—The variation of absorption coefficients with wavelength at $\tau_{0.5\mu} = 0.07$. The combined hydrogen and metal opacity is represented by a continuous line, the molecular opacities by dashed-dotted line, the empirically determined opacity by long-dashed line, the non-LTE opacity of H_2^+ by dashed line, and the LTE opacity of H_2^+ by dotted line.

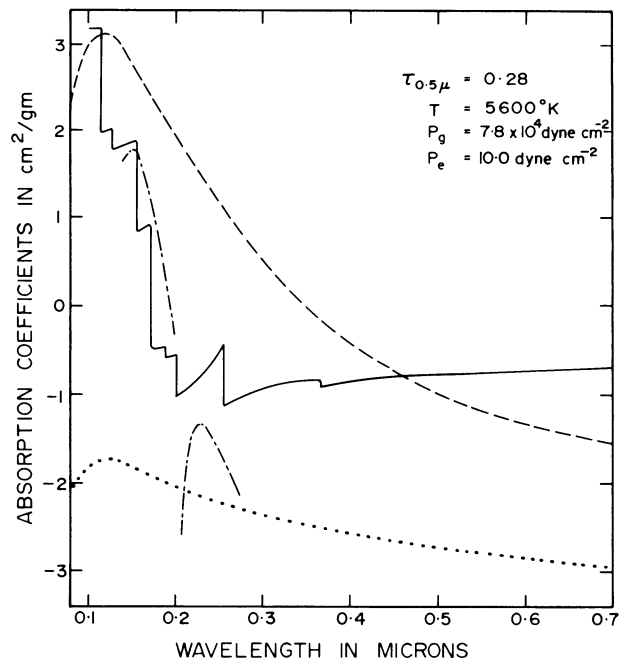


FIG. 2.—Same as in Fig. 1 except for $\tau_{0.5\mu} = 0.28$

0.07 and 0.28, respectively. The figures show that the LTE opacity of H_2^+ is not only smaller than the molecular opacities (Tarafdar and Vardya 1972*a, b*) but also smaller than the combined hydrogen and metal opacity. The non-LTE opacity of H_2^+ is larger than the corresponding LTE opacity by a factor of about 10^5 at 1200 Å and about 100 at 4000 Å. This implies that the non-LTE abundance of H_2^+ is more than its LTE value by a factor of 10^5 for $\nu'' = 0$ and this enhancement decreases as ν'' increases, as the photodissociation cross sections (Dunn 1968) used are the same. From equations (8) and (10), the maximum enhancement of $N(\nu'')$ occurs when $X = 0$ and by a factor $R_p(\nu'')/R(\nu'')$. Table 1 gives the solar emergent photon emittance as well as the ratio of the Planckian intensity to the solar emergent intensity at two temperatures, 5040 K and 5600 K, for several wavelengths. The solar emergent intensities are the theoretical values of Gingerich *et al.* (1971) except for $1683^+ \leq \lambda \leq 4000$ Å, where the theoretical intensity does not agree with the observed intensity; in this wavelength interval, observed values (Labs and Neckel 1968; Houtgast 1968; Bonnet 1968; Parkinson and Reeves 1969) have been used. The table shows that the emergent intensity is larger than the Planckian intensity at $\tau_{0.5\mu} = 0.07$ except for $1198^+ < \lambda < 2000$ Å, where the emergent intensity is at most 20 times less than the Planckian intensity. Therefore, the non-LTE abundance of H_2^+ at $\tau_{0.5\mu} = 0.07$ cannot be more than 20 times the LTE abundance. This is the case for $\nu'' \leq 2$, as photodissociations from these levels are mainly by the radiation in $\lambda < 2000$ Å. For $\nu'' > 2$ ($\lambda > 2000$ Å), the non-LTE abundance is close to the LTE abundance. The non-LTE abundance at $\tau_{0.5\mu} = 0.28$ is similar except that the maximum enhancement is by a factor 100. These enhancement factors over LTE values will decrease if $R(\nu'')$ is computed by using the actual density of radiation, which should be closer to the Planckian density than to the solar emergent density. Therefore, an increase of H_2^+ density from its LTE value by a factor of 10^5 , as found by Krishna Swamy and Stecher (1974), is not at all possible in the solar atmosphere, even if one neglects the collisional processes, which, however, are not negligible. Krishna Swamy and Stecher (1974) find that the photodissociation, electron collision, and three-body recombination are the most important mechanisms. If this is the case, a careful examination of equation (7) shows that the non-LTE density of H_2^+ is less than or equal to the LTE value, provided both forward and backward reactions are considered correctly (i.e., using relation [4]). Note that their conclusion depends, according to relation (4), on the incompatible extrapolated cross sections used for collisional dissociation. The rate of three-body recombination in the presence of hydrogen may be even larger than $2.5 \times 10^{-33} \text{ cm}^6 \text{ s}^{-1}$, the value used by Krishna Swamy and Stecher (1974), as not only $\text{He}^+ + \text{He} + \text{He} \rightarrow \text{He}_2^+ + \text{He}$ has a rate of about $6 \times 10^{-32} \text{ cm}^6 \text{ s}^{-1}$ (Phelps and Brown 1952) but also $\text{H} + \text{H} \rightarrow \text{H}_2 + \text{H}$ has a rate of 10^{-32} at $T \approx 5000$ K (cf. Lambert and Pagel 1968). If we assume a value of $10^{-33} \text{ cm}^6 \text{ s}^{-1}$ for $\beta(\text{O}, \text{H})$, then equation (4) with (5) and (6) gives $q(\text{O}, \text{H}) \approx 10^{-12} \text{ cm}^3 \text{ s}^{-1}$ at $T \approx 5000$ K. The density of hydrogen at $\tau_{0.5\mu} = 0.07$ and 0.28 is about 10^{+16} , which gives $q(\text{O}, \text{H})N_{\text{H}} \approx 10^4 \text{ s}^{-1}$. This is much larger than the photodissociation rate of about 0.5 s^{-1} obtained by using the emergent intensity and the cross section given by Dunn (1968). Note that the collisional process dominates, even if we increase the radiation field by a factor 100. The values of $\gamma(0)$ are about 10^{-20} s^{-1} and $5 \times 10^{-20} \text{ s}^{-1}$ from equations (4), (5), and (6) with $R_p(0) \approx 20R(0)$ and $100R(0)$ for $\tau_{0.5\mu} = 0.07$ and 0.28, respectively. These values of $\gamma(0)$ are also smaller than the value of $N(\text{H})\beta(\text{O}, \text{H})$ by three orders of magnitude. Equation (7) with (9) then shows that the density of H_2^+ in the solar photosphere at $\tau_{0.5\mu} = 0.07$ and 0.28 cannot be much different from that obtained from LTE consideration. Note that the inclusion of reaction

TABLE 1
PHOTON EMITTANCE (in $\text{cm}^{-3} \text{ s}^{-1} \text{ sr}^{-1}$)
[$a+n$ implies $a \times 10^n$]

$\lambda(\text{Å})$	EMERGENT PHOTON EMITTANCE	RATIO OF PLANCKIAN INTENSITY TO EMERGENT INTENSITY AT	
		5040 K	5600 K
912—	2.1+20	1.0—3	2.3—2
912+	5.7+18	3.9—2	9.0—1
1100—	3.0+20	7.2—2	9.7—1
1100+	3.8+19	5.8—1	7.9+0
1197+	1.2+20	1.1+0	1.2+1
1239—	2.1+20	2.1+0	5.8+0
1239+	1.5+19	1.7+1	1.7+2
1443+	3.2+20	1.1+1	7.9+1
1527+	3.5+20	2.0+1	1.6+2
1683+	2.2+21	1.4+1	7.9+1
1700+	3.2+21	1.2+1	6.2+1
1800	1.6+22	4.6+0	2.2+1
2077—	3.5+23	9.8—1	3.9+0
2077+	1.5+24	2.3—1	9.0—1
2300	3.0+24	2.9—1	1.0+0
2665	9.1+24	2.9—1	8.5—1
3400	4.9+25	2.1—1	4.8—1
5000	1.0+26	3.1—1	5.5—1
7000	8.8+25	4.8—1	7.2—1

$\text{H}_2^+ + e \rightleftharpoons \text{H} + \text{H}$ and collisional excitation will not give any non-LTE effect. The opacity due to H_2^+ , as shown in Figures 1 and 2, is much smaller than other opacities, including the non-LTE H_2^+ opacity proposed by Krishna Swamy and Stecher (1974). The overestimate of H_2^+ opacity by from two to four orders of magnitude between 2000 to 4000 Å by Krishna Swamy and Stecher (1974) is due to their incomplete and incorrect use of the reaction processes and their rates.

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S. P. TARAFDAR: Department of Applied Mathematics and Astronomy, University College, P.O. Box 78, Cardiff CF1 1XL, U.K.

M. S. VARDYA: Tata Institute of Fundamental Research, Bombay 400 005, India