

# H<sub>2</sub><sup>+</sup> pickup ions in the solar wind: Outgassing of interplanetary dust

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**Abstract.** Heliospheric neutral atoms and molecules can be ionized and picked up by the solar wind plasma flow. A new generation of space plasma instruments allows detailed study of the solar wind pickup ions with high sensitivity. Detection of H<sub>2</sub><sup>+</sup> pickup ions in the solar wind is an exceptionally sensitive tool for the search of molecular hydrogen in the heliosphere. Possible sources of neutral molecular hydrogen include contributions from the local interstellar medium, release from cometary bodies, and outgassing of interplanetary dust. The flux of the solar wind H<sub>2</sub><sup>+</sup> pickup ions due to outgassing of interplanetary dust is theoretically established in this work. Solar wind ions bombard and penetrate dust grains where they are neutralized and subsequently released in the form of neutral atoms and molecules. The processes of molecular hydrogen interaction with the solar radiation and solar wind plasma are considered in detail and the process rates are determined. Solar wind H<sub>2</sub><sup>+</sup> pickup ion fluxes are obtained for heliocentric distances < 5 AU for different heliocentric latitudes. These heliocentric radial and latitudinal dependences would provide guidance for search of the solar wind H<sub>2</sub><sup>+</sup> pickup ions by Ulysses, WIND, and SOHO missions.

## 1. Introduction

Singly charged ions of nonsolar origin that are found in the solar wind are usually assumed to be pickup ions [Holzer and Axford, 1970; Vasyliunas and Siscoe, 1976] produced by ionization of neutrals (photoionization, charge exchange, and electron impact) in interplanetary space. Pickup ions are a distinct ion population in the solar wind with approximately a spherical shell velocity distribution function superimposed on the solar wind bulk velocity. Evolution of this velocity distribution function as the solar wind expands is a complicated phenomenon [e.g., Isenberg, 1986] with the direct experimental data being scarce.

Most of the pickup ions are believed to be interstellar atoms that penetrate the solar system, where they are ionized and picked up by the solar wind plasma flow. The study of pickup ions is thus important for understanding the formation of the anomalous component of cosmic rays [Fisk et al., 1974], processes in the heliospheric interface, interstellar gas (ISG) flow into the solar system, and properties of the expanding solar wind in the outer heliosphere. Helium pickup ions have been studied in some detail [e.g., Moebius et al., 1985, 1995; Moebius, 1990]. Pickup protons and heavy pickup ions (nitrogen, oxygen, neon) were measured only recently [Gloeckler et al., 1993; Geiss et al., 1994] by a new generation of highly sensitive space plasma instruments, such as the solar wind ion composition instrument (SWICS) [Gloeckler et al., 1992] on Ulysses. In addition, these new instruments have made possible accurate measurement of the solar wind ion velocity distribution function across a wide velocity range [Gloeckler et al., 1994, 1995a].

New instrumental capabilities of SWICS [Gloeckler et al., 1992, 1993] on Ulysses, CELIAS (the charge, element, and isotope analysis system) [Hovestadt et al., 1995] on SOHO, and

STICS (the suprathermal ion composition studies instrument) [Gloeckler et al., 1995b] on WIND open the way for the search for molecular hydrogen in the heliosphere. Hydrogen molecules H<sub>2</sub>, if present in the heliosphere, would be ionized, and the hydrogen molecule ions H<sub>2</sub><sup>+</sup> would be picked up by the solar wind flow. As the solar wind propagates from the Sun, the pickup ions accumulate in the solar wind plasma. Even a small presence of neutral molecular hydrogen in interplanetary space may manifest itself by detectable fluxes of H<sub>2</sub><sup>+</sup> pickup ions. Thus pickup ion measurements provide an exceptionally sensitive tool for the search for molecular hydrogen in the heliosphere.

Possible sources of heliospheric molecular hydrogen include outgassing of interplanetary dust, neutral penetration from the local interstellar medium (LISM) surrounding the Sun, and release from cometary bodies. The heliosphere is filled with a permanent population of interplanetary zodiacal dust, which tends to congregate toward the Sun [Banks, 1971; Holzer, 1977; Leinert et al., 1978; Fahr et al., 1981, 1995; Leinert and Grün, 1990; Banaszkiewicz et al., 1994]. Solar wind ions bombard and penetrate dust grains, where they are neutralized and subsequently released as neutral atoms and molecules. Estimates of this neutral particle source suffer from a large uncertainty in the dust grain population and outgassing process details [Banks, 1971; Holzer, 1977; Fahr et al., 1981]. Fahr et al. [1981] were the first to suggest that most of the hydrogen is desorbed in molecular form. Ionization of this molecular hydrogen is a source of the solar wind H<sub>2</sub><sup>+</sup> pickup ions.

Neutral penetration from the LISM is another source of molecular hydrogen in the heliosphere [e.g., Gruntman, 1993]. The LISM is not in full equilibrium, the physics of the LISM is poorly understood [e.g., Frisch, 1990], and some interstellar hydrogen may be present in molecular form. Direct experimental data on H<sub>2</sub> are unavailable for the LISM. There is no observational evidence that molecular hydrogen is present in the LISM, and there are no observational limitations that would preclude presence of some hydrogen in molecular form.

Comets may also serve as a source of molecules in the

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Paper number 96JA01130.  
0148-0227/96/96JA-01130\$09.00

heliosphere. Fowler *et al.* [1979] suggested that comets provided molecular material for the anomalous component of cosmic rays. Recent search for such molecules in the Solar, Anomalous, Magnetospheric Particle Explorer (SAMPEX) data established the upper limit on the possible concentration of  $\text{CO}^+$  molecular ions in anomalous cosmic rays [Looper *et al.*, 1995].

Measurements of  $\text{H}_2^+$  pickup ions in the solar wind will allow us to experimentally test interplanetary dust concepts, understanding of the solar wind interaction with dust grains (bombardment, outgassing), zodiacal dust population in the Sun's vicinity, and material release from and populations of comets in the inner heliosphere, as well as to conduct a search for molecular hydrogen in the LISM. The interest to physical conditions in the Sun's vicinity, including zodiacal dust characteristics and details of dust outgassing, is supported by the anticipated near-Sun flyby mission, which has finally reached the phase of practical implementation (NASA has issued a Research Announcement for instrumentation development, NRA 95-OSS-15, 1995). The Ulysses, WIND, and SOHO missions present exceptionally favorable platforms for search of the solar wind  $\text{H}_2^+$  pickup ions both in and out of the ecliptic plane and at different heliocentric longitudes. Latitudinal and longitudinal dependences of  $\text{H}_2^+$  pickup ion fluxes will allow one to separate contributions from possible interplanetary and interstellar sources of molecular hydrogen.

Hydrogen molecules, both neutrals and ions, interact with the solar radiation and the solar wind plasma. Accurate knowledge of the relevant process rates is indispensable in order to theoretically establish expected abundances of  $\text{H}_2^+$  pickup ions. While many processes of neutral  $\text{H}_2$  interaction with the solar radiation are well understood and the corresponding reaction rates are used in planetary studies [e.g., Shemansky and Hall, 1992], the rates of  $\text{H}_2$  interaction with the solar wind ions and electrons have never been considered in detail. Molecular hydrogen ions,  $\text{H}_2^+$ , usually quickly collide and react with other molecules in planetary atmospheres, and many processes of  $\text{H}_2^+$  ion direct interaction with the solar radiation and with the solar wind plasma have never been discussed. The processes of molecular hydrogen interaction with the solar radiation and solar wind plasma are considered in detail in this work.

The goal of this paper is to theoretically establish the solar wind  $\text{H}_2^+$  pickup ion fluxes due to outgassing of interplanetary dust. A possible contribution of interstellar molecular hydrogen is only briefly discussed; detailed consideration of interstellar hydrogen as well as cometary material release is beyond the scope of this paper. We concentrate first on neutral molecular hydrogen distribution in the inner heliosphere and production of  $\text{H}_2^+$  ions. Then we calculate the survival probabilities for  $\text{H}_2^+$  ions as they are carried by the solar wind. Finally, expected fluxes of the solar

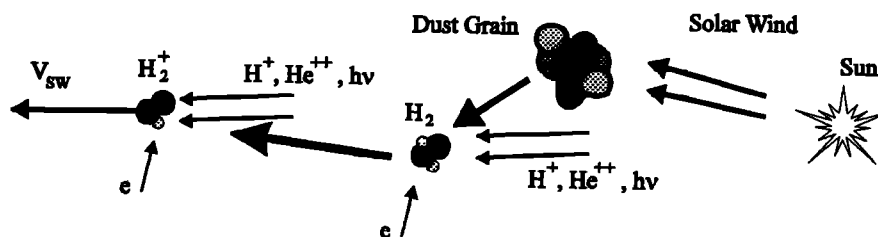
wind  $\text{H}_2^+$  pickup ions are presented for heliocentric distances  $R < 5$  AU.

## 2. Dust-Generated Neutral Molecular Hydrogen in the Inner Heliosphere

Zodiacal dust number density is highest in the ecliptic plane and decreases with increasing the heliocentric latitude [Banks, 1971; Holzer, 1977; Leinert *et al.*, 1978; Fahr *et al.*, 1981, 1995; Leinert and Grun, 1990; Banaszkiewicz *et al.*, 1994]. Interplanetary dust grains are bombarded by solar wind ions with energies of 1–2 keV/nucleon. The ions penetrate down to 100 atomic layers into grains before finally coming to rest. The dust grain surface layer ( $< 500$  Å) is quickly saturated by the bombarding solar wind ions (protons and alpha particles), leading to subsequent desorption of neutral particles, atoms and molecules, from the grain surface (Figure 1). The desorbing flux is usually assumed to be equal to the flux of bombarding ions. The saturation time does not exceed a few years, which is much less than the Poynting-Robertson residence time of dust grains [e.g., Fahr *et al.*, 1981]. Therefore the solar wind plasma is effectively neutralized on interplanetary dust, and the estimates of this neutral particle source suffer from a large uncertainty in the dust grain population and details of the outgassing process [Banks, 1971; Holzer, 1977; Fahr *et al.*, 1981].

Banks [1971] first considered dust-produced neutrals in detail and calculated number densities of interplanetary hydrogen and helium due to dust outgassing. It can be shown that neutral atom number density is scaled by the interplanetary dust geometrical factor,  $\Gamma(R)$ , which is the inverse of the solar wind ion free path against interception by interplanetary dust grains;  $R$  is the distance from the Sun. The uncertainty of this factor, as discussed by Banks [1971], is 4 orders of magnitude,  $\Gamma(1 \text{ AU}) = 10^{-21}$ – $10^{-17} \text{ cm}^{-1}$ . Holzer [1977] favored the value  $\Gamma(1 \text{ AU}) = 2 \times 10^{-19} \text{ cm}^{-1}$ , which was later adopted also by Fahr *et al.* [1981].

While helium desorbs from grains in atomic form, the physics and chemistry of hydrogen desorption are poorly understood. Banks [1971] initially assumed that dust-emitted hydrogen is in atomic form. Later, Fahr *et al.* [1981] reconsidered hydrogen desorption and concluded that most hydrogen is desorbed in molecular form. (The experimentally established low erosion rate of lunar material [e.g., Leinert and Grun, 1990] justifies the assumption that hydrogen release from stony grains in the form of molecules carrying grain atoms, e.g.,  $\text{SiH}$ , can be neglected.) Single ionization of  $\text{H}_2$  molecules results in the solar wind  $\text{H}_2^+$  pickup ion flux (Figure 1). To the best of my knowledge, the number density of  $\text{H}_2^+$  ions in the heliosphere was mentioned only once in the past, by Fahr and Ripken [1985, Figure 2]. No sufficient details of how the number density was obtained and



**Figure 1.** Bombardment of interplanetary dust grains by the solar wind protons and alpha particles. The grain surface layer is quickly saturated by bombarding ions, leading to subsequent desorption of neutral particles, outgassing from dust. Neutral  $\text{H}_2$  molecules are ionized, and  $\text{H}_2^+$  ions are picked up by the solar wind plasma flow.

what model and rates used were given. The H<sub>2</sub><sup>+</sup> number density of *Fahr and Ripken* [1985] is 2–3 orders of magnitude higher than the number density obtained in this work. Such a discrepancy results from an apparent omission in the earlier work of the essential details of H<sub>2</sub><sup>+</sup> ion production and loss.

The spatial distribution of interplanetary dust can be described by various dependences [e.g., *Giese et al.*, 1985; *Leinert and Grün*, 1990; *Fahr et al.*, 1995]. *Fahr et al.* [1981] favored the distribution derived by *Leinert et al.* [1978] from the zodiacal light measurements on Helios. The dust number density distribution  $N_{\text{DUST}}(R, \chi)$  in the inner heliosphere can be fitted by the formula [*Fahr et al.*, 1981] allowing convenient separation of the radial and latitudinal dependences

$$N_{\text{DUST}}(R, \chi) = n_{\text{DUST}}(R) \times v_{\text{DUST}}(\chi) \\ = n_{\text{DUST}}(R_E) \times (R_E/R)^{1/3} \times \exp(-2.1 \sin \chi) \quad (1)$$

where  $n_{\text{DUST}}(R) = n_{\text{DUST}}(R_E) \times (R_E/R)^{1/3}$  is the heliocentric radial dependence of the dust number density,  $v_{\text{DUST}}(\chi) = \exp(-2.1 \sin \chi)$  is the latitudinal dependence,  $R$  and  $\chi$  are the heliocentric distance and heliocentric latitude, respectively; and  $n_{\text{DUST}}(R_E)$  is the dust number density at  $R_E = 1$  AU in the ecliptic plane ( $\chi = 0$ ). This simplification is possible only in the absence of inclinational drifts of dust particles by the plasma Poynting-Robertson effect [*Fahr et al.*, 1995]. The dust number density is an integral over the local distribution of the size of dust grains. The dust-generated pickup ion flux is calculated in the ecliptic plane first; the latitudinal variation of the pickup ion flux can then be easily obtained by scaling by a factor  $v_{\text{DUST}}(\chi)$ .

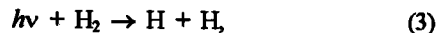
We will adopt the dust distribution (equation (1)) and the dust-generated H<sub>2</sub> source rate (in reciprocal seconds) of *Fahr et al.* [1981], which was obtained as a solution of the solar wind plasma expansion including interaction with interplanetary dust and interstellar gas. The heliocentric radial distribution of molecular hydrogen,  $n_{\text{H}_2}(R)$ , was not directly given by *Fahr et al.* [1981]. (Unfortunately, it is presently impossible (H.J. Fahr, private communication, 1995) to directly retrieve the original H<sub>2</sub> source rate, which was obtained in the past as an intermediate result.) However, this distribution can be derived from the given distribution,  $n_{\text{H}}(R)$ , of atomic hydrogen.

The distribution  $n_{\text{H}}(R)$  can be approximated [*Gruntman*, 1994]

$$n_{\text{H}}(R) = 4.13 \times 10^{-6} \times (R_E/R)^{1.15} \text{ cm}^{-3} \quad (2)$$

for  $0.023 \text{ AU} < R < 1 \text{ AU}$  in the ecliptic plane. The distribution  $n_{\text{H}_2}(R)$  can be obtained following the exact model and using exact rates of *Fahr et al.* [1981]. Then from  $n_{\text{H}_2}(R)$ , the source or production rate  $\rho(R)$  of neutral H<sub>2</sub> can finally be reconstructed.

Dust outgassing occurs predominantly through desorption of molecular hydrogen H<sub>2</sub>, as was argued by *Fahr et al.* [1981]. Molecular hydrogen is lost in two processes, photodissociation and photoionization. The photodissociation process,



is the only source of atomic hydrogen in the model of *Fahr et al.* [1981]; the symbol “ $h\nu$ ” stands for a photon. In equilibrium, production of hydrogen atoms is equal to their loss, i.e.,

$$n_{\text{H}_2} \times 2 \times \kappa_{\text{H}_2} = n_{\text{H}} \times \beta_{\text{H}} \quad (4)$$

where  $\beta_{\text{H}}$  is the atomic hydrogen loss rate and  $\kappa_{\text{H}_2}$  is the photodissociation rate (both in reciprocal seconds). Consequently,

$$n_{\text{H}_2} = n_{\text{H}} \times \beta_{\text{H}} / (2 \times \kappa_{\text{H}_2}) \quad (5)$$

Since hydrogen molecule loss is exactly compensated in equilibrium by molecule production, the neutral H<sub>2</sub> source rate,  $\rho_{\text{H}_2}$  (reciprocal cubic centimeters per second) is

$$\rho_{\text{H}_2} = n_{\text{H}_2} \times \beta_{\text{H}_2} = n_{\text{H}} \times \beta_{\text{H}} \times \beta_{\text{H}_2} / (2 \times \kappa_{\text{H}}) \quad (6)$$

where  $\beta_{\text{H}_2}$  is the total loss rate (reciprocal seconds) of molecular hydrogen.

The most important contribution to the atomic hydrogen loss rate  $\beta_{\text{H}}$  is by charge exchange with the solar wind protons [e.g., *Rucinski and Fahr*, 1991]. For the solar wind characteristics, as used by *Fahr et al.* [1981], this charge-exchange loss rate was  $3.6 \times 10^{-7} \text{ s}^{-1}$  at 1 AU, and the corresponding total loss rate of atomic hydrogen can be assumed to be  $\beta_{\text{H}}(R_E) = 5.4 \times 10^{-7} \text{ s}^{-1}$ . For  $\kappa_{\text{H}_2}(R_E) = 0.34 \times 10^{-7} \text{ s}^{-1}$  [*Fahr et al.*, 1981], one obtains  $n_{\text{H}_2} \approx 8.0 \times n_{\text{H}}$  from (5). Using  $\beta_{\text{H}_2}(R_E) = 6.64 \times 10^{-7} \text{ s}^{-1}$  [*Fahr et al.*, 1981], the neutral H<sub>2</sub> source rate in the ecliptic plane,  $\rho_{\text{H}_2}(R)$ , can then be established

$$\rho_{\text{H}_2}(R) = 2.2 \times 10^{-11} \times (R_E/R)^2 \times (R_E/R)^{1.15} \text{ cm}^{-3} \text{ s}^{-1} \quad (7)$$

The estimates above are valid for identical heliocentric radial dependences of various rates. This simplifying assumption may introduce uncertainty, which does not exceed 30%, in the neutral molecular hydrogen number density and source rate. The accurate calculations would require use of a detailed model [*Fahr et al.*, 1981].

No direct experimental data on dust-produced neutrals are available, and the uncertainty of their number density estimates remains high. Remote optical detection of dust-generated neutral particles is difficult because the light scattering region is very close (only 5°–10° offset angle) to the Sun. The experimental concept to optically measure such neutrals by registering emission in helium and atomic hydrogen resonance lines (584 and 1216 Å) was developed by *Fahr et al.* [1980] and *Fahr et Ripken* [1985].

Two sounding rocket (Skylark 12) launches were attempted in 1985 and 1989 from the Barreira do Inferno range in Natal, Brazil. The first launch failed on account of problems with the separation of the third rocket stage. Experimental data obtained during the second launch in 1989 were inconclusive because of a malfunctioning on-board computer and unexpectedly strong signal contamination by high-energy particles [*Lay et al.*, 1989, 1991]. The feasibility of a direct, in situ measurement of the dust-produced neutral particles on the planned near-Sun flyby mission (Solar Probe, or its latest downscaled version, Fire) is unclear because of spacecraft protective shield sputtering and ablation [*Gruntman*, 1993].

Neutral molecular hydrogen distribution in the heliosphere is determined by the production process and by loss due to interaction with the solar radiation and collisions with the solar wind ions and electrons. The loss occurs either by single ionization with the formation of a hydrogen molecule ion, H<sub>2</sub><sup>+</sup>, or by molecule dissociation, with or without fragment ionization. The single ionization process would contribute to the population of H<sub>2</sub><sup>+</sup> pickup ions in the solar wind. Interaction of H<sub>2</sub><sup>+</sup> ions with the solar radiation and the solar wind plasma would determine the probability for H<sub>2</sub><sup>+</sup> ions to reach an observer (the survival probability).

H<sub>2</sub> interaction with radiation and plasma is complicated by the existence of hydrogen molecules in vibrationally excited states of the ground electronic state. This essentially molecular feature makes consideration of the elementary processes (rates) substantially different from the treatment of heliospheric neutral atoms. Neutral atoms can be found in the ground state only, since

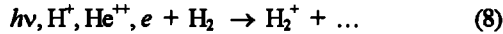
their metastable states are short-lived (e.g., the lifetime of the  $H(2S)$  metastable state is 0.12 s) as compared with characteristic times of other processes involved. The only exception seems to be two-step photoionization of hydrogen atoms in the Sun's vicinity, where the metastable state has to be taken into account [Gruntman, 1990; Ogawa *et al.*, 1995].

The lifetime of an  $H_2^+$  ion in a vibrationally excited state against spontaneous transitions is  $10^7$ – $10^8$  s [Bates and Poots, 1953], and the corresponding lifetimes for neutral  $H_2$  molecules are even longer [e.g., Field *et al.*, 1966]. The characteristic loss time ( $\approx 1/\beta_{H_2}$ ) for molecules and the characteristic time for an  $H_2^+$  ion to be carried away from the Sun by the solar wind are much smaller than the characteristic time of spontaneous transitions. Therefore neutral and ionized hydrogen molecules should be considered as being in the "frozen" vibrational states. This latter requirement significantly complicates the problem, since one has to consider not a single species, i.e., molecular hydrogen, but many species, neutral and ionized molecules in various vibrational states, each state being characterized by its own process rates and cross sections. Many required cross sections and reaction rates are not readily available for all possible vibrational states.

Available cross sections are identified and the corresponding collision frequencies and process rates are determined in this work. The lower limit on the solar wind  $H_2^+$  pickup ion flux is established by considering  $H_2^+$  ions in the ground vibrational state ( $v = 0$ ). Comparison with  $H_2^+$  ions with the Franck-Condon distribution of the vibrational states is used to demonstrate importance of treating molecules as different species according to their vibrational states.

### 3. Model

It is assumed that the only source of molecular hydrogen is interplanetary dust outgassing (equation (7)). Solar photoionization and collisions with the solar wind ions (protons and alpha particles) lead to formation (by single ionization) of hydrogen molecule ions  $H_2^+$ ,



It is assumed that  $H_2^+$  ions are picked up by the solar wind plasma flow instantaneously after their "birth." The pickup ion flux (reciprocal square centimeters per second)  $F_{H_2^+}$  at a given (observation) point  $R_0$  in the ecliptic plane is an integral over the distance from the Sun to this point  $R_0$ ,

$$F_{H_2^+}(R_0) = \int_{\text{Sun}}^{R_0} \eta(R) n_{H_2}(R) (R/R_0)^2 P(R_0, R) dR \quad (9)$$

where  $\eta(R)$  is the local  $H_2^+$  ion production rate (reciprocal seconds), the factor  $(R/R_0)^2$  allows for spherical expansion of the solar wind, and  $P(R_0, R)$  is the probability (survival probability) for an  $H_2^+$  ion born at  $R$  to reach the observation point  $R_0$  without loss.

The rates of various processes due to interaction with the solar radiation are usually inversely proportional to the square of the distance from the Sun. As will be shown below, the same assumption can also be applied to the processes of interaction with the solar wind plasma. Substituting  $\eta(R) = \eta(R_E) \times (R_E/R)^2$  in (9), one obtains

$$F_{H_2^+}(R_0) = \eta(R_E) (R_E/R_0)^2 \int_{\text{Sun}}^{R_0} n_{H_2}(R) P(R_0, R) dR \quad (10)$$

The  $H_2^+$  ion survival probability is

$$P(R_0, R) = \exp \left[ - \int_R^{R_0} \frac{\delta(R)}{V_{sw}(R)} dR \right] \quad (11)$$

where  $\delta(R)$  is the local  $H_2^+$  ion loss rate (reciprocal seconds) and  $V_{sw}(R)$  is the solar wind velocity.

We will be considering below only hydrogen molecules, therefore the subscript "H2" (e.g.,  $\beta_{H_2}$ ) will not be used anymore. The subscripts  $h\nu$ ,  $H^+$ ,  $He^{++}$ , and  $e$  will be used to describe separate contributions to the rates ( $\beta$ ,  $\eta$ , and  $\delta$ ) by solar photons, solar wind protons, solar wind alpha particles, and solar wind electrons, respectively.

## 4. Interaction of $H_2$ Molecules With Solar Radiation and Solar Wind

### 4.1. Vibrational State of Neutral Hydrogen Molecules

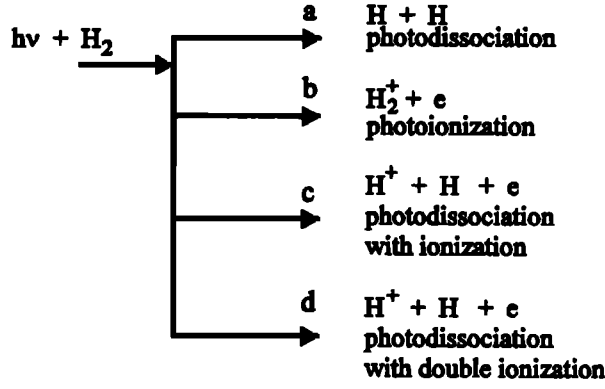
The vibrational state of  $H_2$  molecules leaving grains remains poorly understood. It was suggested long ago that hydrogen molecules born in recombination on the surfaces of cold interstellar dust grains would leave the grain surface in vibrationally and rotationally excited states [e.g., Barlow and Silk, 1976; Hunter and Watson, 1978]. The division of recombination energy between translational, vibrational and rotational degrees of freedom determines the efficiency of an important heating mechanism of interstellar clouds.

The properties of interstellar dust grains are, however, essentially different from those of zodiacal dust around the Sun. The temperature of interplanetary dust grains is  $>300$  K for  $R < 1$  AU, while the temperature of the interstellar dust does not exceed 100 K. Another essential difference is the surface structure. The surface layer of interplanetary grains is saturated by the bombarding solar wind protons and alpha particles. This continuous bombardment may lead to multiple cracks in the surface layer as well as to blistering and flaking effects similar to those observed in materials exposed to high particle doses [e.g., Guseva and Martynenko, 1981].

A significant fraction of hydrogen would thus desorb from the inside surfaces of the cracks in interplanetary dust grains. Consequently, a typical desorbed  $H_2$  molecule would collide several times with the crack walls before escaping to interplanetary space. Such collisions would result in a distribution of  $H_2$  vibrational states that is in thermal equilibrium with the dust grain temperature. Since the energy of the first  $H_2$  vibrational level is almost 0.3 eV (equivalent temperature 3400 K), most of the outgassing  $H_2$  molecules would be in the ground electronic and ground vibrational state. Therefore we will assume that desorbing hydrogen molecules are in the vibrational ground state ( $v=0$ ) only; implications of some molecules being in vibrationally excited states are discussed below.

### 4.2. Solar Extreme Ultraviolet (EUV) Radiation

Possible branches of solar photon interaction with  $H_2$  molecules are shown in Figure 2. The molecular hydrogen photodissociation rate (channel a) is  $3.09 \times 10^{-7} \text{ s}^{-1}$  at 1 AU for the moderate solar activity conditions [Dalgarno and Allison, 1969; Shemansky and Hall, 1992; Gruntman, 1994]. The rates for branches b and c are  $0.49 \times 10^{-7} \text{ s}^{-1}$  and  $0.09 \times 10^{-7} \text{ s}^{-1}$  at 1 AU, respectively [Shemansky and Hall, 1992]. Branch d has a much higher energy threshold and can be disregarded. Branch b is the only process that results

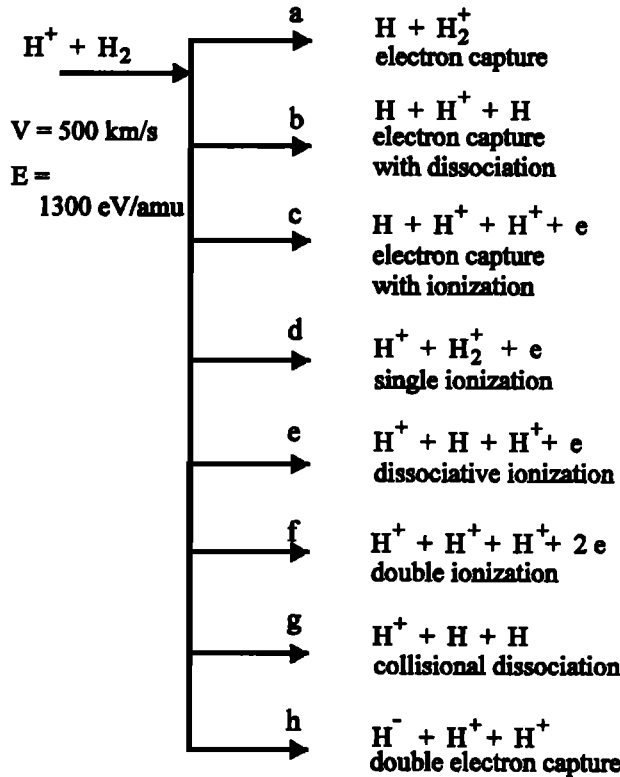


**Figure 2.** Reaction branches for interaction of photons with H<sub>2</sub> molecules.

in production of H<sub>2</sub><sup>+</sup> ions. The H<sub>2</sub> total loss rate due to radiation would be  $\beta_{\text{hv}}(R) = \beta_{\text{hv}}(R_E) \times (R_E/R)^2$ , where  $\beta_{\text{hv}}(R_E) = 3.67 \times 10^{-7} \text{ s}^{-1}$ ; the H<sub>2</sub><sup>+</sup> ion production rate (branch b) would be  $\eta_{\text{hv}}(R_E) = 0.58 \times 10^{-7} \text{ s}^{-1}$ .

#### 4.3. Collisions With the Solar Wind Protons and Alpha Particles

It is assumed that the solar wind velocity is constant,  $V_{\text{sw}} = 500 \text{ km s}^{-1}$ ; the solar wind ion number density is inversely proportional to the square of the distance from the Sun; the solar wind proton number density is  $N_{\text{H}^+}(R_E) = 5 \text{ cm}^{-3}$  at 1 AU; and the alpha particle number density is 5 % of that of the protons,  $N_{\text{He}^{++}} = 0.05 \times N_{\text{H}^+}$ . The fluxes of the solar wind protons and alpha particles at 1 AU are  $F_{\text{H}^+}(R_E) = 2.5 \times 10^8$  and  $F_{\text{He}^{++}}(R_E) = 1.25 \times 10^7 \text{ cm}^{-2} \text{ s}^{-1}$ , respectively.



**Figure 3.** Reaction branches for interaction of the solar wind protons with H<sub>2</sub> molecules.

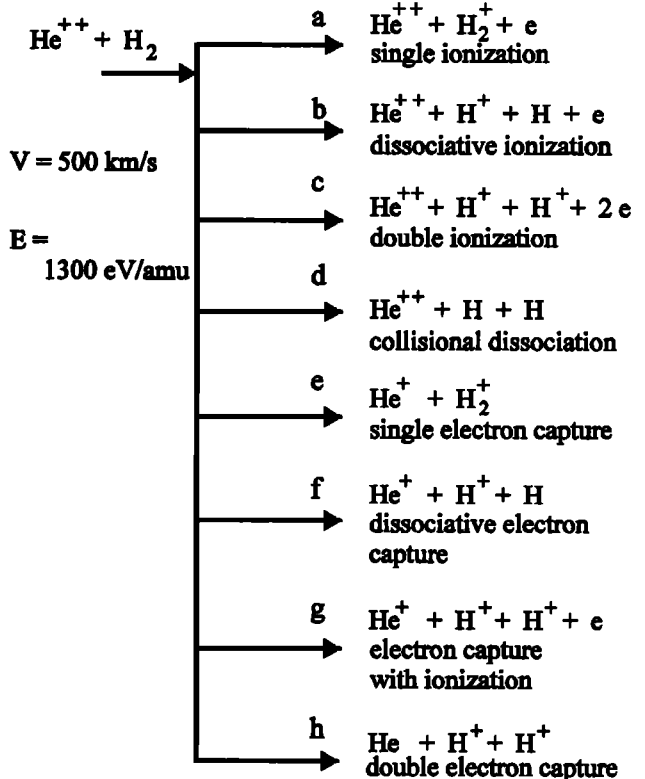
**Table 1.** Cross Sections for H<sub>2</sub> Collisions With Solar Wind Protons

Branch Sum	Cross Section, cm <sup>2</sup>	Reference
$\sigma_a + \sigma_b + \sigma_c$	$5.5 \times 10^{-16}$	Gealy and Van Zyl [1987]
$\sigma_c + \sigma_d + \sigma_e + \sigma_f$	$4.8 \times 10^{-18}$	Barnett et al. [1990]
$\sigma_h$	$1.5 \times 10^{-19}$	Barnett et al. [1990]
$\sigma_g$	?	

Possible reaction branches for H<sub>2</sub> collisions with the solar wind protons are shown in Figure 3. It is convenient to describe collisions by cross sections  $\sigma$  (square centimeters) and a specific reaction rate (reciprocal seconds) would be a product of the cross section and the local particle (ion, electron, photon) flux. The hydrogen molecule total loss rate is determined by the sum of reaction branches a through h, with the corresponding total loss cross section equal to  $(\sigma_a + \dots + \sigma_h)$ . The H<sub>2</sub><sup>+</sup> ion production cross section is  $(\sigma_a + \sigma_d)$ .

The cross sections for all possible individual branches are sometimes unknown, while the sums of certain branch cross sections may be available. For the proton velocity  $V_{\text{sw}} = 500 \text{ km/s}$  (energy 1.3 keV/nucleon), the cross sections that can be found in the literature are shown in Table 1.

The H<sub>2</sub> total loss rate is determined mostly by branches a and b. The cross section of collisional dissociation (branch g), to the best of my knowledge, has never been established. The total cross section of the production of molecular H<sub>2</sub><sup>+</sup> ions  $(\sigma_a + \sigma_d)$  was measured to be larger than that of the proton production  $(\sigma_b + \sigma_c + \sigma_e + \sigma_f + \sigma_h)$  by a factor of ~15 for the incident proton energy 5



**Figure 4.** Reaction branches for interaction of the solar wind alpha particles with H<sub>2</sub> molecules.

keV [Afrosimov *et al.*, 1969]. Since the cross section of proton production falls faster than that of  $H_2^+$  production with the collision energy decrease, one can assume that the  $H_2$  total loss rate  $\beta_{H_2}$ , as well as the total production rate of  $H_2^+$ ,  $\eta_{H_2^+}$ , are entirely determined by the electron capture process (reaction branch a) with the cross section  $\sigma_a = 5.5 \times 10^{-16} \text{ cm}^2$ . This cross section is known with 15% accuracy [Gealy and Van Zyl, 1987].

The cross section of the collisional dissociation (branch g) should be of the same order of magnitude as other dissociation cross sections, e.g., branches b and e, that are much less than the cross section of branch a. Thus the contribution of collisional dissociation can be disregarded. The loss rate due to collisions with the solar wind protons would be  $\beta_{H_2}(R) = \beta_{H_2}(R_E) \times (R_E/R)^2$ , and  $\beta_{H_2}(R_E) = F_{H^+}(R_E) \times \sigma_a = 1.38 \times 10^{-7} \text{ s}^{-1}$ . Similarly, the  $H_2^+$  ion production rate is  $\eta_{H_2^+}(R) = \eta_{H_2^+}(R_E) \times (R_E/R)^2$ , and  $\eta_{H_2^+}(R_E) = 1.38 \times 10^{-7} \text{ s}^{-1}$ .

Possible reaction branches for  $H_2$  collisions with the solar wind alpha particles are shown in Figure 4. The  $H_2^+$  ion production rate  $\eta_{H_2^+}$  is determined by the cross section ( $\sigma_a + \sigma_d$ ). The cross sections for individual branches, as derived from Afrosimov *et al.* [1980], are shown in Table 2 for alpha particle velocity  $V_{sw} = 500 \text{ km s}^{-1}$ . The cross section of collisional dissociation (branch d), to the best of my knowledge, has never been established.

The cross section sum ( $\sigma_f + \sigma_g$ ) =  $3.6 \times 10^{-16} \text{ cm}^2$  was directly measured by Afrosimov *et al.* [1980]. This cross section is approximately 50% larger than the value for the same cross section sum,  $2.3 \times 10^{-16} \text{ cm}^2$ , as derived from other cross sections given by Afrosimov *et al.* [1980] and Table 2. The uncertainty resulting from this inconsistency, which is close to the experiment errors, is about 30 %.

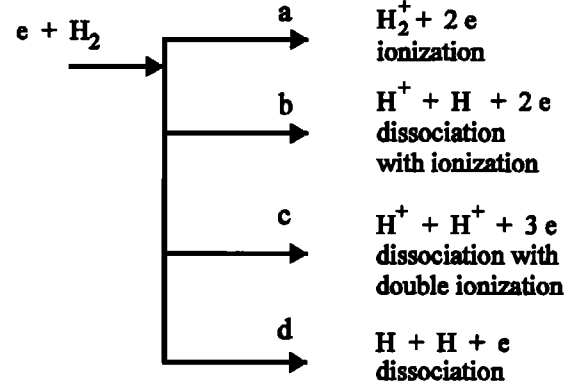
The total  $H_2$  loss rate  $\beta_{H_2}$  is determined mostly by dissociative electron capture (branch f) and electron capture with ionization (branch g) with some contribution of branches e and h. The total cross section of  $H_2$  loss in collisions with the solar wind alpha particles is  $3.2 \times 10^{-16} \text{ cm}^2$ . Similarly to the collisions with the solar wind protons, the unknown cross section of collisional dissociation (branch d) would be of the same order of magnitude as other dissociation (without electron transfer) cross sections, e.g. branches b and c, and thus branch d can be safely disregarded.

The production rate of  $H_2^+$  ions  $\eta_{H_2^+}$  is determined mostly by single electron capture (branch e) with some contribution of single ionization (branch a). The total cross section for this process is  $5.5 \times 10^{-17} \text{ cm}^2$ . Some of the  $He^+$  ions produced in single electron capture (branch e) are in the excited state [Afrosimov *et al.*, 1980] and would decay to the ground state with emission of 30.4-nm photons.

The  $H_2$  collisions with the solar wind alpha particles lead to molecule loss with relatively small production of molecular ions.

**Table 2.** Cross Sections for  $H_2$  Collisions With Solar Wind Alpha Particles

Branch	Cross Section, $\text{cm}^2$
$\sigma_a$	$5 \times 10^{-18}$
$\sigma_b$	$< 10^{-19}$
$\sigma_c$	$< 10^{-19}$
$\sigma_d$	?
$\sigma_e$	$5 \times 10^{-17}$
$\sigma_f$	$1 \times 10^{-16}$
$\sigma_g$	$1.3 \times 10^{-16}$
$\sigma_h$	$4 \times 10^{-17}$



**Figure 5.** Reaction branches for interaction of the solar wind electrons with  $H_2$  molecules.

This is different from the collisions with the solar wind protons, where  $H_2$  loss occurs essentially through the  $H_2^+$  ion producing branch. The hydrogen molecule loss rate due to collisions with the solar wind alpha particles is  $\beta_{H_2}(R) = \beta_{H_2}(R_E) \times (R_E/R)^2$ , and  $\beta_{H_2}(R_E) = 0.04 \times 10^{-7} \text{ s}^{-1}$ . The production rate of  $H_2^+$  ions is  $\eta_{H_2^+}(R_E) = 0.007 \times 10^{-7} \text{ s}^{-1}$ .

#### 4.4. Collisions With the Solar Wind Electrons

Possible reaction branches for  $H_2$  collisions with the solar wind electrons are shown in Figure 5. The total loss rate is determined by an integral over electron collision velocities

$$\beta_e(R) = \int_0^{\infty} q_e(v_e) F(v_e) v_e dv_e \quad (12)$$

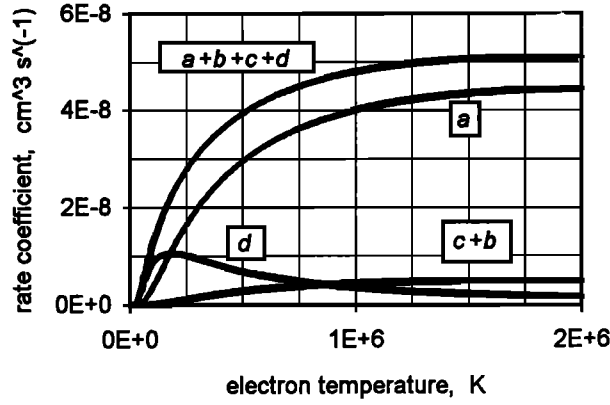
where  $q_e(v_e)$  is the velocity-dependent electron impact loss cross section (branches a through d),  $v_e$  is the electron velocity, and  $F(v_e)$  is the solar wind electron velocity distribution function, which depends on the heliocentric distance  $R$ . Correspondingly, the rates  $\beta_e(R)$  and  $\eta_e(R)$  would also depend on the heliocentric distance.

The number density  $N_e$  of the solar wind electrons is exactly equal to the number density (weighted by ion charge) of the solar wind ions,  $N_e = N_{H^+} + 2 \times N_{He^{++}}$ , to maintain charge neutrality of the solar wind plasma;  $N_e(R) = N_e(R_E) \times (R_E/R)^2$ , where  $N_e(R_E) = 5.5 \text{ cm}^{-3}$ . The solar wind electron distribution function is not accurately known for  $R < 0.5 \text{ AU}$ . It was argued that simple electron temperature models [e.g., Holzer, 1977] have to be modified to include a contribution of hot electrons [Rucinski and Fahr, 1989]. The hot electrons have been shown to be important in defining the ionization rates of heliospheric neutral atoms [Askew and Kunc, 1984].

We follow in this work the solar wind electron model adopted by Rucinski and Fahr [1989]. It is assumed that the solar wind electrons can be described by a bi-Maxwellian distribution (the solar wind velocity is much smaller than the velocity of electron thermal motion) with the so called "core" and "halo" electrons. The core electrons constitute 96% of all electrons,  $N_C = 0.96 \times N_e$ , while the remaining 4% are the halo electrons,  $N_H = 0.04 \times N_e$ . The core and halo electrons are described by temperatures  $T_C$  and  $T_H$ , respectively. It is assumed that the radial temperature dependence is

$$T_{C,H}(R) = T_{C,H}(R_E) \times (R_E/R)^{1/3} \quad (13)$$

where  $T_C(R_E) = 1.5 \times 10^5 \text{ K}$  and  $T_H(R_E) = 7.0 \times 10^5 \text{ K}$  [Rucinski and



**Figure 6.** Electron temperature dependence of the rate coefficients for electron interaction with H<sub>2</sub> molecules. The curves a, b, c, and d correspond to the process branches given in Figure 5.

Fahr, 1989]. Using electron distribution with respect to electron energies  $E_e$ , the H<sub>2</sub> ionization rate can then be expressed as

$$\beta_e(R) = (8\pi / m_e^2) \int_0^\infty q_e(E_e) g(E_e) E_e dE_e \quad (14)$$

where  $q_e(E_e)$  is the energy-dependent electron impact ionization cross section,  $m_e$  is the electron mass, and

$$g(E_e) = N_C (m_e / 2\pi k_B T_C)^{3/2} \exp(-E_e / k_B T_C) + N_H (m_e / 2\pi k_B T_H)^{3/2} \exp(-E_e / k_B T_H) \quad (15)$$

where  $N_C$ ,  $N_H$ ,  $T_C$ , and  $T_H$  depend on the heliocentric distance  $R$ ;  $k_B$  is the Boltzmann constant. A similar expression can be written for the H<sub>2</sub><sup>+</sup> production rate,  $\eta_e(R)$ , by substituting the total loss cross section  $q_e$  by the H<sub>2</sub><sup>+</sup> production cross section (branch a).

The H<sub>2</sub> single ionization cross section (branch a) was measured by Adamczyk *et al.* [1966]. The results of these measurements were recently confirmed by Krishnakumar and Srivastava [1994], who used modern experimental arrangement. These recent measurements of Krishnakumar and Srivastava [1994], however, suggest that the cross section for the proton-producing branches (b and c) is actually higher by a factor of 2–3 than the cross sections measured in the past by Rapp *et al.* [1965] and Adamczyk *et al.* [1966]. We will use the cross section of Adamczyk *et al.* [1966] for branch a (Figure 5) and the cross section of Krishnakumar and Srivastava [1994] for branches b and c. The cross section of hydrogen molecule dissociation without ionization (branch d) was obtained by Corrigan [1965].

**Table 3.** Contribution of Various Processes to H<sub>2</sub> Total Loss Rate  $\beta$  and H<sub>2</sub><sup>+</sup> Ion Production Rate  $\eta$  at 1 AU

Interaction	$\beta(R_E)$ , s <sup>-1</sup>	$\eta(R_E)$ , s <sup>-1</sup>
$h\nu$	$3.67 \times 10^{-7}$	$0.58 \times 10^{-7}$
H <sup>+</sup>	$1.38 \times 10^{-7}$	$1.38 \times 10^{-7}$
He <sup>++</sup>	$0.04 \times 10^{-7}$	$0.007 \times 10^{-7}$
$e$	$1.09 \times 10^{-7}$	$0.50 \times 10^{-7}$
Total	$6.18 \times 10^{-7}$	$2.47 \times 10^{-7}$

The electron temperature dependence of the rate coefficients (cubic centimeters per second) for the reaction branches shown in Figure 5 is presented in Figure 6. Single ionization (branch a) is the dominating process at high temperatures ( $T_e > 4 \times 10^5$  K), while collisional dissociation without ionization (branch d) is most important at smaller temperatures,  $T_e < 2 \times 10^5$  K.

#### 4.5. Molecular Hydrogen Total Loss Rate $\beta(R)$ and H<sub>2</sub><sup>+</sup> Total Production Rate $\eta(R)$

The heliospheric H<sub>2</sub> total loss rate  $\beta(R)$  and the H<sub>2</sub><sup>+</sup> ion production rate  $\eta(R)$  are

$$\beta(R) = \beta_{h\nu}(R) + \beta_{H^+}(R) + \beta_{He^{++}}(R) + \beta_e(R) \quad (16)$$

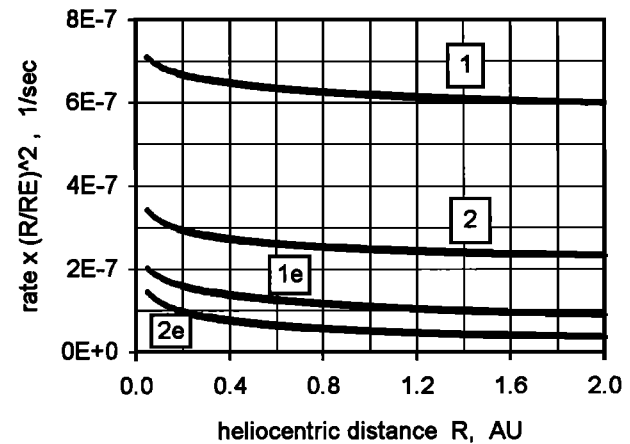
$$\eta(R) = \eta_{h\nu}(R) + \eta_{H^+}(R) + \eta_{He^{++}}(R) + \eta_e(R) \quad (17)$$

Table 3 summarizes contributions of all these processes at 1 AU. The heliocentric radial dependence of the rates can be conveniently presented [e.g., Gruntman, 1990] by using normalized rates that are the rates multiplied by a dimensionless factor  $(R/R_E)^2$ . For processes with the rates inversely proportional to the square of the distance from the Sun, the normalized rates are constants. In our model, only the electron impact rates would deviate from the inverse square dependence. The heliocentric dependence of the total loss  $\beta(R)$  and H<sub>2</sub><sup>+</sup> production  $\eta(R)$  normalized rates as well as corresponding contributions of electron impact processes are shown in Figure 7.

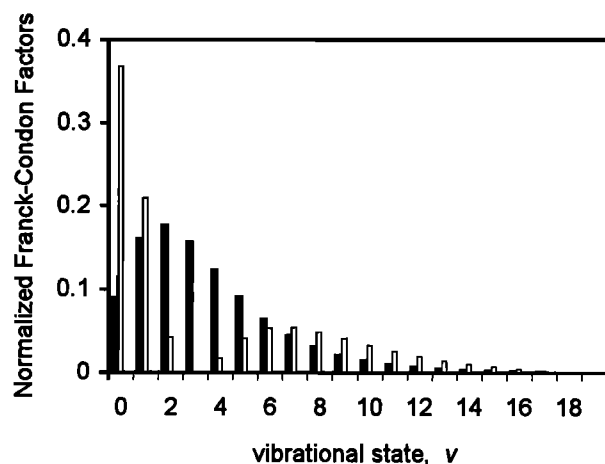
Electron impact processes become increasingly important with the approach to the Sun (up to 40% for the H<sub>2</sub><sup>+</sup> production rate and 25% for the H<sub>2</sub> total loss rate). As one can see from Table 3, solar radiation is most important for total loss of hydrogen molecules, while charge exchange with the solar wind protons is the most important process for H<sub>2</sub><sup>+</sup> ion production.

#### 4.6. Electronic and Vibrational States of H<sub>2</sub><sup>+</sup> Molecules

Charge exchange on the solar wind protons is responsible for the formation of almost 60% of H<sub>2</sub><sup>+</sup> ions, while photoionization and electron impact ionization contribute the remaining 40% to this process (Table 3). It was experimentally established that charge exchange collisions with the solar wind protons produce H<sub>2</sub><sup>+</sup> ions in the electronic ground state [Afrosimov *et al.*, 1969].



**Figure 7.** Normalized H<sub>2</sub> loss rate  $\beta(R) \times (R/R_E)^2$  (curve 1) and normalized H<sub>2</sub><sup>+</sup> ion production rate  $\eta(R) \times (R/R_E)^2$  (curve 2) as a function of the heliocentric distance  $R$ . Contributions of electron collisions are shown for H<sub>2</sub> loss (1e) and for H<sub>2</sub><sup>+</sup> production (2e).



**Figure 8.** Normalized Franck-Condon factors  $G(v)$  for  $\text{H}_2$  ionization. The hatched bars correspond to the initial vibrational state  $v = 0$  of neutral  $\text{H}_2$  molecules; the open bars correspond to the initial vibrational state  $v = 1$ .

Most of the molecular ions produced by photoionization and electron impacts will also be in the electronic ground state as a result of the significantly higher energy threshold for production of  $\text{H}_2^+$  ions in the excited electronic state.

$\text{H}_2^+$  ions can be produced in various vibrationally excited states of the ground electronic state. For a given vibrational state of neutral  $\text{H}_2$  molecules, the distribution of  $\text{H}_2^+$  ion vibrational states,  $G(v)$ , would depend on the exact energy distributions of the solar wind protons and electrons and on the exact spectral distribution of the solar radiation. When electron or photon energies are not very close to the ionization threshold, the assumption of  $\text{H}_2^+$  ion vibrational state distribution according to the Franck-Condon factors is usually valid. The validity of the Franck-Condon distribution assumption was verified for  $\text{H}_2^+$  ion production by electron bombardment under a wide variety of experimental conditions [e.g., *Dumm and Van Zyl*, 1967; *Von Busch and Dumm*, 1972]. The vibrational state distribution of  $\text{H}_2^+$  ions produced in charge exchange with protons has never been established for solar wind proton energies. We will assume that heliospheric  $\text{H}_2^+$  ions are distributed according to the Franck-Condon factors, and possible deviations from this assumption are considered in section 7 (discussion).

The Franck-Condon factors for hydrogen ionization were calculated for various initial neutral molecule vibrational and rotational states [e.g., *Villarejo*, 1968]. The Franck-Condon distributions,  $G_0(v)$  and  $G_1(v)$ , of the  $\text{H}_2^+$  vibrational states are shown in Figure 8 for  $\text{H}_2$  initial vibrational states  $v = 0$  [*Dumm*, 1966] and  $v = 1$  [*Von Busch and Dumm*, 1972].

## 5. Interaction of $\text{H}_2^+$ Ions With Solar Radiation and Solar Wind

### 5.1. $\text{H}_2^+$ Ion Vibrational States

The loss rate of  $\text{H}_2^+$  pickup ions strongly depends on the initial ion vibrational state.  $\text{H}_2^+$  ions in highly excited vibrational states are quickly lost, while the lifetime of the remaining ions in the lower vibrational states is much longer. Therefore the total loss rate determined by formal averaging over the Franck-Condon distribution does not describe correctly the survival of the heliospheric  $\text{H}_2^+$  ions. Rather, one has to treat loss of molecular

ions in different vibrationally excited states as loss of different species. Many required cross sections are not readily available from the literature. We will consider in detail the loss rate of  $\text{H}_2^+$  ions in the ground vibrational state  $v = 0$ , which will allow us to establish the lower limit on the solar wind  $\text{H}_2^+$  pickup ion flux.

### 5.2. Interaction of Solar Photons With $\text{H}_2^+$

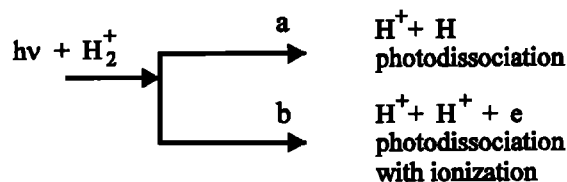
Solar photons may dissociate  $\text{H}_2^+$  ions with or without ionization of the fragment atoms (Figure 9). For a given radiation wavelength,  $\text{H}_2^+$  ion photodissociation is usually efficient from a few ion vibrational states only. Dissociation of  $\text{H}_2^+$  ions in the high vibrationally excited states is possible (cross section  $\sim 10^{-18} \text{ cm}^2$ ) by solar photons in the visible spectral range. For example, at  $\lambda = 600 \text{ nm}$ , approximately 57% of the contribution to photodissociation comes from the vibrational state  $v = 8$ ; 18% comes from  $v = 7$ ; and 15% comes from  $v = 10$  [*Von Busch and Dumm*, 1972]. Consequently, the dissociation rate from such states is very efficient under intense solar illumination in the visible wavelength range, resulting in an exceptionally high  $\text{H}_2^+$  ion photodissociation rate obtained by formal averaging over the Franck-Condon distribution. This averaged photodissociation rate would be  $0.33 \text{ s}^{-1}$  at 1 AU.

The spectral dependence of the cross section for photodissociation of  $\text{H}_2^+$  ions in the ground vibrational state  $v = 0$  without fragment ionization (branch a in Figure 9) was calculated by *Dumm* [1968], the process being efficient in the wavelength range 60–210 nm. The process rate is obtained by convolution of the cross section with the solar photon flux spectral distribution.

The solar photon flux for moderate solar activity was constructed in the following way. The solar flux in the wavelength range 6–99 nm was measured by *Von Tassel et al.* [1981] under the moderate solar activity conditions. The solar flux between 100 and 210 nm was compiled by *Hall et al.* [1985] for the solar activity minimum. *Hinteregger* [1981] determined typical variations of the solar radiation between solar maximum and solar minimum. The photon flux between 100 and 194 nm of *Hall et al.* [1985] was corrected by a factor corresponding to the middle of the solar flux variations as determined by *Hinteregger* [1981]. It is assumed that the solar flux for  $\lambda > 194 \text{ nm}$  does not change during the solar cycle.

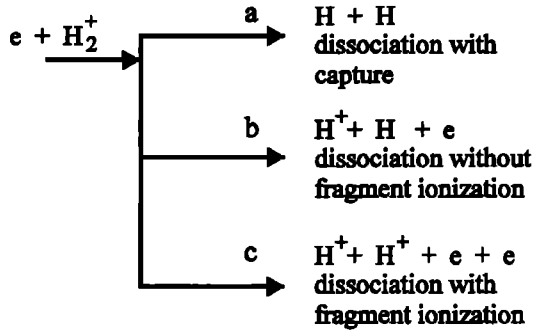
The  $\text{H}_2^+$  ion ( $v = 0$ ) photodissociation rate is calculated to be  $4.63 \times 10^{-6} \text{ s}^{-1}$  at 1 AU (compare with  $0.33 \text{ s}^{-1}$  for the rate obtained by formal averaging over the Franck-Condon distribution). Approximately two thirds of photodissociation is due to the solar hydrogen Lyman alpha line (121.6 nm); the significant contribution is provided also by the solar radiation continuum between 140 and 200 nm.

Photodissociation of  $\text{H}_2^+$  ions ( $v = 0$ ) with the ionization of the fragment (branch b in Figure 9) was considered by *Bates and Opik* [1968]. This process has a threshold at  $\lambda = 45 \text{ nm}$ , and one obtains the dissociation rate  $9 \times 10^{-9} \text{ s}^{-1}$  at 1 AU. This dissociation rate is much smaller than the rate of branch a and can thus be



**Figure 9.** Reaction branches for interaction of photons with the  $\text{H}_2^+$  ions.





**Figure 10.** Reaction branches for interaction of the solar wind electrons with the  $\text{H}_2^+$  ions.

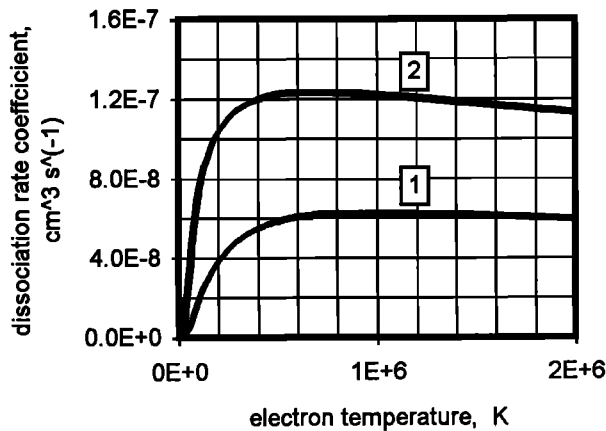
neglected. The total  $\text{H}_2^+$  ion ( $\nu = 0$ ) loss rate due to solar radiation is  $\delta_{\text{H}_2^+}(R) = \delta_{\text{H}_2^+}(R_E) \times (R_E/R)^2$ , and  $\delta_{\text{H}_2^+}(R_E) = 4.63 \times 10^{-6} \text{ s}^{-1}$ .

### 5.3. $\text{H}_2^+$ Ion Collisions With the Solar Wind Electrons

Hydrogen molecule ions are known to efficiently interact with low energy electrons; possible reaction branches are shown in Figure 10. The cross sections for these processes significantly depend on the initial vibrational state of the  $\text{H}_2^+$  ion. The cross sections for  $\text{H}_2^+$  dissociation by electron impact are given, for example, by *Dunn and Van Zyl* [1967]. Electron temperature dependence of the dissociation rate coefficient (cubic centimeters per second) for  $\text{H}_2^+$  ions in the ground vibrational state and the dissociation rate coefficient obtained by averaging over ions with the Franck-Condon distribution of the vibrational states are shown in Figure 11. The difference in initial vibrational states is less important for electron impact processes than for solar photodissociation. The heliocentric radial dependence of the electron impact  $\text{H}_2^+$  loss rate can be calculated similarly to the calculation of the neutral  $\text{H}_2$  electron impact ionization rate (equation 14).

### 5.4. Collisions of $\text{H}_2^+$ Ions With the Solar Wind Protons and Alpha Particles

$\text{H}_2^+$  pickup ions are gyrating about magnetic field lines and colliding with the solar wind protons and alpha particles; the



**Figure 11.** Electron temperature dependence of the electron impact dissociation rate coefficient for  $\text{H}_2^+$  ions in the ground vibrational state  $\nu = 0$  (curve 1) and averaged over the Franck-Condon distribution (curve 2).

**Table 4.** Contribution of Various Processes to Total  $\text{H}_2^+$  Ion Loss Rate at 1 AU

Interaction	$\delta(R_E)$ , $\text{s}^{-1}$
$h\nu$	$4.63 \times 10^{-6}$
$\text{H}^+$	negligible
$\text{He}^{++}$	negligible
$e$	$5.15 \times 10^{-7}$
Total	$5.15 \times 10^{-6}$

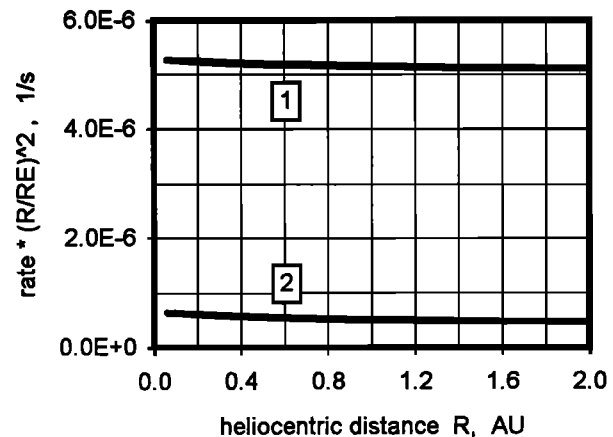
average collision velocity is equal to that of the solar wind. The cross sections of  $\text{H}_2^+$  dissociation by such collisions have not been established. However, one can show that the contribution of such collisions to  $\text{H}_2^+$  ion loss rate is negligible. The  $\text{H}_2^+$  ion loss rate due to the solar wind proton collisions would be similar to the solar photodissociation rate if the proton collision dissociation cross section were  $2 \times 10^{-14} \text{ cm}^2$ . This cross section is 1–2 orders of magnitude higher than the cross section that can be expected for such a process ( $\sim 10^{-16} \text{ cm}^2$ ). Hence the  $\text{H}_2^+$  ion collisions with the solar wind protons can be disregarded. Similar arguments show that the collisions with the solar wind alpha particles can be neglected as well.

### 5.5. Hydrogen Molecule Ion Loss Rate $\delta(R)$

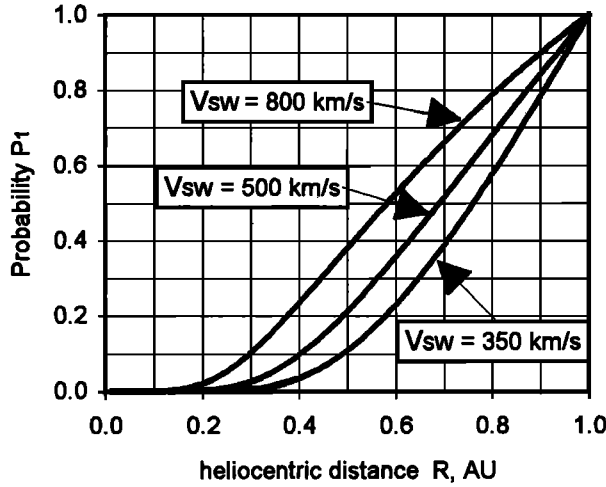
The total  $\text{H}_2^+$  ion loss rate  $\delta(R)$  is

$$\delta(R) = \delta_{\text{H}_2^+}(R) + \delta_{\text{H}^+}(R) + \delta_{\text{He}^{++}}(R) + \delta_e(R) \quad (18)$$

Table 4 summarizes contributions of different processes at 1 AU. The heliocentric radial dependence of the normalized total loss rate  $\delta(R) \times (R/R_E)^2$ , as well as the contribution of electron collisions, is shown in Figure 12. The importance of the electron impact processes increases only slightly with the approach to the Sun. Since electron collisions account for approximately 10% of the  $\text{H}_2^+$  loss rate only, one can assume that the total  $\text{H}_2^+$  loss rate  $\delta(R)$  is inversely proportional to the square of the distance from the Sun. Such an approximation significantly simplifies calculations of  $\text{H}_2^+$  ion survival probabilities.



**Figure 12.** Normalized total loss rate  $\delta(R) \times (R/R_E)^2$  of  $\text{H}_2^+$  ions in the ground vibrational state  $\nu = 0$  as a function of the heliocentric distance (curve 1). The contribution of the solar wind electron collisions is curve 2.



**Figure 13.** Probability for an  $\text{H}_2^+$  ion carried by the solar wind ( $V_{\text{sw}} = 350, 500$ , and  $800 \text{ km s}^{-1}$ ) to reach 1 AU as a function of the ion place of birth (at the distance  $R$  from the Sun).

### 5.6. $\text{H}_2^+$ Ion Survival Probability

The survival probability  $P(R_0, R)$  (equation 11) can be conveniently presented as a product of two probabilities

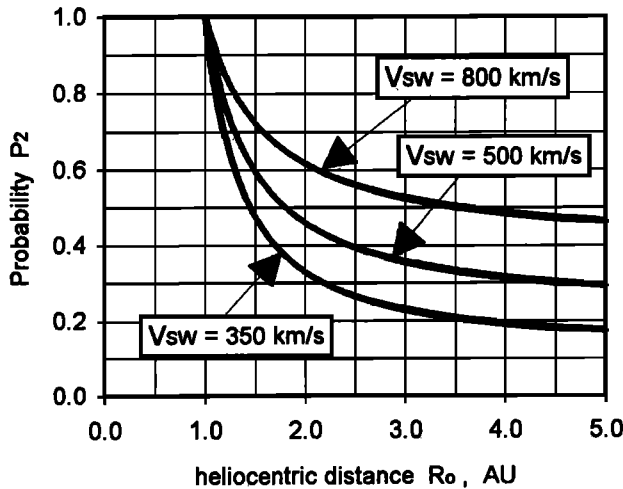
$$P(R_0, R) = P_1(R) \times P_2(R_0) \quad (19)$$

where  $P_1(R) = P(R_E, R)$  is the probability for an  $\text{H}_2^+$  ion to reach  $R_E = 1 \text{ AU}$  from the point of ion birth,  $R$ , and  $P_2(R_0) = P(R_0, R_E)$  is the probability of reaching the observation point  $R_0$  from the Earth's orbit. For pickup ions at  $R_0 = 1 \text{ AU}$ , the probability  $P_2 = 1$  and  $P(R_0, R) = P_1(R)$ .

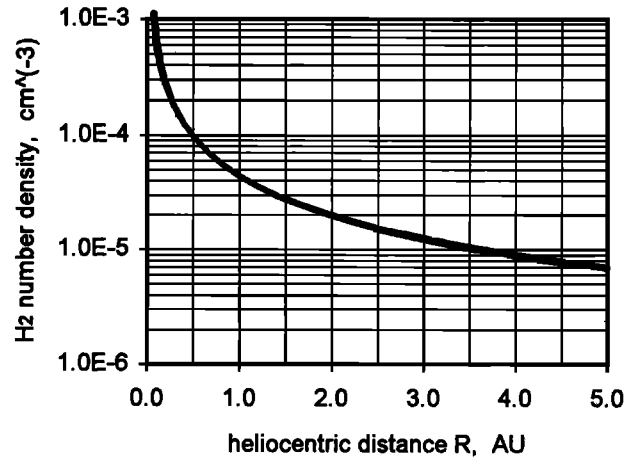
For the constant solar wind velocity and  $\delta(R) = \delta(R_E) \times (R_E/R)^2$ , one obtains from (11)

$$P_1(R) = \exp \left[ \frac{\delta(R_E) R_E}{V_{\text{sw}}} \left( 1 - \frac{R_E}{R} \right) \right] \quad (20)$$

$$P_2(R_0) = \exp \left[ \frac{\delta(R_E) R_E}{V_{\text{sw}}} \left( \frac{R_E}{R_0} - 1 \right) \right] \quad (21)$$



**Figure 14.** Probability for an  $\text{H}_2^+$  ion carried by the solar wind ( $V_{\text{sw}} = 350, 500$ , and  $800 \text{ km s}^{-1}$ ) to reach the heliocentric distance  $R_0$  ( $R_0 > 1 \text{ AU}$ ) from 1 AU.



**Figure 15.** Neutral hydrogen molecule number density as a function of heliocentric distance in the ecliptic plane.

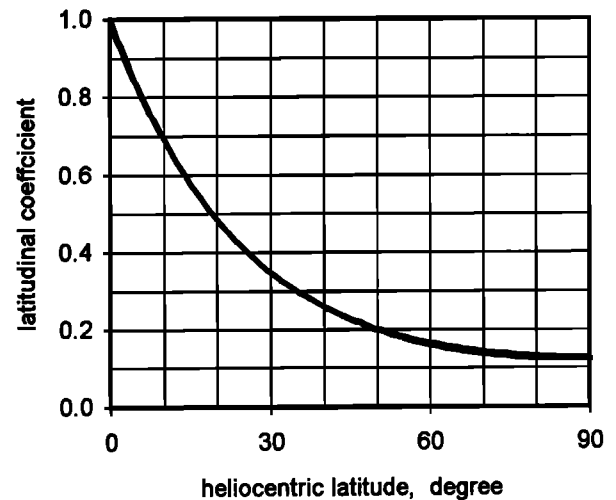
The calculated probabilities  $P_1(R)$  and  $P_2(R_0)$  for  $\text{H}_2^+$  ions in the vibrational ground state are shown in Figures 13 and 14, respectively. The probability  $P_1(R)$  to reach 1 AU decreases dramatically with the approach of the birth point to the Sun. This probability is highly sensitive to the solar wind velocity, especially at  $R < 0.5 \text{ AU}$ . The probability of  $\text{H}_2^+$  ion survival increases with increasing solar wind velocity.

### 6. $\text{H}_2^+$ Pickup Ion Flux in the Solar Wind

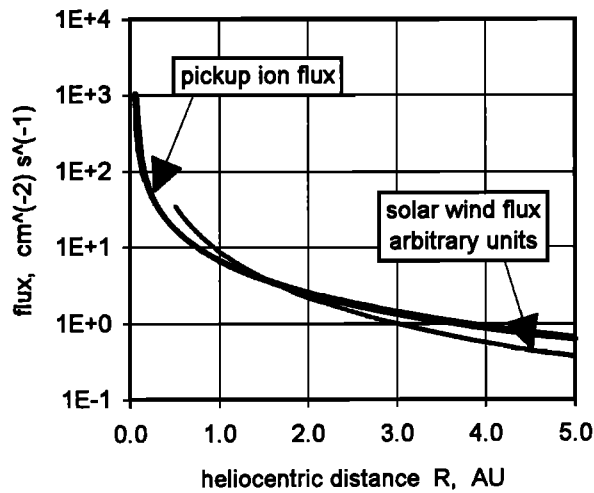
The  $\text{H}_2^+$  pickup ion flux is determined by the integral (10). The neutral  $\text{H}_2$  number density can be obtained (see equation(6)) from the relation

$$n_{\text{H}_2}(R) = \rho_{\text{H}_2}(R) / \beta(R) \quad (22)$$

The  $\text{H}_2$  source rate,  $\rho_{\text{H}_2}(R)$ , in our model is slightly higher than that derived from *Fahr et al.* [1981] (equation 7) because of the higher speed of the solar wind ( $500 \text{ km s}^{-1}$  instead of  $400 \text{ km s}^{-1}$ ). Correspondingly, the source rate is higher by a factor  $500/400 = 1.25$ . For the  $\text{H}_2$  loss rate  $\beta(R_E) = 6.18 \times 10^{-7} \text{ s}^{-1}$  (see Table 3), one obtains  $\text{H}_2$  number density distribution



**Figure 16.** Dust density factor  $v_{\text{DUST}}(\chi)$  dependence on heliocentric latitude.



**Figure 17.** H<sub>2</sub><sup>+</sup> pickup ion flux as a function of heliocentric distance in the ecliptic plane.

$$n_{H_2}(R) = 4.4 \times 10^{-5} \times (R_E/R)^{1.15} \text{ cm}^{-3} \quad (23)$$

Although this number density distribution is based on calculations for heliocentric distances  $R < 1$  AU [Fahr *et al.*, 1981], we will assume that this dependence is valid for a wider range of heliocentric distances,  $R < 5$  AU. The radial dependence of the dust-produced neutral H<sub>2</sub> number density,  $n_{H_2}(R)$ , is shown in Figure 15. The latitudinal dependence of  $n_{H_2}$ , the factor  $v_D(\chi)$ , is shown in Figure 16.

Rapid decrease of the probability  $P_1(R)$  with the approach to the Sun justifies the assumption used throughout this work that the H<sub>2</sub><sup>+</sup> ion production and loss rates are inversely proportional to the square of the distance from the Sun. Deviations from this dependence occur in the Sun's vicinity only. The error introduced by the inverse square assumption would be insignificant, since only a small fraction of H<sub>2</sub><sup>+</sup> ions that are born close to the Sun would survive and reach an observer at 1 AU and beyond.

The lower limit on the solar wind H<sub>2</sub><sup>+</sup> pickup ion flux is obtained by considering H<sub>2</sub><sup>+</sup> ions in the ground vibrational state  $v = 0$  only. The ions are distributed according to the Franck-Condon factors, and all ions in excited vibrational states are assumed to be lost. The heliocentric radial dependence (in the ecliptic plane) of the H<sub>2</sub><sup>+</sup> pickup ion flux obtained under such assumptions is shown in Figure 17. The H<sub>2</sub><sup>+</sup> ion flux (reciprocal square centimeters per second) decreases with the increase of the distance from the Sun. Another curve shown corresponds to a flux that is inversely proportional to the square of the distance from the Sun (for example, the solar wind ion flux). One can see that the relative abundance of H<sub>2</sub><sup>+</sup> pickup ions in the solar wind increases with increasing heliocentric distance.

## 7. Discussion

Neutral H<sub>2</sub> molecules escaping dust grains were assumed to be in the ground vibration state. If some H<sub>2</sub> molecules are in the first vibrationally excited state ( $v = 1$ ) then this would result in increase of the H<sub>2</sub><sup>+</sup> ion flux. Only 9% of H<sub>2</sub><sup>+</sup> ions are produced in the ground vibrational state  $v = 0$  from H<sub>2</sub> molecules in the ground vibration state (Figure 8). If H<sub>2</sub> molecules are initially in the first vibrational state, then 37% of ions will be born in the ground vibrational state, which is a factor of 4 increase. Therefore any

presence of slightly excited ( $v = 1$ ) H<sub>2</sub> molecules will result in increase of H<sub>2</sub><sup>+</sup> ion flux.

An assumption of the H<sub>2</sub><sup>+</sup> ion Franck-Condon distribution is well justified for photoionization and electron impact ionization, these two processes being responsible for almost half of the H<sub>2</sub><sup>+</sup> ions (Table 3). The only vibrationally state-resolved experimental study of proton/hydrogen molecule charge exchange was performed by Niedner *et al.* [1987] for 30-eV protons. The experimental results obtained in that work does not come close to the Franck-Condon predictions. The majority of H<sub>2</sub><sup>+</sup> ions are in the ground vibrational state  $v = 0$  with some ions in the states  $v = 1, 2$ , and 3. Collisions with the solar wind protons are similar to those studied in the experiment of Niedner *et al.* [1987], since both cases (the collision energies are 1300 and 30 eV, respectively) fall into the category of slow adiabatic collisions. Therefore it seems reasonable to assume that the distribution of vibrational states after collisions with the solar wind protons will not be unlike that measured by Niedner *et al.* [1987]. Hence use of the Franck-Condon distribution results in a highly conservative estimate of the expected solar wind H<sub>2</sub><sup>+</sup> pickup ion flux.

The H<sub>2</sub><sup>+</sup> ions in highly excited vibrational states are photoionized practically instantaneously. The H<sub>2</sub><sup>+</sup> ions in the vibrational states  $v=1,2$ , and 3 would have the loss rate that is only slightly higher than that of H<sub>2</sub><sup>+</sup> ions in the ground vibrational state  $v = 0$ . The number of H<sub>2</sub><sup>+</sup> ions produced in states  $v=1,2$ , and 3 is approximately 5 times larger than the number of H<sub>2</sub><sup>+</sup> ions produced in the ground vibrational state for the Franck-Condon distribution and neutral H<sub>2</sub> molecule  $v = 0$  state.

The effects discussed above, namely, (1) possible presence of some neutral H<sub>2</sub> molecules in slightly excited vibrational states, (2) much higher probability of producing H<sub>2</sub><sup>+</sup> ions in the ground vibrational state in charge exchange, and (3) significant survival probability of H<sub>2</sub><sup>+</sup> ions in low vibrational states ( $v=1,2,3$ ), suggest that the solar wind H<sub>2</sub><sup>+</sup> pickup ion flux obtained under an assumption of the Franck-Condon distribution of the vibrational states is likely to be smaller by a factor of 2–5 than the “real” pickup ion flux.

The solar wind H<sub>2</sub><sup>+</sup> pickup ion flux would depend on the solar wind velocity. Let us consider different solar wind velocities,  $V_{sw} = 350, 500$ , and  $800 \text{ km s}^{-1}$ , but assume that the solar wind ion flux is the same, i.e.,  $F_{H^+}(R_E) = 2.5 \times 10^8 \text{ cm}^{-2} \text{ s}^{-1}$ . The neutral H<sub>2</sub> production rate  $\rho(R)$  is independent of the solar wind velocity under an assumption of constant solar wind proton flux (see equation 7). A fraction of H<sub>2</sub> molecules that is converted to H<sub>2</sub><sup>+</sup> ions is proportional to the rate ratio  $\eta(R)/\beta(R)$ , which does depend on the solar wind velocity. Interaction with the solar radiation is independent of the solar wind velocity. The rates due to collisions with the solar wind ions are proportional to the solar wind flux and would depend on the solar wind velocity only because of the velocity dependence of the collision cross sections. The loss rate due to electron collisions would depend on the

**Table 5.** Production and Loss Rates, and H<sub>2</sub><sup>+</sup> Pickup Ion Fluxes at 1 AU for Various Solar Wind Velocities

$V_{sw}$ km s <sup>-1</sup>	$\beta(R_E), \text{s}^{-1}$	$\eta(R_E) \text{s}^{-1}$	$\eta / \beta$	$\delta(R_E), \text{s}^{-1}$	$F_{H_2^+}(R_E)$ cm <sup>-2</sup> s <sup>-1</sup>
350	$6.07 \times 10^{-7}$	$2.10 \times 10^{-7}$	0.35	$5.37 \times 10^{-6}$	4.4
500	$6.18 \times 10^{-7}$	$2.47 \times 10^{-7}$	0.40	$5.15 \times 10^{-6}$	6.8
800	$6.57 \times 10^{-7}$	$3.06 \times 10^{-7}$	0.46	$4.95 \times 10^{-6}$	11.7

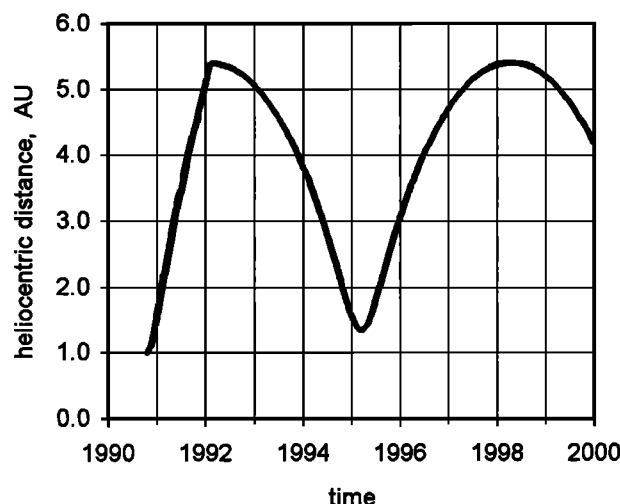


Figure 18. Ulysses heliocentric distance.

electron number density which is inversely proportional to the solar wind velocity (as a result of the plasma charge neutrality requirement). The survival probability,  $P(R_0, R)$  is a strong function of the solar wind velocity, which determines how much time ions are exposed to the radiation and collisions.

Table 5 summarizes the relevant rates for different solar wind velocities and presents fluxes of the solar wind  $\text{H}_2^+$  pickup ions at 1 AU. The rate ratio,  $\eta(R)/\beta(R)$ , changes only slightly with the solar wind velocity. The change in the survival probability of  $\text{H}_2^+$  ions is the most important effect for the pickup ion flux. Not only does  $\text{H}_2^+$  ion survival significantly increase with increasing solar wind velocity (for the constant loss rate; see Figures 13 and 14), but the  $\text{H}_2^+$  ion loss rate  $\delta(R_E)$  would decrease with increasing solar wind velocity. The largest  $\text{H}_2^+$  pickup ion flux would be found in high-speed solar wind streams. It is important to emphasize again that these are conservative estimates of the  $\text{H}_2^+$  pickup ion fluxes.

The Ulysses spacecraft is a unique platform for the study of pickup ion fluxes since its heliocentric distance varies from 1 to 5 AU (Figure 18) and covers practically all possible heliocentric latitudes (Figure 19). Calculated expected dependences of the

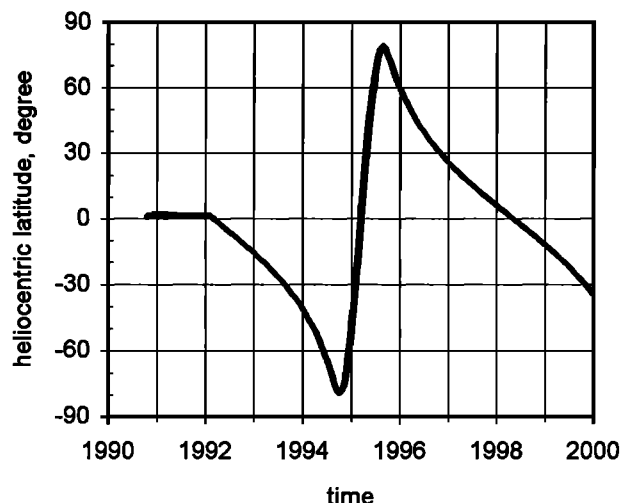


Figure 19. Ulysses heliocentric latitude.

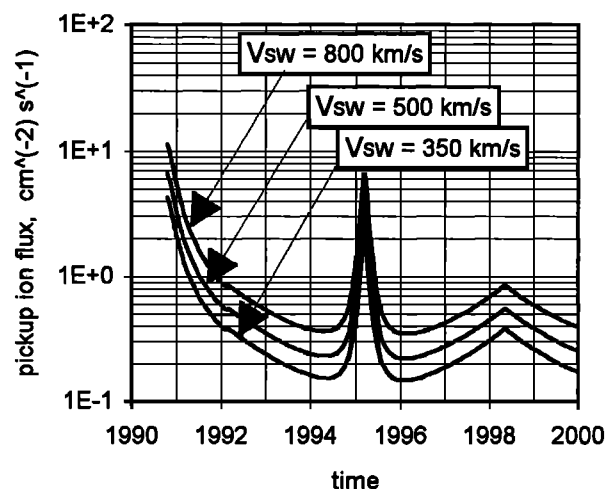


Figure 20. Calculated dependences of the solar wind  $\text{H}_2^+$  pickup ion flux for Ulysses for different solar wind velocities.

solar wind  $\text{H}_2^+$  pickup ion flux as a function of the observation date on Ulysses are shown in Figure 20 for different solar wind velocities. One can see that the most favorable observational conditions for the search of molecular hydrogen are when Ulysses is close to the ecliptic plane and for high solar wind speeds. High-speed streams should also allow one to probe interplanetary dust distribution closer to the Sun. Detection of  $\text{H}_2^+$  ions at high heliocentric latitudes would allow testing of our models of the latitudinal dust distribution.

The Sun is moving through a low-density warm interstellar gas [Frisch, 1990, 1995; Lallement *et al.*, 1990; Bertin *et al.*, 1993]. The number density of interstellar gas, which consists mostly of hydrogen, is  $\sim 0.1 \text{ cm}^{-3}$ . For a  $\text{H}_2/\text{H}$  ratio  $10^{-6}$ – $10^{-5}$  in the LISM, a number density of interstellar molecular hydrogen inside 1 AU would be 2 orders of magnitude smaller than the  $\text{H}_2$  number density of dust-generated hydrogen. It is not excluded, however, that the molecular fraction is much higher in the LISM (LISM is a transitional phase between hot and cold interstellar gas and is not in the full equilibrium), and such a possibility requires careful consideration. The exact distribution of vibrational states of interstellar  $\text{H}_2$  molecules may become an especially important factor determining the survival probability of interstellar molecular hydrogen in the heliosphere.

The distribution of interstellar  $\text{H}_2$  molecules penetrating the heliosphere is highly anisotropic [e.g., Gruntman, 1993] as a result of relative motion between the Sun and LISM. The WIND and SOHO spacecraft are operating in the ecliptic plane and are in an excellent position to study interstellar contribution to the solar wind  $\text{H}_2^+$  pickup ions if interstellar molecular hydrogen is present in substantial quantities in the LISM.

**Acknowledgments.** This work was partially supported by NASA grant NAGW-4380. The author is grateful to Don Shemansky and Bert Van Zyl for useful discussions of elementary processes involving hydrogen molecules.

The Editor thanks H.J. Fahr and another referee for their assistance in evaluating this paper.

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(Received December 15, 1995; revised March 14, 1996; accepted April 8, 1996.)