

## RATE COEFFICIENT FOR $H^+ + H_2(X^1\Sigma_g^+, \nu = 0, J = 0) \rightarrow H(1s) + H_2^+$ CHARGE TRANSFER AND SOME COSMOLOGICAL IMPLICATIONS

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### ABSTRACT

Krستیć has carried out the first quantum mechanical calculations near threshold for the charge transfer (CT) process  $H^+ + H_2(X^1\Sigma_g^+, \nu = 0, J = 0) \rightarrow H(1s) + H_2^+$ . These results are relevant for models of primordial galaxy and first star formation that require reliable atomic and molecular data for obtaining the hydrogen chemistry of the early universe. Using the results of Krستیć, we calculate the relevant CT rate coefficient for temperatures between 100 and 30,000 K. We also present a simple fit that can be readily implemented into early universe chemical models. Additionally, we explore how the range of previously published data for this reaction translates into uncertainties in the predicted gas temperature and  $H_2$  relative abundance in a collapsing primordial gas cloud. Our new data significantly reduce these cosmological uncertainties that are due to the uncertainties in the previously published CT rate coefficients.

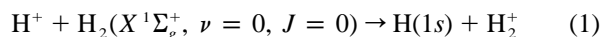
*Subject headings:* atomic data — early universe — galaxies: formation — molecular data — molecular processes — stars: formation

### 1. INTRODUCTION

Molecular hydrogen is an important coolant during the epoch of primordial galaxy and first star formation. Model calculations indicate that radiatively induced cooling due to collisions of  $H_2$ , primarily with  $H$ , dominate the cooling of collapsing primordial gas clouds from temperatures beginning at  $\sim 10^4$  K and going down to  $\sim 5 \times 10^2$  K (e.g., Saslaw & Zipoy 1967; Abel & Haiman 2000; Nakamura & Umemura 2002).

The importance of  $H_2$  in the early universe is supported by the recent *Wilkinson Microwave Anisotropy Probe* (WMAP) measurements which suggest (a) that reionization occurred at high redshift and (b) a large Thompson scattering optical depth. These results require star formation at this redshift to produce the ionizing radiation, which implies that  $H_2$  cooling is important for early star formation (Spergel et al. 2003; Haiman & Holder 2003). Given the pivotal role that  $H_2$  is predicted to play, an accurate understanding of its formation and destruction in the early universe is crucial for understanding the formation of hierarchical structure (Haiman, Thoul, & Loeb 1996; Abel et al. 1997; Abel, Bryan, & Norman 2002; Galli & Palla 1998; Flower 2002; Lepp, Stancil, & Dalgarno 2002; Nakamura & Umemura 2002; Ricotti, Gnedin, & Shull 2002).

The early universe chemistry of  $H_2$  during the epoch of primordial galaxy and first star formation has been reviewed recently by a number of groups (e.g., Abel et al. 1997; Galli & Palla 1998; Lepp et al. 2002; Oh & Haiman 2002). These authors have found that the relative  $H_2$  abundances are determined by only a handful of processes. Of particular interest, Oh & Haiman (2002) point out that the charge transfer (CT) process



is the dominant destruction mechanism of  $H_2$  during the for-

mation at this epoch of halos with viral temperatures  $T_{\text{vir}} > 10^4$  K. This process dominates until a collapsing cloud of primordial gas begins to emit ionizing radiation internally or until the background extragalactic UV radiation field has reached significant levels. Then the dominant destruction mechanism becomes photodissociation through the Lyman-Werner bands via the two-step Solomon process (Haiman, Rees, & Loeb 1997).

Because of the fundamental importance of reaction (1), reliable rate coefficients for this process are needed for our understanding of the formation of structure in the early universe. However, as discussed below, the various rate coefficients adopted by the astrophysics community for this process differ from one another by orders of magnitude. This translates into order-of-magnitude uncertainties in the predicted relative abundance of  $H_2$  at key epochs. Furthermore, this uncertainty directly affects the predicted properties of collapsing gas clouds during primordial galaxy and first star formation.

To help address the need for accurate rate coefficients for reaction (1), Krستیć (2002) has recently carried out the first quantum mechanical calculations for this process at collision energies relevant for the cosmological formation of structure. His results are appropriate for current models of early universe chemistry, which treat all molecules as being in their ground rovibrational state. These models have not yet evolved to the point where they take into account the electronic and rovibrational distribution of molecules (e.g., Oh & Haiman 2002; Lepp et al. 2002). Throughout the rest of this Letter, only ground electronic configurations are considered.

In § 2, we give a brief review of the previous experimental and theoretical work for reaction (1). A short description of the theoretical calculations by Krستیć (2002) is given in § 3. In § 4, we present our new rate coefficient, provide a simple fitting formula that can readily be incorporated into early universe chemistry models, and comment on our results. Lastly, in § 5, we briefly discuss some of the cosmological implications of our results.

### 2. REVIEW OF PREVIOUS WORK

CT of  $H^+$  on  $H_2(\nu = 0, J = 0)$  is an endothermic process with a threshold of 1.83 eV (Janev et al. 1987, p. 142). Cosmologically, reaction (1) is important at temperatures of

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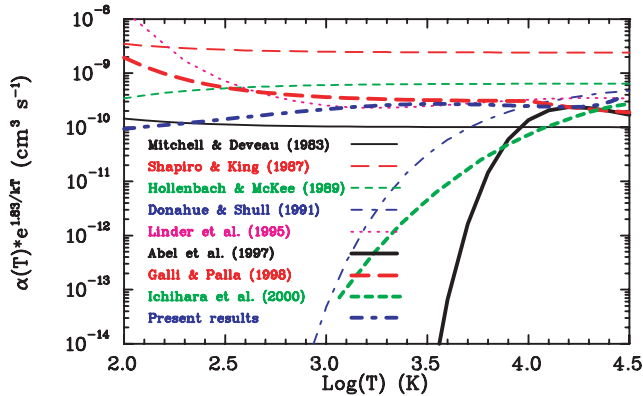


FIG. 1.—Recommended rate coefficients for  $\text{H}_2 + \text{H}^+ \rightarrow \text{H}_2^+ + \text{H}$ . All data have been multiplied by  $\exp(1.83/kT)$  to remove the effects of the 1.83 eV threshold for this process.

$kT < 1$  eV, where  $k$  is the Boltzmann constant. Hence, it is the behavior of the cross section just above threshold that is most important for primordial chemistry. The only cross section measurements in this energy range have been carried out by Holliday, Muckerman, & Friedman (1971). A rate coefficient measurement for the reverse of reaction (1) has been carried out at a temperature of  $T = 300$  K by Karpas, Anicich, & Huntress (1979). Rate coefficients for reaction (1) have been presented by a number of different groups. In Figure 1, we present the various published data multiplied by  $\exp(1.83/kT)$  to remove the effects due to the threshold for this reaction.

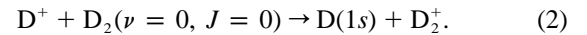
Mitchell & Deveau (1983), Shapiro & Kang (1987), and Hollenbach & McKee (1989) appear to present data derived using detailed balance between the forward and reverse directions of reaction (1) and the rate coefficient measurement for the reverse direction by Karpas et al. (1979). However, reading their papers and their cited sources, how their data are actually derived is unclear. Donahue & Shull (1991) state explicitly that their data are derived from detailed balance between the forward and reverse directions of reaction (1) and the measurements of Karpas et al. Yet, as shown in Figure 1, these four recommended rate coefficients all differ from one another dramatically in both magnitude and temperature dependence, despite their all apparently being based on detailed balance between the forward and reverse directions of reaction (1) and despite the use of the same single-temperature laboratory measurement.

We note that the application of detailed balance is only strictly valid for state-to-state reactions, i.e., when the  $\nu, J$  level of the reactant and product molecules are known. While typical laboratory conditions are such that  $\nu = 0$  and  $J$  is likely to be small for the reactant, the product  $\nu, J$  is usually unknown. For example, Krstić (2002) finds that for the reverse of reaction (1), the product  $\text{H}_2$  is primarily formed into  $\nu = 4$ , not  $\nu = 0$ . Therefore, estimation of reaction (1) by the application of detailed balance to the measured rate coefficient for the reverse reaction gives the rate coefficient for  $\text{H}_2(\nu = 4)$ , which can be as much as an order of magnitude larger than for  $\text{H}_2(\nu = 0)$ . Rate coefficients that are estimated by detailed balance are therefore suspect.

Some groups have derived the needed rate coefficients using the cross section measurements of Holliday et al. (1971). Abel et al. (1997) integrated the recommended cross section data of Janev et al. (1987), which are based on the measurements by Holliday et al. Galli & Palla (1998) directly integrated the data of Holliday et al. Hence, it is unclear why the rate coefficients

of Abel et al. and Galli & Palla differ so dramatically in both temperature dependence and absolute magnitude.

Linder, Janev, & Botero (1995) have presented a recommended cross section for reaction (1) that we have integrated to produce a rate coefficient using the method discussed in § 3. Their cross section is based primarily on published experimental work for both this reaction and the isotopically identical reaction



But as pointed out by Krstić (2002), several eV above the threshold, the recommended cross section of Linder et al. is over an order of magnitude larger than the measurements of Holliday et al. (1971). So the relative agreement between the rate coefficients of Linder et al. (1995) and Galli & Palla (1998), despite their being based on cross section data sets that differ significantly from one another, is surprising.

More recently, theoretical calculations have been carried out using the classical trajectory-surface-hopping (TSH) model of Ichihara, Iwamoto, & Janev (2000). In Figure 1, we have plotted their results as a function of plasma temperature for an  $\text{H}_2$  temperature of 0.1 eV. We expect that at this  $\text{H}_2$  temperature, their results are nearly equivalent to the results for ground-state  $\text{H}_2$ . The TSH method, however, is expected to provide only qualitative results for center-of-mass (CM) energies  $E_{\text{CM}} \lesssim 10$  eV. Early universe chemical models need rate coefficients for these reactions at temperatures  $\lesssim 10^4$  K. This corresponds to  $E_{\text{CM}} \lesssim 1$  eV.

To summarize, it is clear that more sophisticated theoretical calculations and new laboratory measurements for reaction (1) are needed.

### 3. THEORETICAL METHOD

Cross sections for vibrationally resolved CT of protons with  $\text{H}_2(\nu_i)$  and of atomic hydrogen with  $\text{H}_2^+(\nu_i)$  have been obtained by solving the Schrödinger equation for the nuclear and electronic motions on the two lowest diabatic electronic surfaces of  $\text{H}_3^+$  (Krstić 2002). The calculations were performed using a fully quantal, coupled-channel approach by expanding the nuclear wave functions in a large vibrational basis of all discrete  $\text{H}_2(\nu = 0-14)$  and  $\text{H}_2^+(\nu' = 0-18)$  states and corresponding discretized continua pseudostates (altogether 900 states of positive and negative energy). As a consequence, all inelastic processes (CT, excitation, and dissociation) were calculated on the same footing, enabling both proper population dynamics and normalization of the full  $S$ -matrix (Krstić 2002; Krstić & Janev 2003). Discretized vibrational continua and large configuration spaces (40 atomic units [a.u.] in length) were used along with the bound states to account for transitions through the “closed” channels and for nuclear particle exchange. The price paid for using a diabatic vibrational basis is the large number of closed channels needed to achieve the convergence of the cross sections (typically 200 at lower energy to 600 at the highest energies considered here). This is partially a consequence of the large number of quasi-continuum states for representing particle-exchange channels, which are certainly present in the large, 40 a.u.  $\times$  40 a.u., quantization box.

The main approximation used was the sudden approximation for rotations, often referred as the Infinite Order Sudden Approximation (IOSA). This technique freezes target molecule rotations during the collision and then post-collisionally averages the cross sections over all possible molecular orienta-

TABLE 1  
FIT PARAMETERS FOR EQUATION (4)

Parameter	Value
$a$ .....	2.1237150E+04
$b_0$ .....	-3.3232183E-07
$b_1$ .....	3.3735382E-07
$b_2$ .....	-1.4491368E-07
$b_3$ .....	3.4172805E-08
$b_4$ .....	-4.7813720E-09
$b_5$ .....	3.9731542E-10
$b_6$ .....	-1.8171411E-11
$b_7$ .....	3.5311932E-13

NOTE.—The units for  $a$  are K, and the units for  $b_i$  are  $\text{cm}^3 \text{s}^{-1}$ .

tions (Pack 1974; Secrest 1975; Chu & Dalgarno 1975; Kupperman, Schatz, & Baer 1976; Schatz & Kupperman 1976; Khare 1978; Kouri 1979; Baer 1985; Baer & Nakamura 1987; Sidis 1989). This approximation sets the lower limit of the appropriate range for calculations to a fraction of eV. In principle, there is no upper limit. With the IOSA prescriptions and by expansion of the nuclear functions in the vibrational basis, the resulting system of coupled second-order ordinary differential equations in  $R$  (the distance from the projectile to the molecular CM) reduces to uncoupled equations for each partial wave  $\ell$  of the projectile CM motion. These were solved using as many partial waves as needed until convergence of the cross section was achieved (going up to  $\ell = 600$  for the highest value of  $E$ ). The proper plane-wave boundary conditions were applied at the entrance-exit of the reactant configuration (i.e., at  $R = R_{\text{max}} = 40$  a.u.), utilizing multichannel logarithmic derivatives, for both open and closed channels (Johnson 1973). The open-open submatrix of the resulting  $K$ -matrix is then used to obtain the  $S$ -matrix for each  $\ell$ .

A number of different definitions of the plasma rate coefficient exist in the literature. Here we have calculated the rate coefficients  $\alpha(T)$  by taking the Maxwellian average of the cross section  $\sigma(E)$  over the relative energy distribution of the  $H^+$  and  $H_2$  particles using

$$\alpha(T) = \frac{1}{\sqrt{\pi\mu}} \left(\frac{2}{kT}\right)^{3/2} \int_{E_i}^{\infty} \sigma(E) E \exp(-E/kT) dE, \quad (3)$$

where  $\mu$  is the reduced mass of the system,  $E_i$  is the threshold energy for the considered process, and  $E = \mu v^2/2$  is the CM energy. Our calculated data for  $\sigma$  extend from 2 to 9.5 eV. We integrated from 1.83 to 9.5 eV, by assuming  $\sigma(E_i) = 0$ . A spline-fit parabolic curve was used to interpolate  $\sigma$  between the calculated values. We estimate that the cutoff of the integration at 9.5 eV introduces a less than 1% error in our results.

Further details of this calculation can be found elsewhere (Krstić 2002). Also available for both the  $H^+ + H_2$  and  $H + H_2^+$  collision systems are the final and initial vibrational state resolved cross sections for CT (Krstić 2002), excitation (Krstić 2002), dissociation (Krstić & Janev 2003), and elastic transport (Krstić & Schultz 1999, 2003). The three-body association rate coefficients for  $H^+ + H + H$  forming  $H_2$  in the temperature range 200–20,000 K have also been calculated (Krstić, Janev, & Schultz 2003).<sup>5</sup>

<sup>5</sup> All the cross section data can be downloaded in tabular and graphic form from <http://www-cfadc.phy.ornl.gov>.

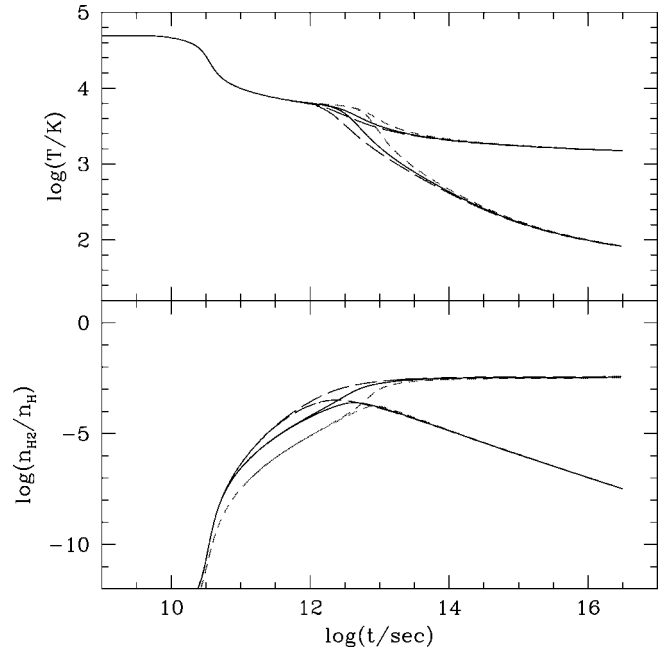


FIG. 2.—Calculated gas temperature (*top*) and  $H_2$  relative abundance (*bottom*) for a parcel of gas starting with a density of  $10 \text{ cm}^{-3}$ . In the top (bottom) plot, the lower (upper) set of curves corresponds to a nonexternal UV field, and the upper (lower) set of three curves corresponds to a field of  $10^{-21} \text{ ergs s}^{-1} \text{ cm}^{-2} \text{ sr}^{-1}$  in the Lyman-Werner bands of  $H_2$  (11.2–13.6 eV). The short-dashed curves use the rate coefficient for reaction (1) of Shapiro & Kang (1987), the long-dashed curves use the values of Abel et al. (1997), and the solid curves uses the present results. See § 5 for further details.

#### 4. RESULTS AND DISCUSSION

We have calculated the rate coefficient for reaction (1) for temperatures of  $10^2$ – $3 \times 10^4$  K. This covers the range of temperatures for which reaction (1) is cosmologically important. We present our results in Figure 1.

The calculated CT rate coefficient has been fitted using

$$\alpha(T) = \exp(-a/T) \sum_{i=0}^7 b_i (\log_{10} T)^i. \quad (4)$$

The best-fit values are listed in Table 1. The fit is accurate to better than 4% for  $10^2 \text{ K} \leq T \leq 3 \times 10^4 \text{ K}$ .

Our calculated results represent the most sophisticated theoretical treatment of reaction (1) at the present time. Previous rate coefficient calculations, based on detailed balance or the TSH method, are unreliable for the reasons discussed in § 2 and cannot be used to verify the validity of our results. Similarly, Linder et al. (1995) raise questions about the reliability of the laboratory measurements by Holliday et al. (1971). Hence, in our opinion, rate coefficients derived from the cross section data of either Holliday et al. (1971) or Linder et al. (1995) cannot be used to verify the reliability of our calculated results. In short, new laboratory measurements are needed to benchmark our new calculations.

#### 5. COSMOLOGICAL IMPLICATIONS

Using the models of Oh & Haiman (2002), we have investigated how our new results for reaction (1) affect the predicted gas temperature and  $H_2$  relative abundance of a collapsing gas cloud during the epoch of primordial galaxy and first star formation. Calculations have been carried out first in the absence

of any external UV field and then assuming an external field of  $10^{-21}$  ergs  $s^{-1}$   $cm^{-2}$   $sr^{-1}$  in the Lyman-Werner bands of  $H_2$  (11.2–13.6 eV). The flux chosen for the UV field is roughly that needed to reionize the universe (Haiman, Abel, & Rees 2000). When using an external UV field, we assumed a hydrogen column density of  $10^{22}$   $cm^{-2}$  to mimic the interior of a dense, initially neutral clump. We used a cosmic H/He ratio of  $Y_{He} = 0.24$ . For reaction (1), we have used the adopted data of Shapiro & Kang (1987), Abel et al. (1997), and our new results. The rest of the chemical network is from Oh & Haiman (2002).

In Figure 2, we show the predicted gas temperature and  $H_2$  relative abundance using these three different rate coefficients. We note that using the rate coefficient of Galli & Palla (1998) yields results similar to those using our new data. Here our model follows a parcel of gas at an initial density of  $10$   $cm^{-3}$ . This is about  $10^4$  times denser than the background intergalactic medium at a redshift  $z \approx 20$ . Assuming that  $z \approx 20$  at  $t = 0$  s, then the evolution of the gas is followed until  $t = 10^{16}$  s. Using the *WMAP* results and the  $\Lambda$ CDM cosmological model of Spergel et al. (2003), this corresponds to a final redshift of  $z \approx 5$ . The asymptotic values for the predicted gas temperature and  $H_2$  relative abundance are little affected by the atomic physics uncertainties (a well-known result; e.g., Abel et al. 1997; Galli & Palla 1998; Oh & Haiman 2002). But as can be readily seen from the

figure, for times between  $10^{11}$  and  $10^{13}$  s, both the predicted gas temperature and the  $H_2$  relative abundance are highly sensitive to the rate coefficient chosen. These timescales are short compared with cosmic timescales but could well be relevant for the formation of the first stars (Haiman et al. 2000). For example,  $10^{13}$  s corresponds to the dynamical time for gas at overdensities of a few times  $10^5$  relative to the cosmic mean at redshift  $z \approx 20$ , and the actual star formation process may proceed on even shorter timescales (Abel et al. 2002). Our new theoretical results for reaction (1) significantly reduce the uncertainties in the predicted gas temperature and  $H_2$  relative abundance that are due to the adopted rate coefficient.

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In equation (4) of the above-mentioned Letter, “ $\log_{10}$ ” should be replaced with “ $\ln$ ” so that it reads

$$\alpha(T) = \exp(-a/T) \sum_{i=0}^7 b_i (\ln T)^i. \quad (4)$$

Also, the second sentence of the caption to Figure 2 of the above-mentioned Letter should read as follows: “In the top (bottom) plot, the lower (upper) set of curves corresponds to no external UV field, and the upper (lower) set of three curves corresponds to a UV field of  $10^{-21}$  ergs  $\text{s}^{-1}$   $\text{cm}^{-2}$   $\text{sr}^{-1}$  in the Lyman-Werner bands of  $\text{H}_2$  (11.2–13.6 eV).”