RATE COEFFICIENTS FOR $D(1s) + H^+ \leftrightarrows D^+ + H(1s)$ CHARGE TRANSFER AND SOME ASTROPHYSICAL IMPLICATIONS

DANIEL WOLF SAVIN

Columbia Astrophysics Laboratory, 550 West 120th Street, Columbia University, New York, NY 10027; savin@astro.columbia.edu

ABSTRACT

We have calculated the rate coefficients for $D(1s) + H^+ \leftrightarrows D^+ + H(1s)$ using recently published theoretical cross sections. We present results for temperatures T from 1 K up to 2×10^5 K and provide fits to our data for use in plasma modeling. Our calculations are in good agreement with previously published rate coefficients for $25 \leq T \leq 300$ K, which covers most of the limited range for which those results were given. Our new rate coefficients for $T \gtrsim 100$ K are significantly larger than the values most commonly used for modeling the chemistry of the early universe and of molecular clouds. This may have important implications for the predicted HD abundance in these environments. Using our results, we have modeled the ionization balance in high-redshift QSO absorbers. We find that the new rate coefficients decrease the inferred D/H ratio by $\lesssim 0.4\%$. This is a factor of $\gtrsim 25$ smaller than the current $\gtrsim 10\%$ uncertainties in QSO absorber D/H measurements.

Subject headings: atomic data — atomic processes — early universe — ISM: molecules —
plasmas — quasars: absorption lines

1. INTRODUCTION

Deuterium plays an important role in addressing several fundamental questions in astrophysics. The deuterium abundance is a key constraint for models of big-bang nucleosynthesis. Primordial D/H measurements provide the most sensitive probe of the baryon-to-photon density ratio η. This, in combination with the cosmic microwave background measurement of the photon density, can be used to determine the cosmological baryon density (Burles & Tytler 1998; Lemoine et al. 1999; Tytler et al. 2000). Deuterium may also be important in the formation of structure in the postrecombination era of the early universe. HD is the second-most abundant primordial molecule after H_2, and cooling radiation from it may play a role in the formation of the first collapsing objects (Puy et al. 1993; Stancil, Lepp, & Dalgarno 1998). Finally, as the universe evolves, deuterium is slowly destroyed in stars, where it is burned into ^{3}He. Mapping the temporal and spatial variations in the D/H abundance ratio can shed light on the time history of star formation in different regions of the cosmos (Tosi 1998; Tosi et al. 1998; Lemoine et al. 1999).

Investigations into these issues are carried out through studies of gas-phase deuterium and deuterated molecules in, for example, the early universe (Galli & Palla 1998; Stancil et al. 1998), QSO absorption systems (O'Meara et al. 2001), molecular clouds (Tielens 1992; Bertoldi et al. 1999; Wright et al. 1999), and the interstellar medium (Linsky et al. 1995). Stancil et al. (1998) have given a recent listing of deuterium models for the early universe, molecular clouds, and the interstellar medium. Recent reviews of deuterium observations have been given by Lemoine et al. (1999) and Tytler et al. (2000).

Interpreting these studies requires an accurate knowledge of all collision processes involving deuterium. Particularly significant is the near-resonant charge-transfer (CT) process

$$D(1s) + H^+ \rightarrow D^+ + H(1s) \qquad (1)$$

and the reverse process

$$D^+ + H(1s) \rightarrow D(1s) + H^+ . \qquad (2)$$
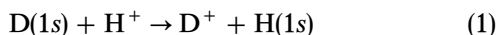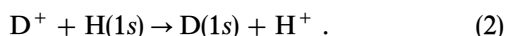
In the early universe, these are two of the most important processes involving deuterium (Galli & Palla 1998). In molecular clouds, the process in equation (1), followed by the exothermic reaction

$$H_2 + D^+ \rightarrow HD + H^+ , \qquad (3)$$
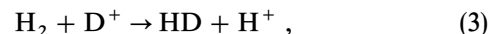
is a major source of HD (Black & Dalgarno 1973; Dalgarno, Black, & Weisheit 1973; Watson 1973). This is also an important source of HD in the early universe (Stancil et al. 1998).

Recently, Igarashi & Lin (1999) and Zhao, Igarashi, & Lin (2000) have carried out cross section calculations for reactions (1) (σ_1) and (2) (σ_2) using a hyperspherical close-coupling method. This technique is free from the ambiguities associated with the conventional Born-Oppenheimer approach. Here we use their results to produce CT rate coefficients for reactions (1) (α_1) and (2) (α_2). In § 2 we describe how we evaluated α_1 and α_2. Our results are presented in § 3 and compared with previously published calculations. Some astrophysical implications are discussed in § 4.

2. CALCULATION OF THE RATE COEFFICIENTS

We consider only capture from and into the $1s$ level of hydrogen and deuterium. The reason for this is twofold. First, in the sources discussed in § 1, neutral hydrogen and deuterium are expected to be found essentially only in their ground state. Second, at the low temperatures (i.e., low collision energies) relevant for these sources ($T \lesssim 3 \times 10^4$ K [i.e., $k_B T \lesssim 3$ eV]), CT into the $1s$ level is predicted to be over 4 orders of magnitude greater than capture into other levels. CT into higher levels does not become important until collision energies of $\gtrsim 10^3$ eV (Alt et al. 1994).

We use the results of Igarashi & Lin (1999) and Zhao et al. (2000) for $\sigma_1(E)$ and $\sigma_2(E)$ at center-of-mass energies E from 2.721×10^{-8} to 2.721 eV (A. Igarashi 2001, private communication). Because the binding energy of $D(1s)$ is slightly larger than that of $H(1s)$, reaction (1) is endothermic, with a threshold of 3.7 meV (43 K). Hence, σ_1 is predicted to be smaller than σ_2 at all energies, but particularly at low energies. As E increases, σ_1 and σ_2 converge,

and for $E \gtrsim 2.72$ eV, the two are predicted to lie within $\lesssim 0.1\%$ of one another (Zhao et al. 2000; A. Igarashi 2001, private communication). The energy dependences for σ_1 and σ_2 allow us to extend the results of Igarashi and collaborators to higher energies. We do this using the calculated cross sections of Dalgarno & Yadav (1953) for the related reaction

$$\text{H}^+ + \text{H}(1s) \to \text{H}(1s) + \text{H}^+ . \quad (4)$$
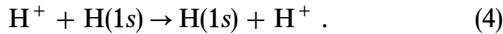
First, to extend the data for σ_2, we multiply the energy scale of Dalgarno & Yadav by $\mu_{\text{HD}}/\mu_{\text{HH}}$, where μ is the reduced mass for the HD and HH systems. This effectively matches the velocity scale for each data set. Then, we multiply the results of Dalgarno & Yadav by a factor of 0.959 to set it equal to the results of Igarashi and collaborators at 1.333 eV. Next, for energies between 1 and ≈ 2.72 eV, we fit the ratio of σ_1/σ_2 from Igarashi to the formula

$$\frac{\sigma_1}{\sigma_2} = 1 - \frac{A}{E} - \frac{B}{E^2} , \quad (5)$$

which yields $A = 2.692 \times 10^{-3}$ and $B = 7.936 \times 10^{-4}$. We calculate σ_1 for energies above ≈ 2.72 eV using the scaled cross sections of Dalgarno & Yadav multiplied by equation (5).

We use the resulting data for σ_1 and σ_2 from energies of 2.721×10^{-8} to 10^3 eV to evaluate the rate coefficients $\alpha_1(T)$ and $\alpha_2(T)$ as a function of the gas temperature T. Rate coefficients are calculated numerically using the desired cross section times the relative velocity, and convolving these results with the appropriate Maxwellian distribution (taking the reduced mass into account). Cross sections for energies not calculated by Igarashi and collaborators or by Dalgarno & Yadav (1953) are evaluated using a spline interpolation method (Press et al. 1992) for $\sigma(E)$ versus $\log (E)$.

3. RESULTS AND COMPARISONS

Our calculated results for $\alpha_1(T)$ and $\alpha_2(T)$ are given in Table 1 from 1 K up to 2×10^5 K. These results are also plotted in Figure 1 from 1 to 30,000 K. As expected, the rate coefficient for the endothermic reaction (1) decreases dramatically for $T \lesssim 10$ K. The rate coefficient for reaction (2) decreases slowly with decreasing temperature down to $T \approx 15$ K. Below this, α_2 begins to increase with decreasing
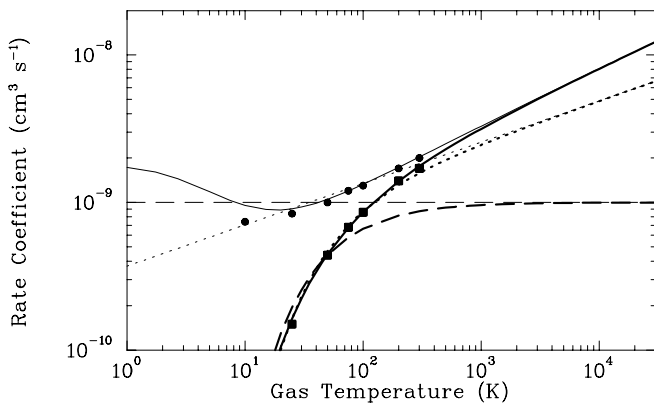

FIG. 1.—Calculated rate coefficients for $\alpha_1(T)$ [D(1s) + H$^+$ → D$^+$ + H(1s)] and the reverse process $\alpha_2(T)$ [D$^+$ + H(1s) → D(1s) + H$^+$] vs. gas temperature T. Results for α_1 are from this work (*thick solid curve*), Watson (1976; *thick dashed curve*), Watson et al. (1978; *squares*), and Galli & Palla (1998; *thick dotted curve*). Results for α_2 are from this work (*thin solid curve*), Watson (1976; *thin dashed curve*), Watson et al. (1978; *circles*), and Galli & Palla (1998; *thin dotted curve*).

TABLE 1

CALCULATED RATE COEFFICIENTS FOR $\alpha_1(T)$ [D(1s) + H$^+$ → D$^+$ + H(1s)] AND THE REVERSE PROCESS $\alpha_2(T)$ [D$^+$ + H(1s) → D(1s) + H$^+$] VERSUS GAS TEMPERATURE T

T (K)	α_1 (cm^3 s^{-1})		α_2 (cm^3 s^{-1})	
	Present	Watson et al. (1978)	Present	Watson et al. (1978)
1	3.88E−28		1.73E−09	
2.7	1.79E−16		1.45E−09	
5	2.21E−13		1.18E−09	
10	1.30E−11	1.0E−11	9.55E−10	7.4E−10
15	5.12E−11		8.95E−10	
20	1.04E−10		8.90E−10	
25	1.63E−10	1.5E−10	9.06E−10	8.4E−10
30	2.22E−10		9.31E−10	
35	2.81E−10		9.59E−10	
40	3.38E−10		9.89E−10	
45	3.93E−10		1.02E−09	
50	4.45E−10	4.4E−10	1.05E−09	1.0E−09
75	6.75E−10	6.8E−10	1.20E−09	1.2E−09
100......	8.63E−10	8.6E−10	1.32E−09	1.3E−09
200......	1.40E−09	1.4E−09	1.73E−09	1.7E−09
300......	1.76E−09	1.7E−09	2.03E−09	2.0E−09
400......	2.05E−09		2.28E−09	
500......	2.29E−09		2.49E−09	
600......	2.50E−09		2.68E−09	
700......	2.68E−09		2.85E−09	
800......	2.85E−09		3.01E−09	
900......	3.01E−09		3.15E−09	
1000	3.15E−09		3.29E−09	
1500	3.75E−09		3.86E−09	
2000	4.23E−09		4.32E−09	
3000	5.00E−09		5.07E−09	
4000	5.61E−09		5.67E−09	
5000	6.13E−09		6.18E−09	
6000	6.59E−09		6.63E−09	
7000	7.00E−09		7.04E−09	
8000	7.37E−09		7.41E−09	
9000	7.72E−09		7.75E−09	
10000	8.04E−09		8.07E−09	
11000	8.34E−09		8.37E−09	
12000	8.62E−09		8.65E−09	
13000	8.89E−09		8.92E−09	
14000	9.15E−09		9.17E−09	
15000	9.39E−09		9.42E−09	
20000	1.05E−08		1.05E−08	
25000	1.14E−08		1.14E−08	
30000	1.22E−08		1.23E−08	
35000	1.30E−08		1.30E−08	
40000	1.37E−08		1.37E−08	
50000	1.49E−08		1.49E−08	
75000	1.73E−08		1.74E−08	
100000...	1.93E−08		1.93E−08	
200000...	2.50E−08		2.50E−08	

temperature. We attribute this to the rapid increase in σ_2 with decreasing collision energy (see Fig. 2 of Igarashi & Lin 1999).

We have fitted our calculated CT rate coefficients using the formula

$$\alpha(T) = aT^b \exp (-c/T) + dT^e . \quad (6)$$

The best-fit values are listed in Table 2. The fits for α_1 and α_2 are accurate to better than 6% and 4%, respectively, for $2.7 \le T \le 2 \times 10^5$ K.

Several other groups have carried out detailed calcu-

TABLE 2

FIT PARAMETERS FOR OUR CALCULATED RATE COEFFICIENTS $\alpha_1(T)$
[$D(1s) + H^+ \to D^+ + H(1s)$] AND THE REVERSE PROCESS
$\alpha_2(T)$ [$D^+ + H(1s) \to D(1s) + H^+$]

Rate Coefficient	a ($\mathrm{cm^3\ s^{-1}}$)	b	c (K)	d ($\mathrm{cm^3\ s^{-1}}$)	e
α_1.................	2.00E−10	0.402	37.1	−3.31E−17	1.48
α_2.................	2.06E−10	0.396	33.0	2.03E−09	−0.332

lations for σ_1 and σ_2. Davis & Thorson (1978) published results for σ_1 from 3.7 to ≈ 100 meV. Results for σ_1 and σ_2 were reported by Hunter & Kuriyan (1977) for energies from 10^{-3} to 7.5 eV, by Hodges & Breig (1993) from 10^{-3} to 10 eV, and by Esry et al. (2000) from ≈ 3.7 meV to 8 eV. In general, the calculations of Igarashi and collaborators are in good to excellent agreement with these published results. The most significant difference is for energies above 10^{-3} eV, for which the results of Hunter & Kuriyan (1977) can fall as much as 15% below those of Igarashi and collaborators (Igarashi & Lin 1999; Zhao et al. 2000; A. Igarashi 2001, private communication). This is partially due to the accidental overlap of minima in the oscillating cross sections with the energy points published by Hunter & Kuriyan (1977).

There have been a couple of experimental measurements of σ_1. We are unaware of any experimental results for σ_2. Absolute measurements of σ_1 have been carried out by Newman et al. (1982) for energies between ≈ 0.1 and 10 eV. The theoretical results of Zhao et al. (2000) and Esry et al. (2000) are in good agreement with these measurements. Relative measurements for σ_1 have been carried out by Wells et al. (2001) for energies between threshold and 1 eV. Good agreement was found with the calculations of Esry et al. (2000) between ≈ 0.02 and 1 eV. Uncertainties in background subtraction limit the reliability of the experimental results below 0.02 eV.

Using the results of Hunter & Kuriyan (1977), Watson et al. (1978) calculated α_1 and α_2 for a number of temperatures between 10 and 300 K. These results are listed in Table 1 and are also plotted in Figure 1. For $T \geq 50$ K, the results of Watson et al. agree with ours to better than 5%. At 25 K, their results differ from ours by $\approx 8\%$ and at 10 K by $\approx 30\%$. The differences for $T \leq 25$ K are most likely due to the uncertainty associated with extrapolating the results of Hunter & Kuriyan (1977) to energies below those published (Watson et al. 1978).

Galli & Palla (1998) fit the results of Watson et al. (1978) for α_1 and α_2. The resulting fitted rate coefficients are plotted in Figure 1. Between 10 and 300 K, these fitted rate coefficients agree with our results not quite as well as the results of Watson et al. Agreement with our results becomes progressively worse the further one extrapolates these fitted rates outside this temperature range.

Watson (1976) presented an estimate for α_1 and α_2, which we plot in Figure 1. These estimated rate coefficients are in poor agreement with our results here, differing significantly in both the values and temperature dependences of α_1 and α_2.

4. SOME ASTROPHYSICAL IMPLICATIONS

4.1. The Early Universe

Recently, results from a number of different chemical models of the early universe have been published. For these models, Puy et al. (1993) and Stancil et al. (1998) used the estimated rate coefficients of Watson (1976). Galli & Palla (1998) used their fits to the results of Watson et al. (1978). For redshifts $z \gtrsim 50$, above which the gas temperature is predicted to be $\gtrsim 50$ K (Puy et al. 1993), the rate coefficients used by Puy et al. and Stancil et al. (1998) begin to differ significantly from our newly calculated results. At $z \approx 400$ ($T \approx 1000$ K; Puy et al. 1993), the rate coefficients used by them are a factor of ≈ 3 smaller than our results. In contrast, the extrapolated rate coefficients used by Galli & Palla (1998) are only $\approx 22\%$ smaller. Determining the full implications of our new rate coefficients will require rerunning updated versions of these various chemical models of the early universe.

4.2. Molecular Clouds

Modeling studies of molecular clouds have been carried out recently by Millar, Bennett, & Herbst (1989), Pineau des Forêts, Roueff, & Flower (1989), Heiles, McCullough, & Glassgold (1993), Rodgers & Millar (1996), and Timmermann (1996). These studies have all used the results of Watson (1976) for α_1 and α_2, and hence significantly underestimate these two rate coefficients for $T \gtrsim 100$ K. Because reaction (1) followed by reaction (3) is predicted to be a major source of HD in molecular clouds (Black & Dalgarno 1973; Dalgarno, Black, & Weisheit 1973; Watson 1973), underestimating α_1 could in turn lead to an underestimate in the amount of HD produced in these clouds.

4.3. High-Redshift QSO Absorption Systems

Observations of high-redshift QSO absorption systems are used to infer the primordial D/H ratio. These studies are carried out assuming that the D I/H I ratio is identical to that of D/H (Burles & Tytler 1998). Here we investigate the validity of this assumption in light of the different values for α_1 and α_2.

The D/H ratio inferred from these observations is given by

$$\frac{n_{\mathrm{D}}}{n_{\mathrm{H}}} = \frac{f_{\mathrm{H\,I}}}{f_{\mathrm{D\,I}}} \frac{N(\mathrm{D\,I})}{N(\mathrm{H\,I})}, \qquad (7)$$

where n_{D} is number density of deuterium, $N(\mathrm{D\,I})$ is the column density of D I, and $f_{\mathrm{D\,I}}$ is the abundance of D I relative to the total abundance of D. Similar definitions exist for H and H I. We can write $f_{\mathrm{D\,I}}$ as

$$\frac{1}{f_{\mathrm{D\,I}}} = 1 + \frac{n_{\mathrm{D\,II}}}{n_{\mathrm{D\,I}}}. \qquad (8)$$

A similar expression can be written for $f_{\mathrm{H\,I}}$.

Currently, there are believed to be six reliable measurements of D/H in high-redshift QSO absorbers (Pettini & Bowen 2001). These measurements all assume $f_{\mathrm{D\,I}} = f_{\mathrm{H\,I}}$. To determine the validity of this assumption, we evaluate

$$\frac{f_{\mathrm{H\,I}}}{f_{\mathrm{D\,I}}} = \frac{1 + n_{\mathrm{D\,II}}/n_{\mathrm{D\,I}}}{1 + n_{\mathrm{H\,II}}/n_{\mathrm{H\,I}}}, \qquad (9)$$

using our new results for α_1 and α_2.

At the inferred temperatures in these six absorbers ($T \approx 1.1 \times 10^4$ K), the gas is predicted to have an insignificant abundance of molecules (Petitjean, Srianand, & Ledoux 2000). The ionization balance of deuterium in these

QSO absorbers can therefore be written

$$\frac{n_{D\,II}}{n_{D\,I}} = \frac{\beta_{D\,I} + n_e C_{D\,I} + n_{H\,II}\alpha_{D+H^+} + \sum_{X^{q+}} n_{X^{q+}}\alpha_{D+X^{q+}}}{n_e R_{D\,II} + n_{H\,I}\alpha_{H+D^+} + \sum_X n_X \alpha_{X+D^+}}.$$
(10)

In the numerator on the right hand side (RHS) of this equation, $\beta_{D\,I}$ is the photoionization (PI) rate of D I due to the radiation field and accounts for further ionization due to the resulting nonthermal photoelectrons, n_e is the electron density, $C_{D\,I}$ is the electron impact ionization (EII) rate coefficient due to thermal electrons, α_{D+H^+} is the rate coefficient for D + H$^+$ collisions producing D$^+$, and similarly for $\alpha_{D+X^{q+}}$, where X^{q+} represents a q-times charged ion of element X, and the sum over X^{q+} includes the ions of all elements except for those of hydrogen and deuterium. Here, α_{D+H^+} and $\alpha_{D+X^{q+}}$ are purely CT rate coefficients. This is because collisions that leave both colliding particles in an ionized state are predicted to be insignificant at the temperatures of interest (Janev, Presnyakov, & Shevelko 1985). In the denominator on the RHS, $R_{D\,II}$ is the radiative-recombination (RR) rate coefficient for D II, α_{H+D^+} is the CT rate coefficient for H + D$^+$ collisions producing D, and similarly for α_{X+D^+}.

The PI rates and EII and RR rate coefficients for deuterium and hydrogen are expected to be essentially identical (Galli & Palla 1998; Stancil et al. 1998). The differences in the energy-level structure of deuterium and hydrogen have an insignificant effect on these processes. Thus, in equation (10) we can substitute

$$\beta_{H\,I} = \beta_{D\,I},$$
(11)

$$C_{H\,I} = C_{D\,I},$$
(12)

and

$$R_{H\,II} = R_{D\,II}.$$
(13)

Next, we add and subtract

$$n_{D\,II}\alpha_{H+D^+} + \sum_{X^{q+}} n_{X^{q+}}\alpha_{H+X^{q+}}$$
(14)

to the numerator on the RHS of equation (10) and

$$n_{D\,I}\alpha_{D+H^+} + \sum_X n_X \alpha_{X+H^+}$$
(15)

to the denominator. We note that using equation (10), we get $n_{H\,II}/n_{H\,I}$ by interchanging all charge states of D with the corresponding charge states of H (and vice versa). Hence, we can rewrite equation (10) as

$$\frac{n_{D\,II}}{n_{D\,I}} = \frac{n_{H\,II}}{n_{H\,I}}\left(\frac{1+\gamma_1/\delta}{1+\gamma_2/\delta}\right),$$
(16)

where

$$\gamma_1 = \alpha_{D+H^+} - \frac{n_{D\,II}}{n_{H\,II}}\alpha_{H+D^+} + \sum_{X^{q+}}\frac{n_{X^{q+}}}{n_{H\,II}}(\alpha_{D+X^{q+}} - \alpha_{H+X^{q+}}),$$
(17)

$$\gamma_2 = \alpha_{H+D^+} - \frac{n_{D\,I}}{n_{H\,I}}\alpha_{D+H^+} + \sum_X \frac{n_X}{n_{H\,I}}(\alpha_{X+D^+} - \alpha_{X+H^+}),$$
(18)

and

$$\delta = \frac{n_e}{n_{H\,I}}R_{H\,II} + \frac{n_{D\,II}}{n_{H\,I}}\alpha_{D+H^+} + \sum_X \frac{n_X}{n_{H\,I}}\alpha_{X+H^+}.$$
(19)

We can simplify γ_1 and γ_2. First we note that $\alpha_{D+H^+} = \alpha_1$ and $\alpha_{H+D^+} = \alpha_2$, and at the temperatures of interest, $\alpha_1 \approx \alpha_2 \approx 8.3 \times 10^{-9}$ cm^3 s^{-1}. Now, to a first approximation, $n_{D\,II}/n_{H\,II}$ and $n_{D\,I}/n_{H\,I}$ are equal to the primordial D/H value that we take to be $\approx 2 \times 10^{-5}$ (from Pettini & Bowen 2001). Hence, the second term in equations (17) and (18) is roughly 5 orders of magnitude smaller than the first term and can be dropped.

At energies important for $T \approx 1.1 \times 10^4$ K, we note that $\sigma_1 \approx \sigma_2$. Similarly, we expect at these temperatures $\sigma_{D+X^{q+}}(v) \approx \sigma_{H+X^{q+}}(v)$ and $\sigma_{X+D^+}(v) \approx \sigma_{X+H^+}(v)$, where v is the relative velocity. As a result, we have $\alpha_{D+X^{q+}}(\mu_{DX})^{1/2} \approx \alpha_{H+X^{q+}}(\mu_{HX})^{1/2}$ and $\alpha_{X+D^+}(\mu_{DX})^{1/2} \approx \alpha_{X+H^+}(\mu_{HX})^{1/2}$. Here, $\mu_{HX} \approx 1$ and $\mu_{DX} \approx 2$ are the reduced masses. For those ions in which CT is important in photoionized plasmas (e.g., QSO absorbers), we estimate that $\alpha_{D+X^{q+}}$, $\alpha_{H+X^{q+}}$, α_{X+D^+}, and α_{X+H^+} will all be $\lesssim 10^{-9}$ cm^3 s^{-1} (Kingdon & Ferland 1996). The expressions in the parentheses in the third term in equations (17) and (18) are thus $\lesssim 4 \times 10^{-10}$ cm^3 s^{-1}. Furthermore, we note that the metallicity in these absorbing systems are $\approx 10^{-2}$ solar (Pettini & Bowen 2001) and that we expect $n_{X^{q+}}/n_{H\,II}$ and $n_X/n_{H\,I}$ to be within a couple of orders of magnitude of these reduced abundances. As a result, we can also drop the third term in equations (17) and (18). With these approximations, we can rewrite equation (16) as

$$\frac{n_{D\,II}}{n_{D\,I}} \approx \frac{n_{H\,II}}{n_{H\,I}}\left(\frac{\alpha_1}{\alpha_2}\right)\left(\frac{1+\delta/\alpha_1}{1+\delta/\alpha_2}\right).$$
(20)

For typical QSO absorption systems, we estimate that $\delta/\alpha_1 \approx \delta/\alpha_2 \lesssim 0.15$, and as α_1 and α_2 differ by $\lesssim 0.4\%$ at $T \approx 1.1 \times 10^4$ K, equation (20) reduces to

$$\frac{n_{D\,II}}{n_{D\,I}} \approx \frac{n_{H\,II}}{n_{H\,I}}\left(\frac{\alpha_1}{\alpha_2}\right).$$
(21)

Because σ_1 has a threshold, in contrast to σ_2, the ratio α_1/α_2 will always be less than 1. For the temperature of interest here, we have

$$\frac{n_{D\,II}}{n_{D\,I}} \approx 0.996\,\frac{n_{H\,II}}{n_{H\,I}}.$$
(22)

Substituting these results into equations (7) and (9), we find

$$\frac{n_D}{n_H} = \begin{cases} \approx 0.996 N(D\,I)/N(H\,I) & n_{H\,II} \gg n_{H\,I}, \\ 1.000 N(D\,I)/N(H\,I) & n_{H\,II} \ll n_{H\,I}. \end{cases}$$
(23)

The uncertainty in the above factor of 0.996 depends on the accuracy of the theoretical cross sections we have used here. Verifying the accuracy of these cross sections will require further theoretical and experimental studies. However, we note that the variation of $\approx 0.4\%$ in n_D/n_H is a factor of $\gtrsim 25$ smaller than the current $\gtrsim 10\%$ uncertainties in QSO absorber D/H measurements. Thus, it is likely to be some time before the subtle differences in reactions (1) and (2) become important for primordial D/H measurements.

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