



# Stimulated Radiative Association of He and H +

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## STIMULATED RADIATIVE ASSOCIATION OF He AND H<sup>+</sup>

B. ZYGELMAN,<sup>1</sup> P. C. STANCIL,<sup>2,3</sup> AND A. DALGARNO<sup>4</sup>

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### ABSTRACT

The enhancement of the rate coefficient for the radiative association of He and H<sup>+</sup> to form HeH<sup>+</sup> arising from stimulated emission due to a blackbody radiation field is calculated. The effects on the fractional abundance of HeH<sup>+</sup> in the early universe, in supernova ejecta, and in planetary nebulae are small. There may occur some enhancement in the abundance of HeH<sup>+</sup> in quasar broad-line clouds.

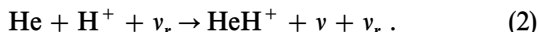
*Subject headings:* atomic processes — early universe — molecular processes — planetary nebulae: general — quasars: general

### 1. INTRODUCTION

Processes that lead to the formation and destruction of the molecular ion HeH<sup>+</sup> in astrophysical environments have been the subject of a number of investigations (Jura & Dalgarno 1971; Dabrowski & Herzberg 1978; Frommhold & Pickett 1978; Roberge & Dalgarno 1982; Zygelman & Dalgarno 1990; Kimura et al. 1993; Juřek, Špirko, & Kraemer 1995; Kraemer, Špirko, & Juřek 1995). At low temperatures, the HeH<sup>+</sup> molecule can be formed via the direct radiative process (1) (Roberge & Dalgarno 1982)



but in this paper we focus on the process whereby the formation of the HeH<sup>+</sup> ion is enhanced via a stimulating background radiation field of frequency  $\nu_r$ ,



We were motivated to consider the second process, which we will call process (2), following a suggestion by V. K. Dubrovich (1996, private communication) that the rate of formation of stable molecules in the early universe may be enhanced through the radiative association of atoms stimulated by the cosmic background radiation (CBR) field. Stancil & Dalgarno (1997) have recently shown, from the value obtained allowing only the spontaneous emission of photons, that the rate for Li and H to associate and form LiH is enhanced when stimulated by the CBR field from the value obtained allowing only the spontaneous emission of photons (Dalgarno, Kirby, & Stancil 1996).

In this paper we extend the theory of radiative association to include stimulated emission and calculate rate coefficients for the formation of HeH<sup>+</sup> as a function of the matter temperature  $T_m$  and blackbody radiation temperature  $T_r$ . Special attention is given to the treatment of long-lived, inverse predissociation resonances (Dabrowski & Herzberg 1978; Roberge & Dalgarno 1982) seen in this system. We explore the possibility for enhancement of the rate of formation for HeH<sup>+</sup> in the early universe when stimulated by the CBR radiation field. We also investigate the role of stimulated association of HeH<sup>+</sup> in supernova

ejecta, planetary nebulae, and quasars. Atomic units are used throughout, unless stated otherwise.

### 2. THEORY

The cross section for the spontaneous radiative association process (1) is (see, e.g., Zygelman & Dalgarno 1990; Gianturco & Giorgi 1996)

$$\sigma_{\text{sp}}(k) = \sum_J \sum_n \frac{64}{3} \frac{\pi^5 \nu^3}{c^3 k^2} [(J+1)M_{J+1,J}^2 + JM_{J-1,J}^2], \quad (3)$$

where the sum extends over the ro-vibrational quantum numbers  $n$  and  $J$  of the bound levels of the HeH<sup>+</sup> ion. The frequency  $\nu$  of the emitted photon is  $2\pi\nu = k^2/2\mu - E_{n,J}$ , where  $k$  is the wavenumber corresponding to the relative motion of H<sup>+</sup> and He during their initial approach,  $\mu$  is the nuclear reduced mass of the molecular ion, and  $E_{n,J}$  is the energy eigenvalue for ro-vibrational level  $(n, J)$  of the molecular ion HeH<sup>+</sup> in its electronic ground  $^1\Sigma^+$  state. The overlap integral  $M_{J,J'}$  is defined by

$$M_{J,J'} = \int_0^\infty dR f_J(kR) D(R) \phi_{J'}^n(R), \quad (4)$$

where  $f_J(kR)$  is a radial, energy-normalized, continuum function that is a solution to the Schrödinger equation

$$\left\{ \frac{d^2}{dR^2} - \frac{J(J+1)}{R^2} - 2\mu[V_X(R) - V_X(\infty)] + k^2 \right\} f_J(kR) = 0, \quad (5)$$

in which  $V_X(R)$  is the potential energy curve for the  $X^1\Sigma^+$  state,  $D(R)$  is the radial electric dipole moment, and  $\phi_J^n(R)$  is a bound state eigensolution with eigenvalue  $E_{n,J}$ .

The spontaneous, dipole-allowed, transition rate from quantum state  $|a\rangle$  to  $|b\rangle$  is given by the Fermi Golden Rule expression (Schiff 1968)

$$A_{\text{sp}} = \frac{4\omega_{ab}^3}{3c^3} |\langle a | \mathbf{d} | b \rangle|^2, \quad (6)$$

where  $\omega_{ab}$  is the angular frequency associated with the transition, and  $\mathbf{d}$  is the dipole operator evaluated with respect to the nuclear center of mass. We assume the Born-Oppenheimer (BO) approximation for the initial state,

$$|a\rangle \equiv |^1\Sigma^+\rangle \sum_{lm} Y_{lm}(\theta\phi) Y_{lm}^*(\theta_{\mathbf{k}}\phi_{\mathbf{k}}) 4\pi i^l f_l(R)/R, \quad (7)$$

where  $|^1\Sigma^+\rangle$  is the BO ground-state wave function and  $\theta_{\mathbf{k}}\phi_{\mathbf{k}}$  are the polar and azimuthal angles that specify the

<sup>1</sup> W. M. Keck Laboratory for Computational Physics, Department of Physics, University of Nevada, Las Vegas, NV 89154-4002; bernard@physics.unlv.edu.

<sup>2</sup> Physics Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6372; stancil@mail.phy.ornl.gov.

<sup>3</sup> Eugene P. Wigner Fellow.

<sup>4</sup> Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138; adalgarno@cfa.harvard.edu.

relative momentum for the  $H^+$  and He fragments in their initial approach. The bound state into which the fragments recombine is

$$|b\rangle \equiv |^1\Sigma^+\rangle [\phi_J^n(R)/R] Y_{JM}(\theta\phi). \quad (8)$$

Inserting equations (8) and (7) into equation (6), making use of the fact that  $\langle ^1\Sigma^+ | \mathbf{d} | ^1\Sigma^+ \rangle$  is directed along the internuclear axis, and dividing the resulting transition probability by the flux,  $2k^2/\pi$ , of the incident wave, we obtain expression (3) for the spontaneous association cross section.

An expression for the cross section for the stimulated process (2) is obtained by replacing equation (6) with the Fermi Golden Rule formula for the stimulated emission rate (Schiff 1968):

$$A_{\text{stim}} = \frac{4\pi^2}{3c} I(\omega_{ab}) |\langle a | \mathbf{d} | b \rangle|^2, \quad (9)$$

where  $I(\omega_{ab})$  is the energy flux per unit frequency of the radiation field at  $\nu = \omega_{ab}/2\pi$ . Using equation (9), we obtain the cross section for stimulated association

$$\sigma_{\text{stim}}(k) = \sum_J \sum_n \frac{8}{3} \frac{\pi^4 I(\nu)}{ck^2} [(J+1)M_{J+1,J}^2 + JM_{J-1,J}^2], \quad (10)$$

where  $\nu$  is defined as above. We add the cross sections defined in equations (3) and (10) to obtain the total cross section,  $\sigma = \sigma_{\text{sp}} + \sigma_{\text{stim}}$ ,

$$\sigma = \sum_J \sum_n \frac{64}{3} \frac{\pi^5 \nu^3}{c^3 k^2} \left(1 + \frac{I}{I_0}\right) [(J+1)M_{J+1,J}^2 + JM_{J-1,J}^2], \quad (11)$$

where  $I_0 = 4h\nu^3/c^2$ . If the radiation field is that of a blackbody characterized by temperature  $T_b$ ,

$$I(\nu) = \frac{4h\nu^3}{c^2} \frac{1}{\exp(h\nu/kT_b) - 1}, \quad (12)$$

and we obtain the expression given by Stancil & Dalgarno (1997):

$$\sigma = \sum_J \sum_n \frac{64}{3} \frac{\pi^5 \nu^3}{c^3 k^2} \left[ \frac{1}{1 - \exp(-h\nu/kT_b)} \right] \times [(J+1)M_{J+1,J}^2 + JM_{J-1,J}^2]. \quad (13)$$

### 3. CALCULATIONS

#### 3.1. Molecular Properties

In order to carry out the sum in equation (13), we need to itemize all the bound states supported by the potential curve of the  $X^1\Sigma^+$  ground electronic state of the  $\text{HeH}^+$  ion. In this calculation we employed the potential curve tabulated by Bishop & Cheung (1979). The reduced mass of the molecular ion is taken to have the value  $\mu = 1467.4243$  a.u. The wave functions, corresponding to the nuclear motion, were obtained using a Numerov integration scheme, and the eigenvalues associated with these states are tabulated in Table 1. In that table, the vibrational and rotational quantum numbers,  $n$  and  $J$ , respectively, are tabulated alongside the eigenenergies  $-E_{n,J}$ . A total of 158 bound states were found, three less than obtained by Juřek et al.

(1995), who also used the potential curve of Bishop & Cheung (1979). A possible explanation for this discrepancy is that the two calculations used different values for the reduced mass. We adopted the radial dipole moment  $D(R)$  tabulated by Juřek et al. (1995).

#### 3.2. Cross Sections

In Figure 1 we illustrate the calculated cross sections for processes (1) and (2) in the collision energy range from 0.01 to 1000 meV and for blackbody temperatures up to 5000 K. The curve corresponding to the value  $T_b = 0$  K is for the spontaneous radiative association cross sections. Throughout the collision energy range considered, the background radiation field produces an enhancement in the association cross section. The effect is most pronounced at low collision energies and diminishes at higher collision energies. At collision energies corresponding to matter temperatures of about 11,600 K, the stimulated radiative association cross section, for the range of radiation temperatures considered, becomes negligible.

The pronounced peak, or resonance, structures seen are due to the existence of quasibound ro-vibrational levels in the  $\text{HeH}^+$  molecule. These resonances are known to contribute significantly to the overall spontaneous association rate coefficients at low matter temperatures. In Figure 1 we do not show resonances whose widths are  $\ll 10^{-3}$  meV; however, these resonances and the parameters that define them are shown separately in Figure 2 and Table 2. In Figure 2 we illustrate the cross section for process (1) in the vicinity of a resonance for collision energy  $E_r = 1.5799469$  meV. The filled circles represent the results of our fully quantal calculation, whereas the solid lines running through these points are nonlinear fits of the data to the Breit-Wigner form

$$\sigma_r(E) = \frac{\Gamma_r \Gamma/2}{(E - E_r)^2 + (\Gamma/2)^2}. \quad (14)$$

In equation (14) the cross sections are expressed in atomic units and the parameters  $E_r$ ,  $\Gamma$ , and  $\Gamma_r$  are given in units of meV energy. The parameters are tabulated in Table 2 for several narrow resonances. We note that the resonance position,  $E_r$ , and total widths,  $\Gamma$ , are essentially independent

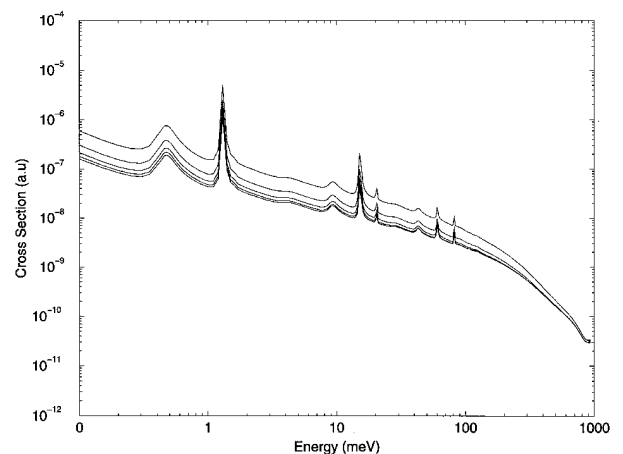


FIG. 1.—Cross sections ( $a_0^2$ ) for stimulated plus spontaneous radiative association of He and  $H^+$  for various blackbody radiation temperatures  $T_b$ .  $T_b = 0, 500, 1000, 2000,$  and  $5000$  K from bottom to top, respectively.

TABLE 1  
RO-VIBRATIONAL LEVELS FOR THE GROUND STATE OF THE HeH<sup>+</sup> ION

<i>n</i>	<i>J</i>	$-E(n, J)$	<i>n</i>	<i>J</i>	$-E(n, J)$	<i>n</i>	<i>J</i>	$-E(n, J)$	<i>n</i>	<i>J</i>	$-E(n, J)$	<i>n</i>	<i>J</i>	$-E(n, J)$
0.....	0	1.84412	1.....	12	0.93243	3.....	1	0.86954	4.....	14	0.13297	7.....	1	0.13431
0.....	1	1.83581	1.....	13	0.84902	3.....	2	0.85706	4.....	15	0.07641	7.....	2	0.12821
0.....	2	1.81923	1.....	14	0.76173	3.....	3	0.83846	4.....	16	0.02054	7.....	3	0.11920
0.....	3	1.79449	1.....	15	0.67106	3.....	4	0.81386	5.....	0	0.42415	7.....	4	0.10749
0.....	4	1.76173	1.....	16	0.57757	3.....	5	0.78346	5.....	1	0.41937	7.....	5	0.09332
0.....	5	1.72112	1.....	17	0.48182	3.....	6	0.74748	5.....	2	0.40985	7.....	6	0.07703
0.....	6	1.67291	1.....	18	0.38441	3.....	7	0.70619	5.....	3	0.39569	7.....	7	0.05904
0.....	7	1.61737	1.....	19	0.28598	3.....	8	0.65989	5.....	4	0.37705	7.....	8	0.03989
0.....	8	1.55479	1.....	20	0.18724	3.....	9	0.60894	5.....	5	0.35411	7.....	9	0.02029
0.....	9	1.48553	1.....	21	0.08898	3.....	10	0.55372	5.....	6	0.32713	7.....	10	0.00126
0.....	10	1.40997	2.....	0	1.16040	3.....	11	0.49466	5.....	7	0.29641	8.....	0	0.05808
0.....	11	1.32851	2.....	1	1.15344	3.....	12	0.43224	5.....	8	0.26229	8.....	1	0.05596
0.....	12	1.24158	2.....	2	1.13958	3.....	13	0.36697	5.....	9	0.22520	8.....	2	0.05178
0.....	13	1.14965	2.....	3	1.11889	3.....	14	0.29940	5.....	10	0.18560	8.....	3	0.04569
0.....	14	1.05318	2.....	4	1.09152	3.....	15	0.23018	5.....	11	0.14406	8.....	4	0.03793
0.....	15	0.95269	2.....	5	1.05765	3.....	16	0.16001	5.....	12	0.10124	8.....	5	0.02879
0.....	16	0.84869	2.....	6	1.01751	3.....	17	0.08971	5.....	13	0.05795	8.....	6	0.01872
0.....	17	0.74172	2.....	7	0.97135	3.....	18	0.02030	5.....	14	0.01522	8.....	7	0.00829
0.....	18	0.63234	2.....	8	0.91949	4.....	0	0.63005	6.....	0	0.25949	9.....	0	0.01753
0.....	19	0.52110	2.....	9	0.86225	4.....	1	0.62451	6.....	1	0.25552	9.....	1	0.01634
1.....	0	1.48323	2.....	10	0.80003	4.....	2	0.61347	6.....	2	0.24763	9.....	2	0.01404
1.....	1	1.47559	2.....	11	0.73322	4.....	3	0.59703	6.....	3	0.23594	9.....	3	0.01078
1.....	2	1.46037	2.....	12	0.66228	4.....	4	0.57532	6.....	4	0.22060	9.....	4	0.00683
1.....	3	1.43765	2.....	13	0.58767	4.....	5	0.54854	6.....	5	0.20183	9.....	5	0.00257
1.....	4	1.40757	2.....	14	0.50990	4.....	6	0.51692	6.....	6	0.17991	10.....	0	0.00321
1.....	5	1.37031	2.....	15	0.42954	4.....	7	0.48072	6.....	7	0.15519	10.....	1	0.00271
1.....	6	1.32611	2.....	16	0.34716	4.....	8	0.44029	6.....	8	0.12807	10.....	2	0.00178
1.....	7	1.27523	2.....	17	0.26341	4.....	9	0.39598	6.....	9	0.09905	10.....	3	0.00060
1.....	8	1.21797	2.....	18	0.17900	4.....	10	0.34822	6.....	10	0.06875	11.....	0	0.00014
1.....	9	1.15467	2.....	19	0.09475	4.....	11	0.29747	6.....	11	0.03794	11.....	1	0.00004
1.....	10	1.08571	2.....	20	0.01164	4.....	12	0.24426	6.....	12	0.00766			
1.....	11	1.01148	3.....	0	0.87581	4.....	13	0.18920	7.....	0	0.13739			

NOTE.—Energies are in electron volts.

of the radiation temperature. The width  $\Gamma_r$  does depend on the temperature, and it is useful to consider  $\Gamma_r$  as an effective radiative lifetime of the quasibound state formed.

The rate coefficient for process (2) is given by

$$k(T) = \sqrt{\frac{8\kappa T}{\mu\pi}} \left(\frac{1}{\kappa T}\right)^2 \int_0^\infty E\sigma(E) \exp\left(\frac{-E}{\kappa T}\right) dE, \quad (15)$$

where  $\sigma(E)$  is given by equation (13). Using the values for

the cross sections shown in Figure 1, we calculated a background rate coefficient,  $k_b$ , which is tabulated in Table 3. To include the contribution to the rate coefficient from resonances whose widths are less than  $10^{-3}$  meV, we use parameterization (14) in formula (15). We get

$$k_i = \sqrt{\frac{8\kappa T}{\mu\pi}} \left(\frac{\Gamma_r^i}{\kappa T}\right) \left(\frac{E_i}{\kappa T}\right) \exp\left(\frac{-E_i}{\kappa T}\right), \quad (16)$$

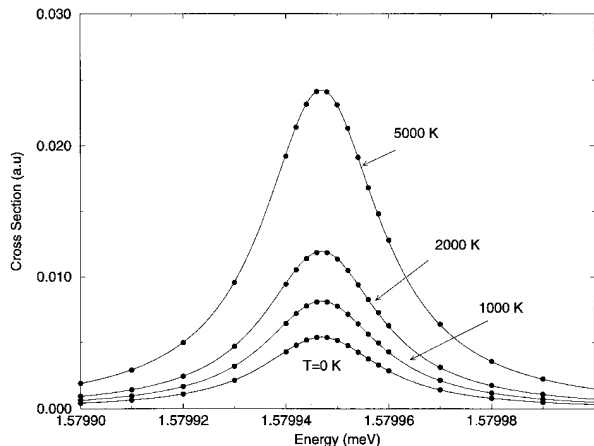


FIG. 2.—Cross sections near a resonance due to the existence of the  $J = 8, n = 8$  quasi-bound state at  $E = 1.5799469$  meV. The cross sections are calculated for blackbody radiation temperatures  $T_b$ .  $T_b = 0, 1000, 2000,$  and  $5000$  K from bottom to top, respectively.

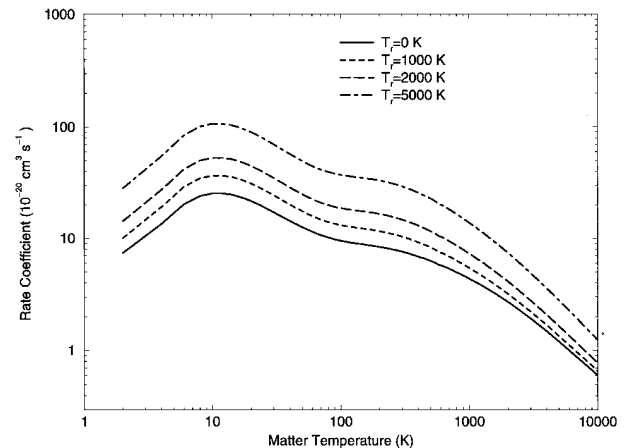


FIG. 3.—Rate coefficients for stimulated plus spontaneous radiative association of He and H<sup>+</sup> for various blackbody radiation temperatures  $T_b$ .  $T_b = 0, 1000, 2000,$  and  $5000$  K from bottom to top, respectively.

TABLE 2  
RO-VIBRATIONAL RESONANCES IN THE GROUND STATE OF THE HeH<sup>+</sup> ION

<i>T</i>	<i>n</i>	<i>J</i>	<i>E<sub>r</sub></i> (meV)	Γ	Γ <sub><i>r</i></sub>	<i>E<sub>r</sub></i> (meV)	Γ <sup>a</sup>
0.....	8	8	1.5799469	2.74 × 10 <sup>-5</sup>	7.423 × 10 <sup>-8</sup>	1.6365083	1.98 × 10 <sup>-5</sup>
1000.....	8	8	1.5799469	2.74 × 10 <sup>-5</sup>	1.112 × 10 <sup>-7</sup>		
2000.....	8	8	1.5799469	2.73 × 10 <sup>-5</sup>	1.627 × 10 <sup>-7</sup>		
5000.....	8	8	1.5799469	2.74 × 10 <sup>-5</sup>	3.322 × 10 <sup>-7</sup>		
0.....	5	15	25.2879286	9.513 × 10 <sup>-4</sup>	2.003 × 10 <sup>-8</sup>	25.576641	1.06 × 10 <sup>-4</sup>
1000.....	5	15	25.2879277	9.559 × 10 <sup>-4</sup>	3.541 × 10 <sup>-8</sup>		
2000.....	5	15	25.2879280	9.315 × 10 <sup>-4</sup>	5.505 × 10 <sup>-8</sup>		
5000.....	5	15	25.2879276	9.553 × 10 <sup>-4</sup>	1.214 × 10 <sup>-7</sup>		
0.....	4	17	33.0473819	1.69 × 10 <sup>-6</sup>	2.21 × 10 <sup>-8</sup>	33.43684	1.89 × 10 <sup>-6</sup>
1000.....	4	17	33.0473819	1.69 × 10 <sup>-6</sup>	3.78 × 10 <sup>-8</sup>		
2000.....	4	17	33.0473819	1.69 × 10 <sup>-6</sup>	6.05 × 10 <sup>-8</sup>		
5000.....	4	17	33.0473819	1.69 × 10 <sup>-6</sup>	1.31 × 10 <sup>-7</sup>		
0.....	3	19	46.63856180	1.63 × 10 <sup>-7</sup>	1.795 × 10 <sup>-8</sup>	47.148795	1.83 × 10 <sup>-7</sup>
1000.....	3	19	46.63856180	1.63 × 10 <sup>-7</sup>	2.973 × 10 <sup>-8</sup>		
2000.....	3	19	46.63856180	1.63 × 10 <sup>-7</sup>	4.753 × 10 <sup>-8</sup>		
5000.....	3	19	46.63856180	1.63 × 10 <sup>-7</sup>	1.029 × 10 <sup>-7</sup>		

<sup>a</sup> Jurek et al. 1995.

where *k<sub>i</sub>* is the contribution to the total rate coefficient from the *i*th resonance.

In Table 3 we tabulate, for several values of the CBR temperature *T<sub>b</sub>*, the background resonance contribution, and total rate coefficients for process (1).

4. ASTROPHYSICAL APPLICATIONS

The role that stimulated effects may play on chemical processes, including radiative association and radiative attachment, in astrophysical environments was discussed by

TABLE 3  
RATE COEFFICIENTS FOR STIMULATED RADIATIVE RECOMBINATION OF THE HeH<sup>+</sup> ION

<i>T<sub>b</sub></i>	<i>T<sub>m</sub></i>	<i>k<sub>b</sub></i>	<i>k<sub>1</sub></i>	<i>k<sub>2</sub></i>	<i>k<sub>3</sub></i>	<i>k<sub>4</sub></i>	<i>k</i>	<i>k<sup>a</sup></i>
0.....	2	7.336	0.083	0.000	0.000	0.000	7.419	6.34
	4	10.666	2.859	0.000	0.000	0.000	13.526	10.53
	8	13.960	10.002	0.000	0.000	0.000	23.962	19.46
	16	12.584	11.123	0.000	0.000	0.000	23.706	20.31
	30	9.755	7.395	0.003	0.000	0.000	17.154	15.30
	60	7.676	3.549	0.156	0.050	0.004	11.435	10.90
500.....	100	6.765	1.864	0.514	0.301	0.071	9.515	9.72
	2	8.318	0.101	0.000	0.000	0.000	8.418	...
	4	12.236	3.484	0.000	0.000	0.000	15.720	...
	8	16.112	12.187	0.000	0.000	0.000	28.300	...
	16	14.432	13.553	0.000	0.000	0.000	27.986	...
	30	11.028	9.011	0.004	0.000	0.000	20.044	...
1000.....	60	8.545	4.325	0.211	0.066	0.005	13.152	...
	100	7.465	2.271	0.695	0.393	0.091	10.915	...
	2	10.003	0.124	0.000	0.000	0.000	10.127	...
	4	14.820	4.284	0.000	0.000	0.000	19.103	...
	8	19.587	14.983	0.000	0.000	0.000	34.570	...
	16	17.468	16.663	0.000	0.000	0.000	34.131	...
2000.....	30	13.217	11.079	0.006	0.000	0.000	24.302	...
	60	10.135	5.317	0.276	0.086	0.007	15.821	...
	100	8.798	2.792	0.909	0.515	0.118	13.132	...
	2	14.134	0.181	0.000	0.000	0.000	14.315	...
	4	21.090	6.267	0.000	0.000	0.000	27.357	...
	8	27.975	21.923	0.000	0.000	0.000	49.898	...
5000.....	16	24.838	24.379	0.000	0.000	0.000	49.217	...
	30	18.599	16.210	0.009	0.001	0.000	34.818	...
	60	14.100	7.779	0.430	0.138	0.011	22.457	...
	100	12.149	4.086	1.413	0.824	0.189	18.661	...
	2	27.901	0.370	0.000	0.000	0.000	28.271	...
	4	41.902	12.795	0.000	0.000	0.000	54.697	...
	8	55.762	44.760	0.000	0.000	0.000	100.522	...
	16	49.311	49.778	0.000	0.000	0.000	99.089	...
	30	36.579	33.097	0.020	0.001	0.000	69.697	...
	60	27.438	15.884	0.947	0.298	0.024	44.591	...
	100	23.481	8.342	3.115	1.785	0.405	37.129	...

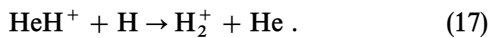
NOTES.—*T<sub>b</sub>* is the radiation temperature, *T<sub>m</sub>* is the matter temperature, *k<sub>b</sub>* is the background contribution to the total rate coefficient, *k<sub>i</sub>* is the contribution of the *i*th resonance tabulated in Table 2, and *k* is the total rate coefficient. Rate coefficients are expressed in units of 10<sup>-20</sup> cm<sup>3</sup> s<sup>-1</sup>.

<sup>a</sup> Jurek et al. 1995.

Stancil & Dalgarno (1998). We describe here a number of particular environments where HeH<sup>+</sup> is expected to be present.

#### 4.1. The Early Universe

Processes (1) and (2) were included in the early universe chemistry model of Stancil, Lepp, & Dalgarno (1998) for the postrecombination era. Figure 4 illustrates the results for model III of Stancil et al. (1998). The HeH<sup>+</sup> abundance is enhanced by a maximum factor of  $\sim 3$  near redshifts of about 2300, but photodissociation, assuming a local thermodynamic equilibrium (LTE) population distribution of ro-vibrational levels, limits its abundance to  $\sim 5 \times 10^{-20}$ . For  $z < 300$ , photodissociation becomes inefficient, so that the HeH<sup>+</sup> abundance rises to  $\sim 4 \times 10^{-15}$ . However, at  $z = 225$ , the radiation temperature is only 620 K, so that the enhancement is reduced to 17%. At this epoch it is primarily removed by



#### 4.2. Supernovae Ejecta

Miller et al. (1992) have tentatively identified two emission features in the spectra of SN 1987A as due to HeH<sup>+</sup>. It is formed by radiative association in the outer hydrogen envelope. The visible and infrared spectrum of the supernova consisted of a 5000 K photospheric emission from the central region and an infrared (IR) excess. The IR excess is believed to be due to dust that formed in the same zone as CO, somewhat inside the hydrogen layer. At 260 days after the explosion, Stancil & Dalgarno (1998) have estimated that the dilution factor from the photosphere to the hydrogen envelope, including geometric dilution and departure from a blackbody intensity, is about  $8 \times 10^{-4}$ . While the dust, which has an effective temperature of 700 K (Wooden et al. 1993), has a large dilution factor of 0.6, Stancil & Dalgarno (1998) estimated that the total HeH<sup>+</sup> production is enhanced only by about 2%.

#### 4.3. Planetary Nebulae and Quasars

HeH<sup>+</sup> is predicted to be formed in planetary nebulae (Cecchi-Pestellini & Dalgarno 1993), but it has so far eluded detection. It may, however, have been observed by the

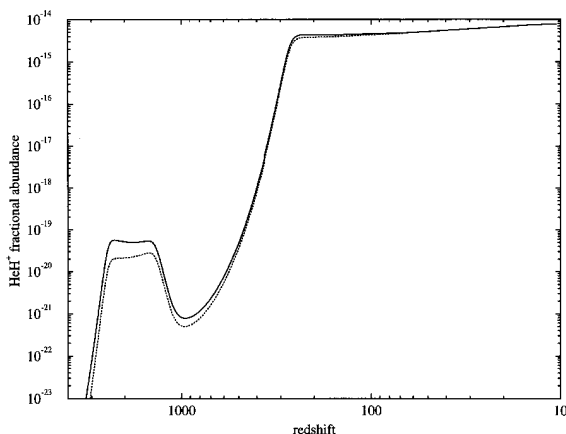


FIG. 4.—Fractional abundance of HeH<sup>+</sup> in the early universe, with (solid line) and without (dashed line) stimulated radiative association of He and H<sup>+</sup>. Model III of Stancil et al. (1998): closure parameter  $\Omega_0 = 1$ , baryonic-matter fraction  $\Omega_b = 0.0367$ , Hubble constant  $H_0 = 67 \text{ km s}^{-1} \text{ Mpc}^{-1}$ , and helium primordial fractional abundance  $\text{He}/\text{H} = 8.04 \times 10^{-2}$ .

*Infrared Space Observatory* in NGC 7027 (Liu et al. 1997). Its identification is complicated by the near-coincidence of its 149.14  $\mu\text{m}$  rotational transition with the 149.09 and 149.39  $\mu\text{m}$  lines of CH. For a stellar effective temperature of 175,000 K, Cecchi-Pestellini & Dalgarno (1993) find that molecules begin to form for distances greater than  $10^{16}$  cm from the white dwarf. This corresponds to a dilution factor of  $10^{-14}$ , suggesting that stimulated radiative association will play no role in the formation of HeH<sup>+</sup>.

Dubrovich & Lipovka (1995) suggest that HeH<sup>+</sup> is formed in high-redshift Ly $\alpha$  clouds at a distance of  $10^{23}$  cm from the nearest quasar. As the abundance produced by spontaneous radiative association is probably not much larger than that produced in the early universe, V. K. Dubrovich (1996, private communication) suggested that the HeH<sup>+</sup> production could be enhanced by stimulated radiative association due to the quasar radiation field. If we assume that the quasar radiates as a blackbody with a radius of  $10^{19}$  cm, the geometric dilution is about  $10^{-8}$ . Therefore stimulated effects appear to be unimportant in these clouds.

Stimulated association may be important in broad-line clouds. Kallman, Lepp, & Giovannoni (1987) predict that the fractional abundance of H<sub>2</sub> can reach 0.5 at a depth of about  $10^{14}$  cm into the cloud. Geometric dilution is therefore negligible, as this distance is much smaller than the quasar radius. In Figure 5 we plot the cross sections for process (1) as a function of radiation temperature up to  $10^6$  K for the values of collision energies,  $E = 1000, 100, 10,$  and  $1 \text{ meV}$ , which correspond to matter temperatures  $T_m \approx 8000, 800, 80,$  and  $8 \text{ K}$ , respectively. At radiation temperatures  $T_r > 10,000 \text{ K}$ , the figure shows that the rate for stimulated association scales as a linear function of the radiation temperature. This can also be demonstrated by assuming that  $h\nu/\kappa T_r \ll 1$  in equation (13). Expanding equation (13) to leading order in  $h\nu/\kappa T_r$ , we get

$$\sigma = T_r \sum_J \sum_n \frac{32 \pi^4 \nu^2}{3 c^3 k^2} [(J+1)M_{J+1,J}^2 + JM_{J-1,J}^2], \quad (18)$$

where  $T_r$  is expressed in atomic units. Figure 5 suggests that the HeH<sup>+</sup> abundance could be enhanced by an order of magnitude for a quasar effective temperature of 50,000 K,

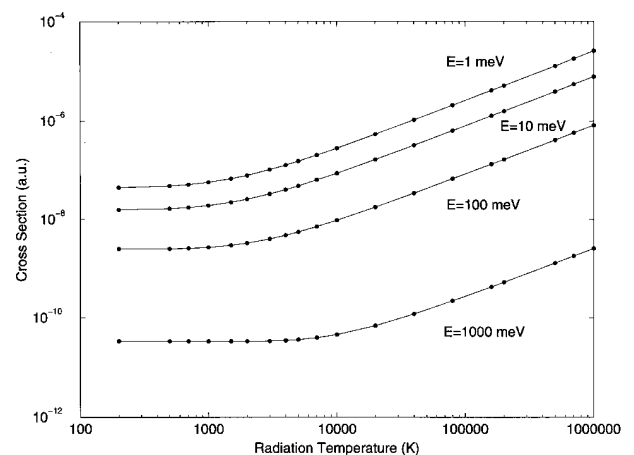


FIG. 5.—Calculated values for the cross sections (filled circles) for processes (1) and (2) as a function of radiation temperature  $T_r$ . The curves are labeled by the collision energy, and from bottom to top correspond to effective matter temperatures  $T_m \approx 8000, 800, 80,$  and  $8 \text{ K}$ , respectively.

but a detailed cloud model is necessary to test this prediction.

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#### REFERENCES

- Bishop, D. M., & Cheung, L. M. 1979, *J. Mol. Spectrosc.*, 75, 462  
Cecchi-Pestellini, C., & Dalgarno, A. 1993, *ApJ*, 413, 611  
Dabrowski, I., & Herzberg, G. 1978, *Ann. NY Acad. Sci.*, 38, 14  
Dalgarno, A., Kirby, K., & Stancil, P. C. 1996, *ApJ*, 458, 397  
Dubrovich, V. K., & Lipovka, A. A. 1995, *A&A*, 296, 309  
Frommhold, L., & Pickett, H. M. 1978, *Chem. Phys.*, 28, 441  
Gianturco, F. A., & Giorgi, G. P. 1996, *Phys. Rev. A*, 54, 4073  
Jura, M., & Dalgarno, A. 1971, *A&A*, 11, 243  
Juřek, M., Špirko, V., & Kraemer, W. P. 1995, *Chem. Phys.*, 193, 287  
Kallman, T., Lepp, S., & Giovannoni, P. 1987, *ApJ*, 321, 907  
Kimura, M., Lane, N. F., Dalgarno, A., & Dixson, R. G. 1993, *ApJ*, 405, 801  
Kraemer, W. P., Špirko, V., & Juřek, M. 1995, *Chem. Phys. Lett.*, 236, 177  
Liu, X., et al. 1997, *MNRAS*, 290, L71  
Miller, S., Tennyson, J., Lepp, S., & Dalgarno, A. 1992, *Nature*, 355, 420  
Roberge, W., & Dalgarno, A. 1982, *ApJ*, 255, 489  
Schiff, L. I. 1968, *Quantum Mechanics* (3d ed.; New York: McGraw-Hill)  
Stancil, P. C., & Dalgarno, A. 1997, *ApJ*, 479, 543  
———. 1998, *Faraday Discussions*, 109, in press  
Stancil, P. C., Lepp, S., & Dalgarno, A. 1998, *ApJ*, in press  
Wooden, D. H., et al. 1993, *ApJS*, 88, 477  
Zygelman, B., & Dalgarno, A. 1990, *ApJ*, 365, 239