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STIMULATED RADIATIVE ASSOCIATION OF Li AND H IN THE EARLY UNIVERSE

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ABSTRACT

The enhancement of the rate coefficient for the radiative association of Li and H to form LiH arising from stimulated emission by the cosmic background radiation field is calculated. It is shown that the effect on the fractional abundance of LiH in the early universe for redshifts z between 1000 and 10 is small.

Subject headings: atomic processes — cosmic microwave background — early universe

1. INTRODUCTION

It has been suggested that the molecule LiH may be formed in the postrecombination epoch of the early universe in sufficient abundance to be detectable through its imprint on the cosmic background radiation (de Bernardis et al. 1993; Maoli, Melchiorri, & Tosti 1994; Signore et al. 1994). Several studies of the lithium chemistry have been carried out (Lepp & Shull 1984; Puy et al. 1993; Palla, Galli, & Silk 1995; Stancil, Lepp, & Dalgarno 1996). The most recent studies concluded that because of the low rate coefficient for the radiative association of lithium and hydrogen,

the fraction of lithium that is converted to LiH is very small, making its detection improbable. In reaction (1), the formation of LiH is stabilized by the spontaneous emission of a photon of frequency ν as the Li and H approach and recede. V. K. Dubrovich (1996, private communication) has suggested that the radiative association of Li and H may be significantly enhanced by stimulated emission because of the cosmic background radiation with frequency ν_b ,

We present here the extension of the theory of radiative association to include stimulated emission and calculate the rate coefficient for the formation of LiH as a function of the matter temperature T_m and the blackbody radiation temperature T_b .

2. THEORY

The cross section for the spontaneous radiative association process (eq. [1]) is given by (see Zygelman & Dalgarno 1990)

$$\sigma^{\text{sp}}(E) = \sum_{N'} \sum_{v''} \sigma_N^{\text{sp}}(v'', E), \quad (3)$$

where

$$\begin{aligned} \sigma_N^{\text{sp}}(v'', E) = & \frac{64}{3} \frac{\pi^5}{c^3} \frac{v^3}{k^2} p[N' M_{v'', N' - 1; k, N'}^2 \\ & + (N' + 1) M_{v'', N' + 1; k, N'}^2], \end{aligned} \quad (4)$$

E is the relative collision energy, k is the wave number of relative motion, p is the probability of approach in the initial electronic state, N' is the initial rotational quantum number, v'' is the final vibrational quantum number, and M is the electric dipole matrix element connecting the initial continuum and final rotational-vibrational states of the ground electronic state. The final rotational level N'' is given by the dipole selection rule $N'' = N' \pm 1$. 929 rotational-vibrational levels are included in the calculation.

The photon density per unit frequency interval ρ of the cosmic background radiation field is given by

$$\rho(\nu, T_b) = \frac{8\pi h \nu^3}{c^3} \frac{1}{\exp(h\nu/k_b T_b) - 1}, \quad (5)$$

and the stimulated cross section is related to the spontaneous cross section by

$$\sigma_N^{\text{st}}(v'', E) = \frac{c^3}{8\pi h \nu^3} \sigma_N^{\text{sp}}(v'', E). \quad (6)$$

Multiplying equations (5) and (6) results in

$$\sigma_N^{\text{st}}(v'', E) \rho(\nu, T_b) = \frac{1}{\exp(h\nu/k_b T_b) - 1} \sigma_N^{\text{sp}}(v'', E), \quad (7)$$

giving, for the spontaneous plus stimulated partial cross section,

$$\sigma_N(v'', E) = \frac{\sigma_N^{\text{sp}}(v'', E)}{1 - \exp(-h\nu/k_b T_b)}. \quad (8)$$

The rate coefficients are obtained by averaging the product of the relative velocity and the cross section over a Maxwellian velocity distribution characterized by the matter temperature T_m .

The potential energy curve of the ground $X^1\Sigma^+$ state of LiH and the dipole moment are described in Dalgarno, Kirby, & Stancil (1996), and their accuracy has been confirmed by Gianturco et al. (1996).

3. RESULTS AND DISCUSSION

The total cross sections for stimulated and spontaneous radiative association are given in Figure 1 as a function of the energy E for radiation temperatures up to 5000 K. The

FIG. 1.—Cross sections (a_0^2) for stimulated plus spontaneous radiative association of Li and H for various blackbody radiation temperatures T_b . $T_b = 0, 300, 500, 1000, 3000, 4000$, and 5000 K (from bottom to top).

cross sections for $T_m = 0$ are those obtained earlier for spontaneous radiative association (Dalgarno et al. 1996). The pronounced structures that appear are a result of shape resonances in the elastic scattering of Li and H.

A comparison of the shape of the blackbody spectrum at $T_b = 440$ K and the spontaneous radiative association spectrum at $E = 30$ meV is given in Figure 2. The overlap of the two spectra illustrates the enhancement that can arise from

FIG. 2.—Shape of the spontaneous radiative association spectrum for a collision energy of 30 meV compared to that of a blackbody radiation spectrum of arbitrary magnitude. T_m and T_b are chosen from the early-universe Model A of Puy et al. (1993) for $z = 160$.

FIG. 3.—Rate coefficients for stimulated plus spontaneous radiative association of Li and H for various blackbody radiation temperatures T_b . $T_b = 0, 300, 500, 1000, 3000, 4000$, and 5000 K (from bottom to top).

stimulated emission from a blackbody. Equation (8) indicates that this enhancement increases with T_b or decreasing ν and to larger ν as T_b is increased.

The rate coefficients are displayed in Figure 3 as functions of T_m and T_b and are listed in Table 1. At $T_b = 500$,

1000, and 5000 K, stimulated emission increases the rate coefficients by factors of about 1.1, 1.3, and 4, respectively.

We have repeated the calculations of Stancil et al. (1996) of the fractional abundance of LiH as a function of the redshift z using the enhanced rate coefficients. Figure 4 illus-

FIG. 4.—Fractional abundance of LiH in the early universe with (solid line) and without (dashed line) stimulated radiative association of Li and H. Model III of Stancil et al. (1996): 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 lithium primordial fractional abundance $\text{Li}/\text{H} = 2.3 \times 10^{-10}$.

TABLE 1

TOTAL, SPONTANEOUS PLUS STIMULATED, RADIATIVE ASSOCIATION RATE
COEFFICIENTS α (10^{-20} cm³ s⁻¹) FOR Li + H AS A FUNCTION OF
MATTER TEMPERATURE T_m AND BLACKBODY RADIATION
TEMPERATURE T_b

T_m/T_b (K)	0	100	300	500	1000	3000	4000	5000
10	2.56	2.56	2.63	2.77	3.35	6.47	8.12	9.79
20	2.78	2.78	2.86	3.03	3.69	7.20	9.05	10.9
30	2.87	2.87	2.96	3.14	3.85	7.55	9.50	11.5
40	2.92	2.93	3.02	3.21	3.95	7.79	9.81	11.8
50	2.97	2.97	3.07	3.27	4.03	7.98	10.1	12.2
60	3.01	3.01	3.11	3.32	4.10	8.16	10.3	12.4
70	3.05	3.05	3.15	3.36	4.17	8.31	10.5	12.7
80	3.08	3.09	3.19	3.41	4.23	8.45	10.7	12.9
90	3.11	3.12	3.22	3.44	4.28	8.57	10.8	13.1
100	3.14	3.15	3.25	3.48	4.33	8.68	11.0	13.3
150	3.25	3.25	3.36	3.59	4.49	9.04	11.4	13.8
200	3.30	3.30	3.40	3.64	4.55	9.17	11.6	14.0
300	3.28	3.28	3.37	3.59	4.47	8.97	11.3	13.7
400	3.14	3.15	3.22	3.43	4.25	8.47	10.7	12.9
500	2.96	2.97	3.03	3.22	3.97	7.87	9.92	12.0
600	2.77	2.77	2.83	3.00	3.68	7.26	9.14	11.0
700	2.58	2.58	2.63	2.78	3.41	6.69	8.41	10.2
800	2.40	2.40	2.45	2.58	3.15	6.17	7.75	9.35
900	2.24	2.24	2.28	2.40	2.92	5.69	7.15	8.62
1000	2.08	2.08	2.12	2.23	2.71	5.26	6.61	7.97
1200	1.82	1.82	1.85	1.95	2.35	4.54	5.70	6.86
1500	1.51	1.51	1.53	1.61	1.93	3.71	4.65	5.59
2000	1.15	1.15	1.16	1.22	1.46	2.77	3.47	4.18
3000	0.74	0.74	0.75	0.78	0.93	1.76	2.19	2.64
4000	0.53	0.53	0.53	0.56	0.66	1.24	1.54	1.85
5000	0.40	0.40	0.40	0.42	0.50	0.93	1.16	1.39
6000	0.32	0.32	0.32	0.33	0.39	0.73	0.91	1.09
7000	0.26	0.26	0.26	0.27	0.32	0.59	0.74	0.89
8000	0.22	0.22	0.22	0.23	0.27	0.50	0.62	0.74
9000	0.18	0.18	0.19	0.19	0.23	0.42	0.53	0.63
10000	0.16	0.16	0.16	0.17	0.20	0.36	0.45	0.54

trates the results for Model III of Stancil et al. (1996). There occurs an increase of about 25% in the fractional abundance at redshifts between 150 and 325. At earlier times, dissociation processes limit the abundance of LiH. At later times, associative detachment,

replaces reactions (1) and (2) as the major source of LiH. The conclusion of Stancil et al. (1996) that the abundance of LiH is negligible in the early universe is unaltered.¹

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¹ In Table 1 of Stancil et al. (1996), the parameter a_2 for the rate coefficient fit of reaction (22), the radiative attachment of Li^- , should be +0.62. The use of the correct rate coefficient for reaction (22) results in a reduction of the fractional abundances of Li^- and LiH for $z < 80$. In addition, an error in our use of the LiH dissociation equilibrium constant shifts the LiH redshift of formation z_f from 450 to 300. These changes are reflected in Figure 4 of the current paper.

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