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MODEL OF EARLY UNIVERSE WITH H_2^+

by

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ABSTRACT

Model of Early Universe with H_2^+

by

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The aim of this thesis is to improve existing models of the Early Universe by adding vibrationally resolved reactions to a standard model. Stancil, Lepp, and Dalgarno (1996, 1998) have developed a standard chemical model for molecules in the Early Universe. Galli and Palla (1998) have shown that vibrational excitation may be important in this model by forcing the vibrational level of H_2^+ to be either v=0 or v=9. I studied a consistent model for the vibrational levels including level dependent formation and destruction as well as trasition between the levels.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

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CHAPTER 1

INTRODUCTION

The correct analysis of atomic and molecular processes is necessary to understand the early universe. At high redshift matter was completely ionized by thermal radiation. As the universe was expanding and cooling, the formation of molecules was possible. The formation of a molecule like H_2 was very important because the presence of the hydrogen molecule was directly related to the cooling properties of the primodial gas, and the most important aspect of H_2 is its role in the formation of the first star. Saslaw and Zippoy (1967) suggested using H_2^+ as a mechanism to create H_2. Therefore, the use of the H_2^+ ion reaction rates based on populations of the rotational-vibrational levels could be important.

The purpose of my study is the analysis of vibrational transitions between the 0 and 19 vibrational level. The H_2^+ ion related reactions are introduced in Chapter 2. The rate calculations of all 190 H_2^+ vibrational modes are in Chapter 3. The radiative association, dissociation, charge transfer, dissociation recombination, and remaining reactions are discussed in Chapter 4. The fittings to find the rate coefficient, K_{ij}, are in Chapter 5. The abundancy comparisons between the previous calculation of the eleven molecules and molecular ions and this work are presented in Chapter 6. I conclude in Chapter 7.

CHAPTER 2

THE EARLY UNIVERSE CHEMICAL REACTIONS WITH H_2^+

H_2 was the first neutral molecule formed in the early universe and became the most abundant. Because of the lack of a dipole moment, molecular hydrogen cannot form directly by a radiative process. The most common reaction to form a hydrogen molecule happens on a grain surface. The minimum requirement is that one hydrogen atom is retained at the surface until a second hydrogen atom arrives and bonds with the first. But in the early Universe there was no grain available to form H_2, so H must be found some other way and H_2^+ and H can act as intermediaries. A bubble diagram in figure 1 shows the hydrogen reactions in the early Universe.

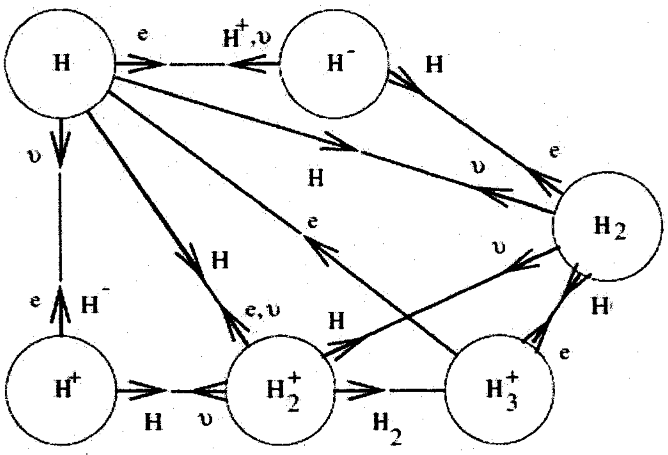

Figure 1 Bubble diagram of H reactions in the early universe (Lepp *et al.*, 2002)

H_2^+ reactions

The H_2^+ ion can be created by

$$H + H^+ \longrightarrow H_2^+ + \text{photon}.$$

The reverse reaction is

$$H_2^+ + \text{photon} \longrightarrow H + H^+.$$

The H_2^+ ion can be created and destroyed by associative and dissociative recombinations,

$$H^+ + H^- \longrightarrow H_2^+ + e^-,$$

and

$$H_2^+ + e^- \longrightarrow H + H.$$

The H_2^+ ion can be converted to H_2 via

$$H_2^+ + H \longrightarrow H_2 + H^+.$$

There are two possibilities between H_2^+ and H^-

$$H_2^+ + H^- \longrightarrow H_2 + H,$$

and

$$H_2^+ + H^- \longrightarrow H + H + H.$$

H_3^+ can be created from H_2^+ by the following reactions

$$H_2^+ + H_2 \longrightarrow H_3^+ + H,$$

$$H_2^+ + H \longrightarrow H_3^+ + \text{photon},$$

$$H_2^+ + H^- \longrightarrow H_3^+ + e^-.$$

The Helium mechanism to create and destroy H_2^+

HeH^+ can form H_2^+ by the reaction

$$HeH^+ + H \longrightarrow He + H_2^+,$$

$$H_2 + He^+ \longrightarrow H_2^+ + He + \text{photon},$$

or He can destroy H_2^+ by the following reaction

$$He + H_2^+ \longrightarrow HeH^+ + H.$$

Deuterium and Lithium related reactions

The following are the Deuterium related reactions

$$H_2^+ + D \longleftrightarrow HD^+ + H,$$

$$H_2^+ + D \longrightarrow H_2D^+ + \text{photon},$$

$$H_2^+ + D \longrightarrow H_2 + D^+,$$

$$H_2^+ + D^- \longrightarrow H_2D^+ + e^-,$$

$$HD + H_2^+ \longrightarrow H_2D^+ + H,$$

$$HD + H_2^+ \longrightarrow H_3^+ + D.$$

There are two Lithium reactions to create H_2^+

$$LiH^+ + H \longrightarrow Li + H_2^+,$$

$$LiH + H^+ \longrightarrow Li + H_2^+.$$

CHAPTER 3

H_2^+ VIBRATIONAL LEVELS

The Einstein transition probability of spontaneous emission coefficients, A_{ij}, for vibrational level data provided by S. Lepp were used to calculate the Einstein transition probabilities, and the stimulated emission, B_{ij}, and absorption, B_{ji}, coefficients. The partial spontaneous emission coefficients given by Lepp are shown in Table 1.

Level i	Level j	Rate Coefficients(sec^{-1})
1	0	5.200E-07
2	1	8.600E-07
3	2	1.000E-06
4	3	1.100E-06
5	4	1.100E-06
6	5	1.000E-06
7	6	9.200E-07
8	7	7.800E-07
9	8	6.400E-07
10	9	4.900E-07
11	10	3.600E-07
12	11	2.400E-07
13	12	1.500E-07
14	13	8.000E-08
15	14	3.600E-08
16	15	1.200E-08
17	16	2.000E-09
18	17	6.000E-11
19	18	7.900E-15

Table 1 The H_2^+ vibrational A_{ij}

Calculation of B_{ji}

The Einstein transition probability of spontaneous emission is related to the matrix element of the transition as follows:

$$\mathrm{A}_{ij} = \frac{64\pi^4\nu_{ij}^3}{3hc^2}|\mathbf{R}_{ij}|^2,$$

where $\mathbf{R}_{ij}$ is the transition moment.

If there are N_i atoms in the i state. A_{ij} is the fraction of atoms in the i state carrying out the trasition to j state per second,

$$I_{ij} = N_i hc\nu_{ij}\mathrm{A}_{ij}.$$

Then the intensity of an emission line with respect to $|\mathbf{R}_{ij}|^2$ will be the following

$$Ie_{ij} \approx \nu_{ij}^4|\mathbf{R}_{ij}|^2.$$

The intensity of absorption from the incident beam is given by

$$Ia_{ij} = \rho_{ij}N_j\mathrm{B}_{ji} \triangle xhc\nu_{ij},$$

where N_j is the number of atoms per cm^3 in the lower state. The factor $\rho_{ij}N_jB_{ji}$ represents the number of transitions per cm^3 per second produced by the incident radiation. If ρ_{ij} is expressed in terms of energy per wave number, then B_{ji} can be written as the following

$$\mathrm{B}_{ji} = \frac{8\pi^3c}{3h^2}|\mathbf{R}_{ij}|^2.$$

If we combine the above equation with $\mathrm{A}_{ij} = \frac{64\pi^4\nu_{ij}^3}{3hc^2}|\mathbf{R}_{ij}|^2$, then B_{ji} will be

$$\mathrm{B}_{ji} = \frac{\mathrm{c}^3}{8\pi h\nu_{ij}^3}\mathrm{A}_{ij}.$$

Calculation of ν_{ij}

To complete the calculation of B_{ji}, we need to know the frequency between level i and j. In order to calculate, the frequency we can use the given energy values and the following relation

$$\nu_{ij} = \frac{E_{ij}}{h}.$$

I downloaded the energies (in Atomic Units) of the vibrational levels calculated by P. Stancil (1994). The first nineteen energy differences were then converted to Joules and are listed in Table 2.

Einstein stimulated coefficients

Absorption

From the Einstein probability coeffients, the total number of induced radiative transitions per cm^3 per sec from i to j is equal to $n_j B_{ij} U_\nu$. The n_j is the number of particles in the j state and U_ν is the density of radiant energy per cm^3 per unit frequency interval. U_ν is related to the intensity, I_ν, by

$$U_\nu = \frac{1}{c}\int I_\nu d\omega.$$

If we solve the above eqution, then it will lead us to the following

$$U_{\nu_{ij}} = \frac{4\pi W B_\nu(T)}{c},$$

where W is called the 'dilution factor' and $B_\nu(T)$ is the Plank function,

Level i	Level j	E_{ij}(a.u.)	E_{ij}(Joules)
1	0	9.986304e-03	4.353773e-20
2	1	9.406298e-03	4.100906e-20
3	2	8.845501e-03	3.856412e-20
4	3	8.300997e-03	3.619022e-20
5	4	7.769801e-03	3.387435e-20
6	5	7.249001e-03	3.160379e-20
7	6	6.735798e-03	2.936636e-20
8	7	6.227102e-03	2.714857e-20
9	8	5.719900e-03	2.493730e-20
10	9	5.210999e-03	2.271862e-20
11	10	4.696900e-03	2.047728e-20
12	11	4.173500e-03	1.819539e-20
13	12	3.636830e-03	1.585565e-20
14	13	3.081960e-03	1.343656e-20
15	14	2.503450e-03	1.091440e-20
16	15	1.895570e-03	8.264200e-21
17	16	1.254394e-03	5.468837e-21
18	17	5.950070e-04	2.594078e-21
19	18	1.041290e-04	4.539758e-22

Table 2 The energy differences between i and j

$$\mathrm{B}_{\nu}(T) = \frac{2h\nu^3}{c^2}\frac{1}{e^{\frac{h\nu}{kT}} - 1}.$$

By substituting $\mathrm{B}_{\nu}(T)$ into $U_{\nu_{ij}}$ and assuming a diluted black body radiation field, we can solve for the energy density

$$U_{\nu_{ij}} = \frac{8\pi W h\nu^3}{c^3}\frac{1}{e^{\frac{h\nu}{kT}} - 1}.$$

I decided to use a perfect black body radiation field in which the dilution factor, W, must be 1. Finally, the rate coefficient of absorption will be

$$U_{\nu_{ij}}\mathrm{B}_{ji} = \frac{8\pi h\nu_{ij}^3}{c^3}\frac{1}{(e^{\frac{h\nu_{ij}}{kT}}-1)}\frac{\mathrm{c}^3}{8\pi h\nu_{ij}^3}\mathrm{A}_{ij}$$

Emission

The number of particles making the transition from i to j per sec by absorbing radiation, $\dot{N}_{ji}$, is proportional to N_i, the number of atoms in the state i, and the energy density, $U_{\nu_{ij}}$, by the following

$$\dot{N}_{ji} = \mathrm{B}_{ji}\mathrm{N}_i U_{\nu_{ij}}.$$

The number of particles making the transition from j to i per sec, $\dot{N}_{ij}$, has two different parts. The first part has the sum of the number of spontaneous transitions per sec, which is independent of $U_{\nu_{ij}}$. The second part consists of the number of stimulated transitions per sec, which is proportional to $U_{\nu_{ij}}$

$$\dot{N}_{ij} = \mathrm{A}_{ij}\mathrm{N}_j + \mathrm{B}_{ij}\mathrm{N}_j U_{\nu_{ij}}.$$

N_j is the total number of particles in the state j, A_{ij} is the Einstein coefficient for spontaneous emission, and B_{ij} is the Einstein coefficient for stimulated emission. Then the above two equations can be expressed as the following

$$\frac{\mathrm{N}_i}{\mathrm{N}_j} = \frac{\mathrm{A}_{ij} + \mathrm{B}_{ij}U_{\nu_{ij}}}{\mathrm{B}_{ji}U_{\nu_{ij}}}.$$

At thermal equilibrium $\mathrm{N}_i/\mathrm{N}_j$ is given by

$$\frac{\mathrm{N}_i}{\mathrm{N}_j} = e^{\frac{h\nu_{ij}}{kT}}.$$

By equating the two equations above, we can find the expression of energy density $\mathrm{U}_{\nu_{ij}}$,

$$U_{\nu_{ij}} = \frac{\mathrm{A}_{ij}}{\mathrm{B}_{ji} e^{\frac{h\nu_{ij}}{kT}} - \mathrm{B}_{ij}}.$$

As derived earlier, the energy density for B_{ji} can be expressed as

$$U_{\nu_{ij}} = \frac{8\pi W h\nu^3}{c^3} \frac{1}{e^{\frac{h\nu}{kT}} - 1},$$

where the dilution factor is 1. In order for the above two energy densities to be equal, the Einstein coefficients for stimulated absorption and emission must be indentical. In other words,

$$\mathrm{B}_{ij} = \mathrm{B}_{ji}.$$

The partial calculated values for B_{ij} and B_{ji} are listed in Table 3.

Level i	Level j	B_{ij} and B_{ji}
1	0	2.965789e+09
2	0	5.296046e+07
3	0	1.589224e+06
4	0	6.054540e+04
5	0	1.893547e+03
6	0	1.077553e-01
7	0	5.734775e+01
8	0	5.498259e+01
9	0	3.933649e+01
10	0	2.512452e+01
11	0	1.765158e+01
12	0	1.231602e+01
13	0	9.181294e+00
14	0	6.624061e+00
15	0	4.510369e+00
16	0	2.874841e+00
17	0	1.570683e+00
18	0	4.626121e-01
19	0	2.520845e-02

Table 3 The first 19 values of B_{ij} and B_{ji}

CHAPTER 4

CREATION AND DISTRUCTION MECHANISMS OF H_2^+

The H_2^+ ion is diatomic, and in the previous chapter all the rate coefficients for the bound states of H_2^+ are calculated. We now must determine the amount of each H_2^+ level, taking into account the radiative and collisional association rates of each level by changing the vibrational quantum numbers, v, the destruction rate by photodissociation, and charge transfer.

Radiative association

The radiative association reaction starts with an H atom and H^+ ion

$$H + H^+ \longrightarrow H_2^+ + \text{photon}.$$

The rate coefficients (from v = 0 to v = 19) in the different temperatures were given by P. Stancil and shown in Table 4 on page 18, and the a, b, and c parameters are listed in Table 9 on page 25.

Radiative dissociation

The destruction of H_2^+ by photodissociation is the reverse of the association reaction

$$H_2^+ + \text{photon} \longrightarrow H + H^+.$$

In order to properly calculate the dipole radiative dissociation (Hirata and Padmanabhan 2006), we need to solve for the unbound final state and the cross section from the bound level with energy, E($v, J = 0$). The equation for the cross section is

$$\sigma_{v,J=0} = \frac{8\pi^3 \nu}{3c} |Q_{v,J=0}|^2,$$

where ν is the photon frequency, v and J are the vibrational and rotational quantum numbers respectively, and

$$|Q_{v,J=0}|^2 = \int_0^\infty \Phi(R) D(R) f_1(R) dR.$$

$\Phi(R)$ is the bound wave function, D(R) is the dipole matrix element between bound and unbound states, and $f_1(R)$ is the unbound wave function. The radiative dissociation rate of thermal contribution, $UB_{v,J=0}$, is given by the following relation

$$UB_{v,J=0} = \frac{8\pi}{c^2} \int_{-E/h}^{\infty} \frac{\nu^2 \sigma_{v,0}(\nu) d\nu}{e^{h\nu/kT} - 1}.$$

Instead, one can use the detailed balance between $\mathrm{H} + \mathrm{H}^+ \rightarrow \mathrm{H}_2^+ +$photon and its reverse reaction, photodissociation. The calculated $K_{v,J=0}$ values for photoassociation are listed in the last section. Now, we need to use $K_{v,J=0}$ values as a spontaneous emission coefficient ($\mathrm{A}^{sp}_{v,J=0}$) for the reverse reaction. The actual technique of the detailed balance is simular to method I introduced in Chapter 3, but unlike the changing of the vibrational levels between i and j of H_2^+, one must consider the number(s) of elements created by these two reactions. Photoassociation creates one element, H_2^+, while the reverse reaction creates H and H^+. The spontaneous coefficient is related to the stimulalted coefficent by phase space factors,

$$K^{st}_{v,J=0}(\nu, T) = \frac{G_{H+H^+}}{G_{H^+_{2(v,J=0)}+\gamma}} \frac{1}{e^{\frac{h\nu}{kT}} - 1} A^{sp}_{v,J=0},$$

where G represents the number of quantum states per unit wavenumber k per unit volume for $\mathrm{H} + \mathrm{H}^+$ and $\mathrm{H}_2^+ + \gamma$. G_{H+H^+} and $G_{H_2^+ + \gamma}$ are given by

$$G_{H_2^+ + \gamma} = 4 g'_{guc} \frac{4\pi k_\gamma^2}{(2\pi)^3}$$

$$G_{H+H^+} = 2\frac{4\pi k^2_{H+H^+}}{(2\pi)^3},$$

where $k_\gamma = 2\pi\nu/c$ is the photon wavenumber, $k^2_{H+H^+} = \sqrt{2\mu E}/\hbar$ is the relative wavenumber of H and H$^+$, and $g^{'}_{guc}(=1/4)$ is the nuclear spin-degeneracy factor, and μ is the reduced mass.

After putting together all the terms, $K^{st}_{v,J=0}$ becomes

$$K^{st}_{v,J=0}(\nu, T) = \frac{4\mu c^2}{\nu h}\frac{1}{e^{\frac{h\nu}{kT}} - 1}A^{sp}_{v,J=0}.$$

Charge transfer

Each vibrational level of H_2^+ can transfer to H_2 and H^+ via the reaction

$$H_2^+ + H \longrightarrow H_2 + H^+.$$

To complete the above calculations, one needs to have the charge transfer reaction rate as a function of the matter temperature for each level of H_2^+. Unfortunately, the rates have not been measured or calculated for all levels yet. Hirata and Padmanabhan (2006) suggested three different cases. For case (1), one can use the value

$$K_{v,J=0} = 6.40 \times 10^{-10}\mathrm{cm}^3/sec,$$

measured by Karpas *et al.* (1979) for all vibrational levels. In case (2) one can use the Langevin rate coefficient

$$K_{v,J=0} = 2.38 \times 10^{-9}\mathrm{cm}^3/sec.$$

For the last case, the reaction rates can be calculated by linearly interpolating the values of σ (Krstić and Janev 2003) and integrating over the Maxwellian energy distribution,

$$K_{v,J=0} = \frac{2}{\sqrt{\pi}(kT)^{3/2}}\int_0^\infty E^{1/2}e^{-E/kT}\sigma_{(v,J=0)}v_{rel}dE,$$

where k is Boltzman constant, $\sigma_{(v,J=0)}$ is cross section for each vibrational level, and v_{rel} is relative velocity. For this study case (3) has been used for each level.

Dissociative recombination

The dissociative recombination

$$\mathrm{H_2^+ + e^- \longrightarrow H + H},$$

is the important reaction that destroys $\mathrm{H_2^+}$ and contributes to a reduction in the abundance of $\mathrm{H_2}$. Schneider *et al.* (1994) have calculated the first 78 rate coefficients out of 423 ro-vibrational levels between 20 and 5,000 Kelvin. There is no published paper available, but according to Hirata and Padmanabhan (2006) the importance of $\mathrm{H_2^+} + e^-$ may not be significant at lower red shifts (in this study red shifts between z = 10 to z = 365 were covered). Their arguement was that at z < 600 the number of electrons, n_e, is less than 10^{-3}. Therefore in order for dissociative recombination to be accountable, $K_{v,J=0}$ must be $\geq \sim 6.00 \times 10^{-7}\ cm^3$/sec. In the previous section, I considered case (1) which $K_{v,J=0}$ is 6.40 $\times 10^{-10}$cm^3/sec, so the rate coefficient given by the file, 'rates.data', was used for all vibrational levels. The actual value of $K_{v,J=0}$ can be found in Table 5 on page 20.

The forward reactions of $\mathrm{H_2^+}$

The following two reactions can be found in Dalgarno and Lepp (1987).

$$\mathrm{H_2^+ + H^- \longrightarrow H_2 + H}$$

$$\mathrm{H_2^+ + H^- \longrightarrow H + H + H}$$

They argued that the rate coefficient of above reactions might be on the order of 5 $\times 10^{-7}(\frac{100}{T})^{\frac{1}{2}} cm^3/sec$. I got the rate coefficient of 2.89 $\times 10^{-7} cm^3/sec$ by fitting the curve created by 5 $\times 10^{-7}(\frac{100}{T})^{\frac{1}{2}} cm^3/sec$.

The experimental associative ionization cross sections and v_{rel} for following reaction can be found in Naji (1998), but the rates have not been measured or calculated for all levels (only $v = 0, J = 0$)

$$\mathrm{H_2^+ + H^- \longrightarrow H_3^+ + e^-}$$

The rate coefficient is obtained by averaging the product of the cross section and v_{rel} over a Maxwellian distribution. The calculated reaction rate was 1.30 $\times 10^{-10} cm^3/sec$, and compared with the rate coefficient of 2.70 $\times 10^{-10} cm^3/sec$ from 'rates.data'.

Thread and Huntress (1974) have calculated the vibrational reaction rates for the following two reactions

$$\mathrm{He + H_2^+ \longrightarrow HeH^+ + H},$$

and

$$\mathrm{H_2^+ + H_2 \longrightarrow H_3^+ + H}.$$

For the second reaction, Thread and Huntress have stated only the vibrational rate coefficients from $v = 0$ to 5, so I decided to use the value of 1.90 $\times 10^{-9} cm^3/sec$ for the rest of levels (from $v = 6$ to 19).

There is one more reaction related to $\mathrm{H_3^+}$,

$$\mathrm{H_2^+ + H \longrightarrow H_3^+ + \gamma}.$$

According to Galli and Palla (1998), the above reaction was irrelevant. Unfortunately, I wasn't able to find any source for all vibrational level except for $v = 0$. I used the rate coefficient of 1.50 $\times 10^{-17} cm^3/sec$ from Stancil *et al.* (1998).

The reaction for charge exchange with Deuterium is

$$\mathrm{H_2^+ + D \longrightarrow H_2 + D^+}.$$

The reaction is very simular to charge exchange between H_2^+ and H. For case (1), I decide to use 6.40 $\times 10^{-10} cm^3/sec$ as the rate coefficient (Stancil *et al.*, 1998), and for case (2), the charge transfer rate coefficients between H_2^+ and H have been applied.

The experimental associative ionization cross sections and v_{rel} ($v = 0$, $J = 0$) for the following reaction can be found in Naji (1998)

$$\mathrm{H_2^+ + D^- \longrightarrow H_2D^+ + e^-}.$$

The rate coefficient is obtained by averaging the product of the cross section and v_{rel} over a Maxwellian distribution.

Because of the similarity in the process of H_2^+ dissociation by D,

$$\mathrm{H_2^+ + D \longrightarrow H_2D^+} + \gamma,$$

one can use the same rate coefficient of 1.50 $\times 10^{-17} cm^3/sec$ for all the reaction levels used in H_2^+ dissociation by H. Probably, it might be over estimated rate because Deuterium to be heavier than Hydrogen, and it will cause the v_{rel} of Deuterium is smaller than Hydrogen. I compare the result from the rate coefficient of 1.50 $\times 10^{-17} cm^3/sec$ with the reaction rate of 7.0 $\times 10^{-18} cm^3/sec$ from Stancil *et al.* (1998).

For the following two reactions, the vibrational reaction rates calculated by Thread and Huntress (1974) have been used and compared with the reaction rate of 1.05 $\times 10^{-9} cm^3/sec$ from Stancil*et al.* (1998)

$$\mathrm{HD + H_2^+ \longrightarrow H_2D^+ + H}$$

$$\mathrm{HD + H_2^+ \longrightarrow H_3^+ + D}.$$

For the next reaction, the rate coefficient of 1.07 $\times 10^{-9} cm^3/sec$ determined from cross section by Linder, Janev, and Botero (Stancil *et al.*, 1998) has been used for all 20 levels,

$$\mathrm{H_2^+ + D \longleftrightarrow HD^+ + H}.$$

The formation reactions

For formations I have considered the case in which the reaction only creates H_2^+ with a vibrational mode of zero. This method will make the populations of H_2^+ in each vibrational level differ from the detailed calculations from populating all available levels with their statistical ratios, but the total abundances of H_2^+ and others (molecules and molecular ions) might be conserved (Hirata and Padmanabhan, 2006).

$$\mathrm{HeH^+ + H \longrightarrow He + H_2^+}$$

$$\mathrm{H_2 + He^+ \longrightarrow H_2^+ + He} + \gamma$$

$$\mathrm{HD^+ + H \longrightarrow H_2^+ + D}$$

$$\mathrm{LiH^+ + H \longrightarrow Li + H_2^+}$$

$$\mathrm{LiH + H^+ \longrightarrow Li + H_2^+}$$

The following associative ionization reaction,

$$\mathrm{H^+ + H^- \longrightarrow H_2^+ + e^-},$$

is discussed by Shapiro and Kang (1987). For $T < 10^4$, the rate coefficient is on the order of $1.00 \times 10^{-8} (T)^{-0.4} cm^3/sec$ for all levels. The values of parameters (a, b, and c) are 1.02×10^{-9}, -0.400, and 0.42 respectively fitting $K_{(v=0,J=0)}(T) = 1.00 \times 10^{-8} (T)^{-0.4} cm^3/sec$.

Levels	Temps. (Kelvin)	Rate Coefficients (cm^3/sec)
0	8.00E+01	2.50837244E-42
0	9.00E+01	6.61330719E-42
0	1.00E+02	1.82654370E-41
0	2.00E+02	2.02590356E-37
0	3.00E+02	9.87475603E-35
0	4.00E+02	8.17486798E-33
0	5.00E+02	2.43846844E-31
0	6.00E+02	3.75409139E-30
0	7.00E+02	3.63649821E-29
0	8.00E+02	2.50157078E-28
0	9.00E+02	1.32319958E-27
1	8.00E+01	9.13835247E-40
1	9.00E+01	2.33990073E-39
1	1.00E+02	6.27230119E-39
1	2.00E+02	5.23705277E-35
1	3.00E+02	1.96094664E-32
1	4.00E+02	1.28629637E-30
1	5.00E+02	3.12126341E-29
1	6.00E+02	3.99091816E-28
1	7.00E+02	3.26505646E-27
1	8.00E+02	1.92377272E-26
1	9.00E+02	8.82071908E-26
19	8.00E+01	3.19616417E-26
19	9.00E+01	6.72232888E-26
19	1.00E+02	1.39287552E-25
19	2.00E+02	3.04755629E-23
19	3.00E+02	6.05605983E-22
19	4.00E+02	4.05872404E-21
19	5.00E+02	1.53254152E-20
19	6.00E+02	4.10022848E-20
19	7.00E+02	8.75986568E-20
19	8.00E+02	1.60152906E-19
19	9.00E+02	2.61602289E-19

Table 4 The partial values of $K_{(v,J=0)}(T)$

Reactions	a (cm^3/sec)	b	c (Kelvin)
$H_2^+ + e^- \longrightarrow H + H$	1.20e-08	-0.40e+00	0.00e+00
$H^+ + H^- \longrightarrow H_2^+ + e^-$	1.02e-09.	-0.40e+00	0.42e+00
$HeH^+ + H \longrightarrow He + H_2^+$	1.04d-09.	0.13d+00	3.31d+04
$H_2 + He^+ \longrightarrow H_2^+ + He + \gamma$	3.60d-16	0.00d+00	0.00d+00
$HD^+ + H \longrightarrow H_2^+ + D$	1.00d-09	0.00d+00	1.54d+02
$LiH^+ + H \longrightarrow Li + H_2^+$	9.00d-10	0.00d+00	6.64d+04
$LiH + H^+ \longrightarrow Li + H_2^+$	1.00d-09	0.00d+00	0.00d+00

Table 5 The dissociative recombination and formation reactions for H_2^+

CHAPTER 5

FITTING

To calculate the rate coefficient one must know the values of the $K_{v,J=0}$ at different temperatures (examples are shown in Table 4). The rate coefficient fits are given by the relation

$$\alpha(\mathrm{cm}^3/sec) = a\left(\frac{T}{300}\right)^b e^{-\frac{c}{T}}.$$

The bound states of H_2^+

The spontaneous emission coefficient, A_{ij}, does not depend on temperature so it can be used as a rate coefficient without fitting (Table 6). For the stimulated emission and the absorption, one needs to calculate the $K_{v,J=0}$ with several different temperatures between 450 (400 for photoassociation) and 900 Kelvin and use the fitting equation. The fitting will give a, b, and c parameters and add to ' rates.data', which is used for 'the early universe code'. The a, b, and c parameters for stimulated emission and absorption are listed in Table 7 and 8 on page 23 and 24. The fitting curves are on page 26 and 27. 'Gnuplot' has been used to find the a, b, and c parameters for the bound states of H_2^+.

Reactions	a (cm^3/sec)	b	c (Kelvin)
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(1,J=0)}$	5.200e-07	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(2,J=0)}$	6.800e-08	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(3,J=0)}$	6.300e-09	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(4,J=0)}$	5.200e-10	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(5,J=0)}$	2.900e-11	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(6,J=0)}$	2.600e-15	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(7,J=0)}$	2.000e-12	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(8,J=0)}$	2.600e-12	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(9,J=0)}$	2.400e-12	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(10,J=0)}$	1.900e-12	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(11,J=0)}$	1.600e-12	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(12,J=0)}$	1.300e-12	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(13,J=0)}$	1.100e-12	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(14,J=0)}$	8.800e-13	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(15,J=0)}$	6.500e-13	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(16,J=0)}$	4.400e-13	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(17,J=0)}$	2.500e-13	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(18,J=0)}$	7.500e-14	0.000E+00	0.000E+00
$\mathrm{H}^+_{2\,(0,J=0)} + \gamma \rightarrow \mathrm{H}^+_{2\,(19,J=0)}$	4.100e-15	0.000E+00	0.000E+00

Table 6 The spontaneous emission, A_{ij}

Photoassociation

By use of the data shown in Table 4, the three parameters a, b, and c, can be found for the reaction $\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_2^+ + \text{photon}$. The parameters are listed in Table 9 on page 24. 'Xmgrace' was used to fit the data points.

Reactions	a (cm^3/sec)	b	c (Kelvin)
$\mathrm{H}_{2\,(1,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.395E-06	0.185E+00	0.306E+04
$\mathrm{H}_{2\,(2,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.670E-07	0.948E-02	0.612E+04
$\mathrm{H}_{2\,(3,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.630E-08	0.422E-03	0.892E+04
$\mathrm{H}_{2\,(4,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.520E-09	0.697E-04	0.115E+05
$\mathrm{H}_{2\,(5,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.290E-10	0.813E-04	0.140E+05
$\mathrm{H}_{2\,(6,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.260E-14	0.300E-04	0.163E+05
$\mathrm{H}_{2\,(7,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.200E-11	0.648E-04	0.184E+05
$\mathrm{H}_{2\,(8,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.260E-11	-0.883E-04	0.204E+05
$\mathrm{H}_{2\,(9,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.240E-11	-0.555E-04	0.222E+05
$\mathrm{H}_{2\,(10,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.190E-11	0.146E-04	0.238E+05
$\mathrm{H}_{2\,(11,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.160E-11	-0.167E-04	0.253E+05
$\mathrm{H}_{2\,(12,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.130E-11.	0.268E-05	0.266E+05
$\mathrm{H}_{2\,(13,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.110E-11	-0.114E-03	0.278E+05
$\mathrm{H}_{2\,(14,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.880E-12	-0.818E-04	0.288E+05
$\mathrm{H}_{2\,(15,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.650E-12	0.224E-03	0.295E+05
$\mathrm{H}_{2\,(16,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.438E-12	0.277E-02	0.301E+05
$\mathrm{H}_{2\,(17,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.247E-12	0.613E-02	0.305E+05
$\mathrm{H}_{2\,(18,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.752E-13	-0.152E-02	0.307E+05
$\mathrm{H}_{2\,(19,J=0)}^{+} + \gamma \rightarrow \mathrm{H}_{2\,(0,J=0)}^{+}$	0.487E-14	-0.934E-01	0.308E+05

Table 7 The stimulated emission, UB_{ij}

Reactions	a (cm^3/sec)	b	c (Kelvin)
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(1,J=0)}^{+}$	0.395E-06	0.185E+00	0.306E+04
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(2,J=0)}^{+}$	0.670E-07	0.948E-02	0.612E+04
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(3,J=0)}^{+}$	0.630E-08	0.422E-03	0.892E+04
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(4,J=0)}^{+}$	0.520E-09	0.697E-04	0.115E+05
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(5,J=0)}^{+}$	0.290E-10	0.813E-04	0.140E+05
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(6,J=0)}^{+}$	0.260E-14	0.300E-04	0.163E+05
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(7,J=0)}^{+}$	0.200E-11	0.648E-04	0.184E+05
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(8,J=0)}^{+}$	0.260E-11	-0.883E-04	0.204E+05
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(9,J=0)}^{+}$	0.240E-11	-0.555E-04	0.222E+05
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(10,J=0)}^{+}$	0.190E-11	0.146E-04	0.238E+05
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(11,J=0)}^{+}$	0.160E-11	-0.167E-04	0.253E+05
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(12,J=0)}^{+}$	0.130E-11	0.268E-05	0.266E+05
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(13,J=0)}^{+}$	0.110E-11	-0.114E-03	0.278E+05
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(14,J=0)}^{+}$	0.880E-12	-0.818E-04	0.288E+05
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(15,J=0)}^{+}$	0.650E-12	0.224E-03	0.295E+05
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(16,J=0)}^{+}$	0.438E-12	0.277E-02	0.301E+05
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(17,J=0)}^{+}$	0.247E-12	0.613E-02	0.305E+05
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(18,J=0)}^{+}$	0.752E-13	-0.152E-02	0.307E+05
$H_{2\,(0,J=0)}^{+} + \gamma \rightarrow H_{2\,(19,J=0)}^{+}$	0.487E-14	-0.934E-01	0.308E+05

Table 8 The stimulated absorption, UB_{ji}

Levels	a (cm^3/sec)	b	c (Kelvin)
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(0,J=0)}^+ + \gamma.$	1.48E-34	8.39E+00	-3.19E+01
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(1,J=0)}^+ + \gamma.$	2.43E-32	8.04E+00	-3.04E+01
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(2,J=0)}^+ + \gamma.$	1.15E-21	4.09E+00	-1.44E+01
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(3,J=0)}^+ + \gamma.$	5.01E-21	3.59E+00	-1.24E+01
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(4,J=0)}^+ + \gamma.$	1.61E-20	3.04E+00	-1.03E+01
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(5,J=0)}^+ + \gamma.$	4.08E-20	2.49E+00	-8.24E+00
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(6,J=0)}^+ + \gamma.$	7.66E-20	1.92E+00	-6.16E+00
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(7,J=0)}^+ + \gamma.$	8.87E-20	1.31E+00	-4.00E+00
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(8,J=0)}^+ + \gamma.$	5.88E-20	7.14E-01	-2.08E+00
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(9,J=0)}^+ + \gamma.$	1.48E-20	2.09E-01	-8.43E-01
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(10,J=0)}^+ + \gamma.$	5.69E-22	2.24E-01	-2.05E+00
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(11,J=0)}^+ + \gamma.$	7.18E-24	4.33E-01	-1.98E+00
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(12,J=0)}^+ + \gamma.$	1.78E-30	7.70E+00	-2.91E+01
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(13,J=0)}^+ + \gamma.$	7.87E-29	7.36E+00	-2.77E+01
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(14,J=0)}^+ + \gamma.$	2.34E-27	7.02E+00	-2.62E+01
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(15,J=0)}^+ + \gamma.$	5.01E-26	6.65E+00	-2.47E+01
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(16,J=0)}^+ + \gamma.$	7.93E-25	6.26E+00	-2.31E+01
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(17,J=0)}^+ + \gamma.$	5.86E-24	5.68E+00	-2.08E+01
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(18,J=0)}^+ + \gamma.$	4.53E-23	5.18E+00	-1.87E+01
$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_{2\,(19,J=0)}^+ + \gamma.$	2.45E-22	4.63E+00	-1.65E+01

Table 9 The a, b, and c parameters for the photoassociation

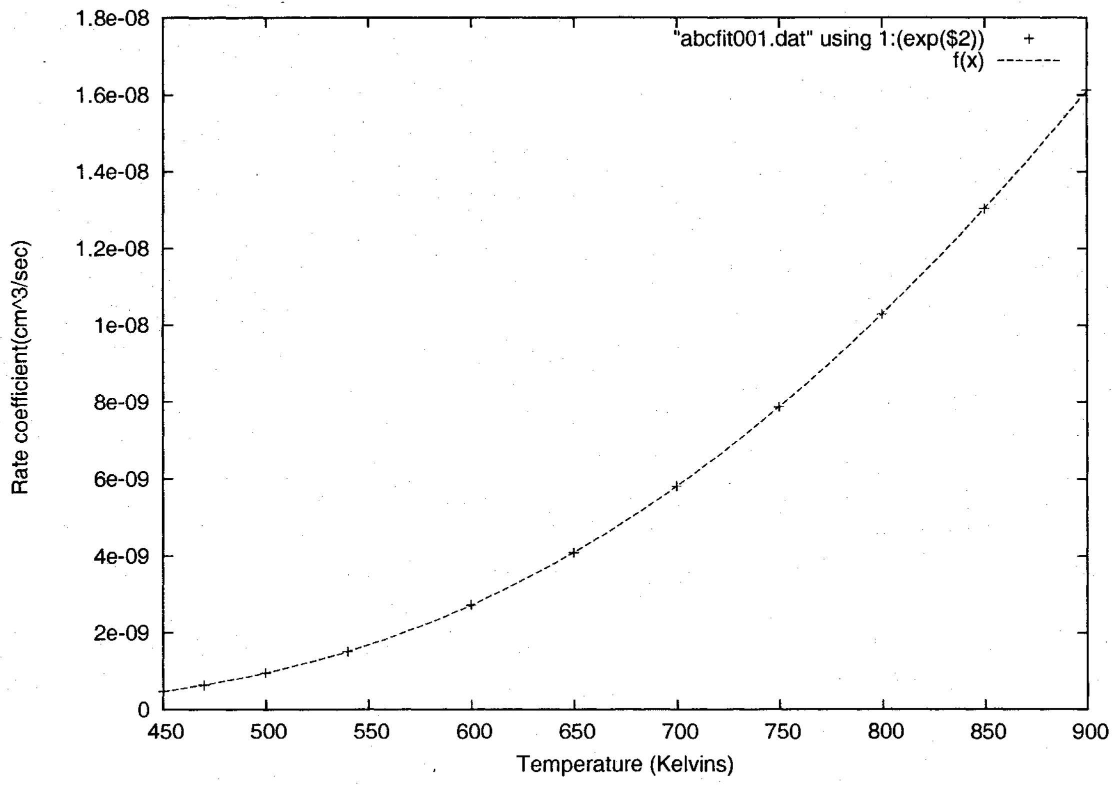

Figure 2 The fitting curve of the bound states of H_2^+

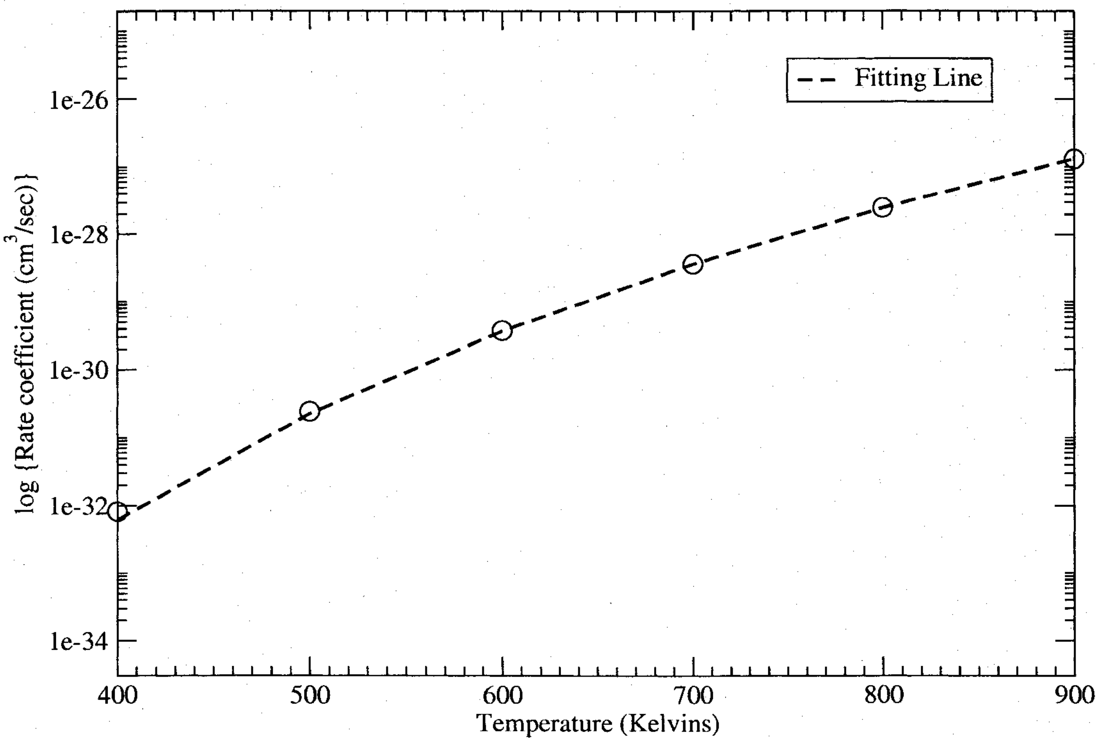

Figure 3 The fitting curve of photoassociation

CHAPTER 6

RESULTS

Figure 4, 5, and 6 show the abundances of all nineteen H_2^+ vibrational levels and the newly calculated H_2 molecule. The comparison between the old calculation and this work of the abundances of the eleven molecules and molecular ions in the early Universe at redshift range $11 \leq z \leq 365$ are presented on the following graphs. There is no change in the abundances of HeH^+, HeD^+, He_2^+, and LiH^+.

I found that the reactions discussed in Chapter 2 (with all the vibrational levels of H_2^+) did not heavily contribute to the creation and destruction of molecules and molecular ions, but one can clearly observe certain differences between previous calculations and this study. The differences of their abundances are shown in Figures 6 to 18.

The comparison between this work and Hirata and Padmanabhan (2006) is shown on page 35. One can see that there is noticable difference in the total abundances of H_2 between my work and Hirata and Padmanabhan. This work is closer to the previous calculation than theirs. Does it mean that the contribution from the vibrational levels is a lot less effective than from rotational and vibrational levels all together? In fact, there was a major difference between this study and Hirata and Padmanabhan (2006) beside of the additional rotational quantum numbers. Their calculation was started from $z = 500$, so at the time it reaches $z = 365$ the abundances of all the elements (include H_2 and H_2^+) were not the same as the initial conditions I used for this calculation.

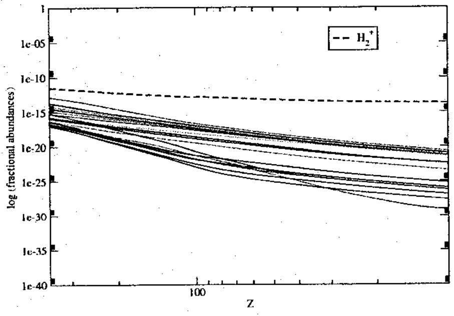

Figure 4 The abundances of 20 H_2^+ vibrational levels for the new1

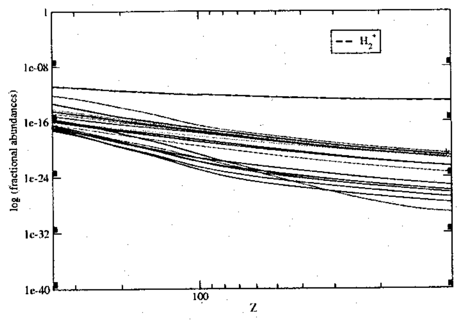

Figure 5 The abundances of 20 H_2^+ vibrational levels for the new2

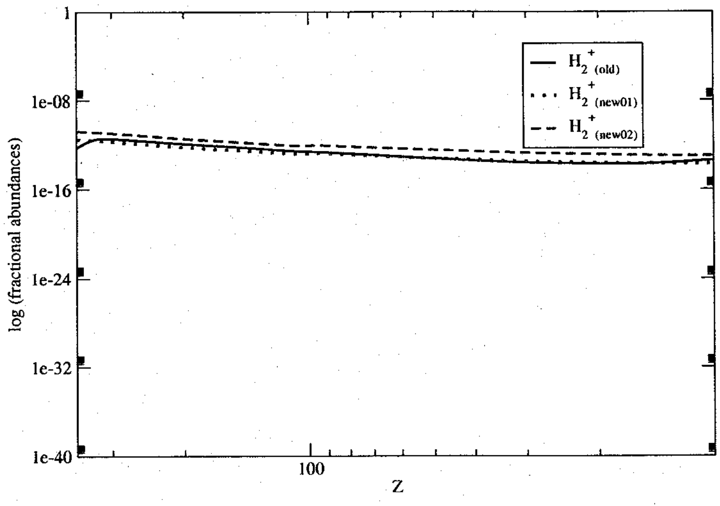

Figure 6 The old and new abundances of H_2^+

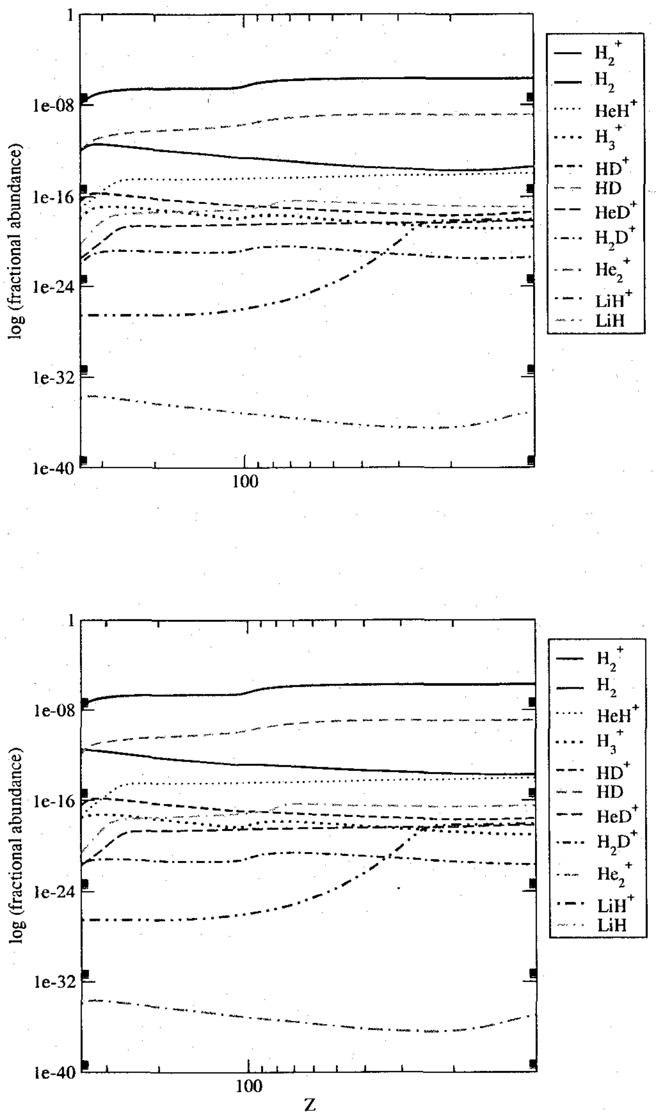

Figure 8 The abundances of 11 molecules (old and new)

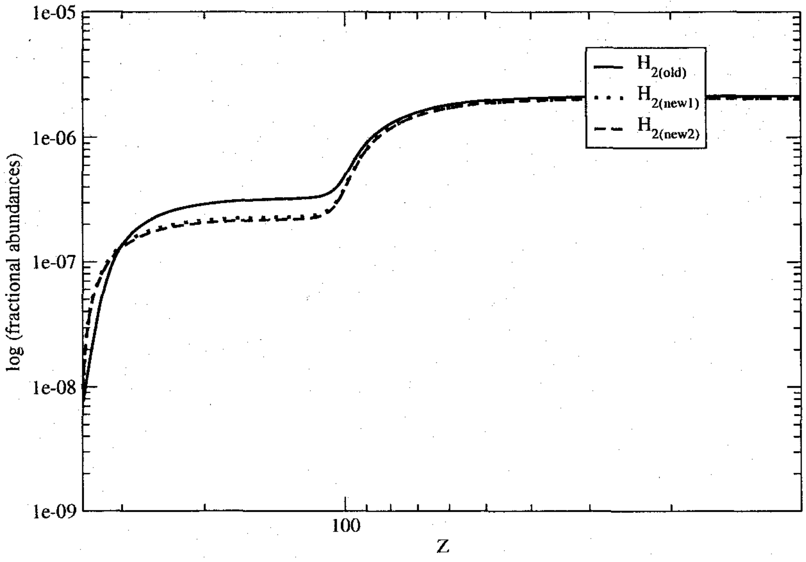

Figure 9 The old and new abundances of H_2

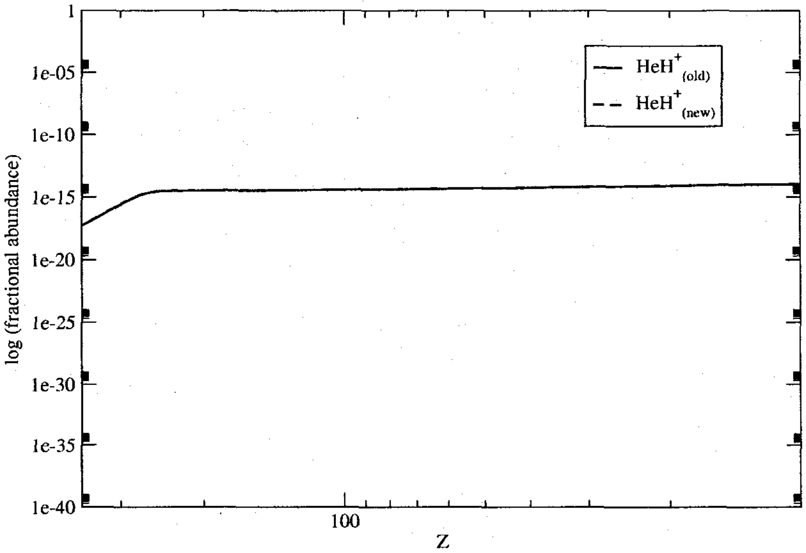

Figure 10 The old and new abundances of HeH^+

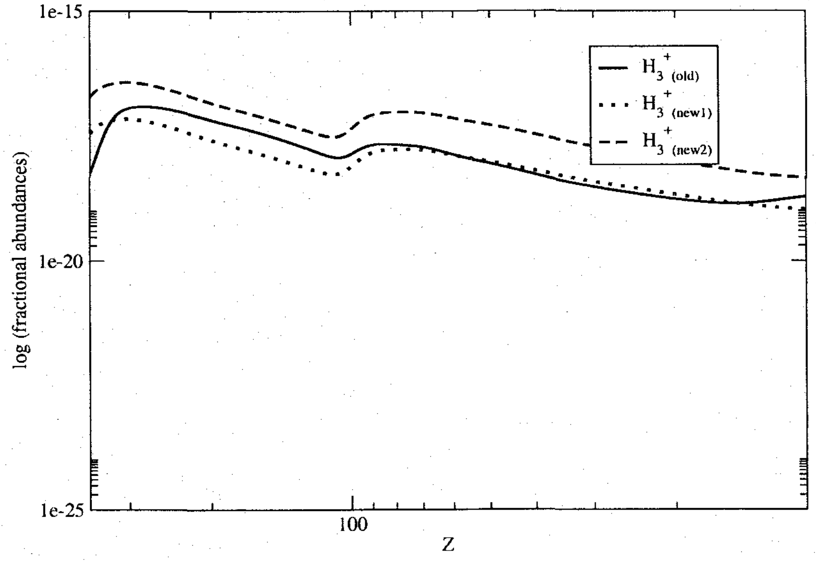

Figure 11 The old and new abundances of H_3^+

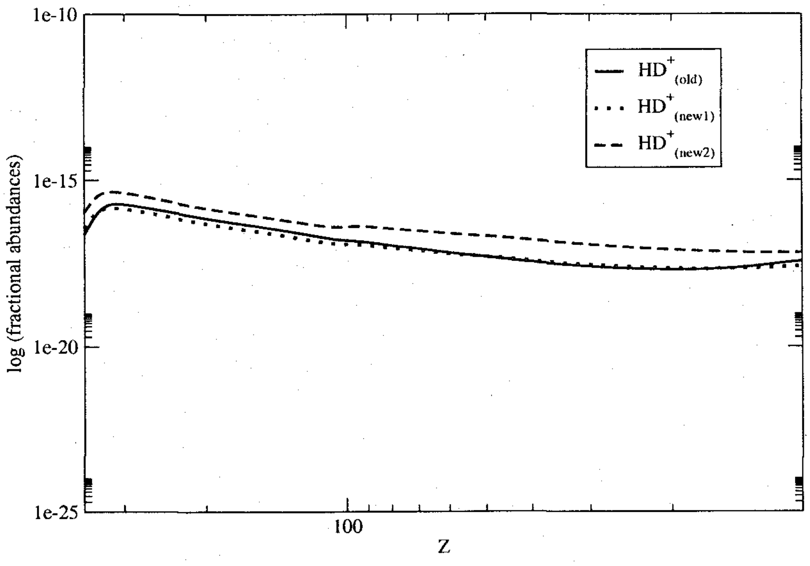

Figure 12 The old and new abundances of HD^+

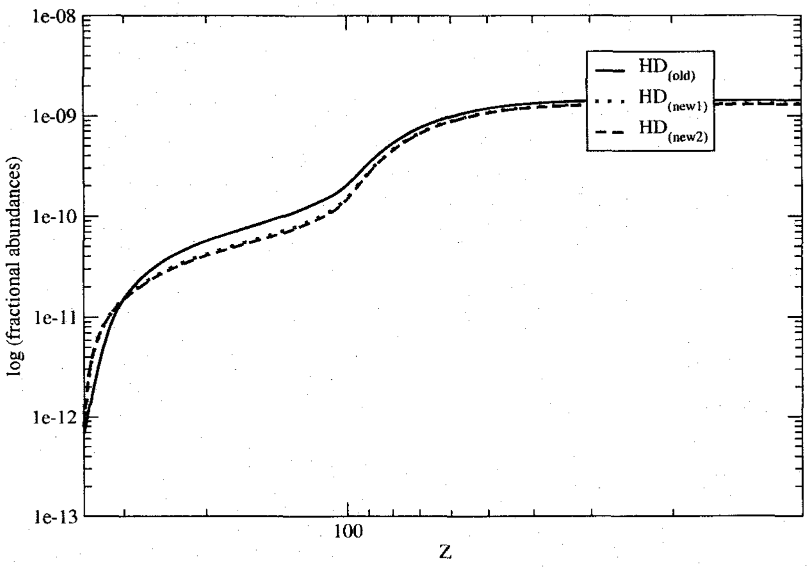

Figure 13 The old and new abundances of HD

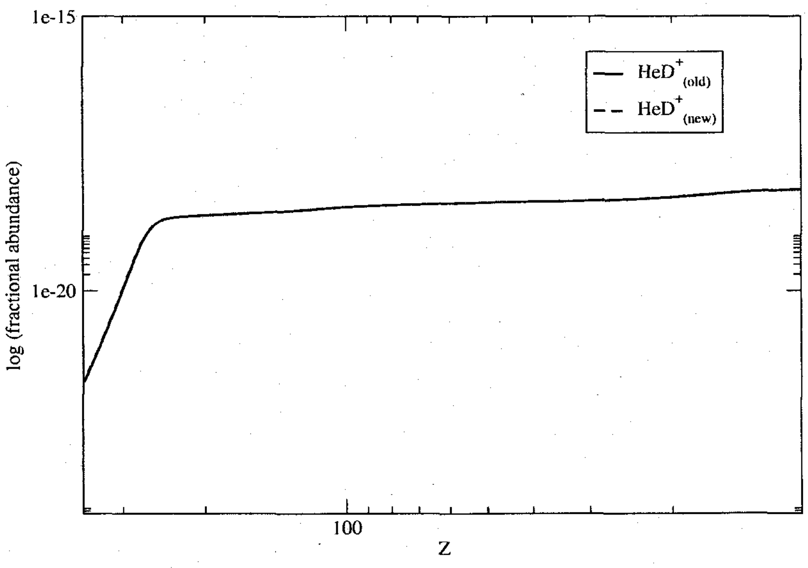

Figure 14 The old and new abundances of HeD^+

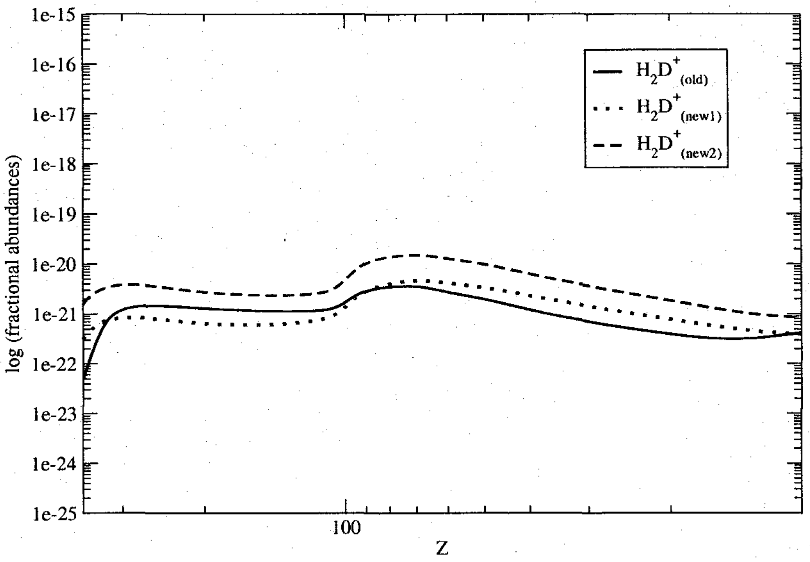

Figure 15 The old and new abundances of H_2D^+

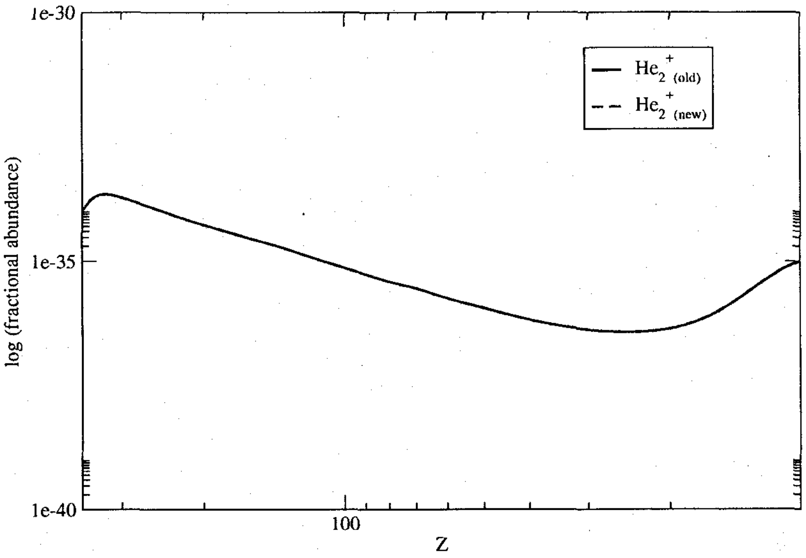

Figure 16 The old and new abundances of He_2^+

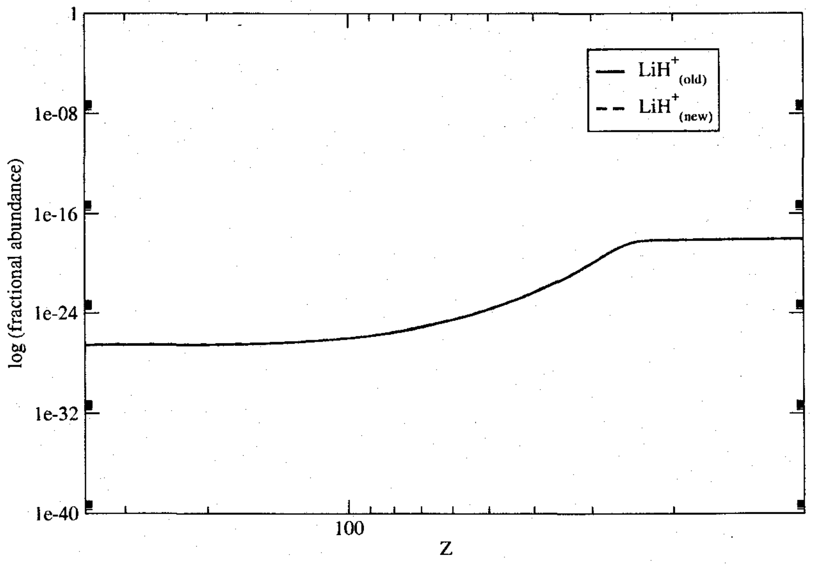

Figure 17 The old and new abundances of LiH$^+$

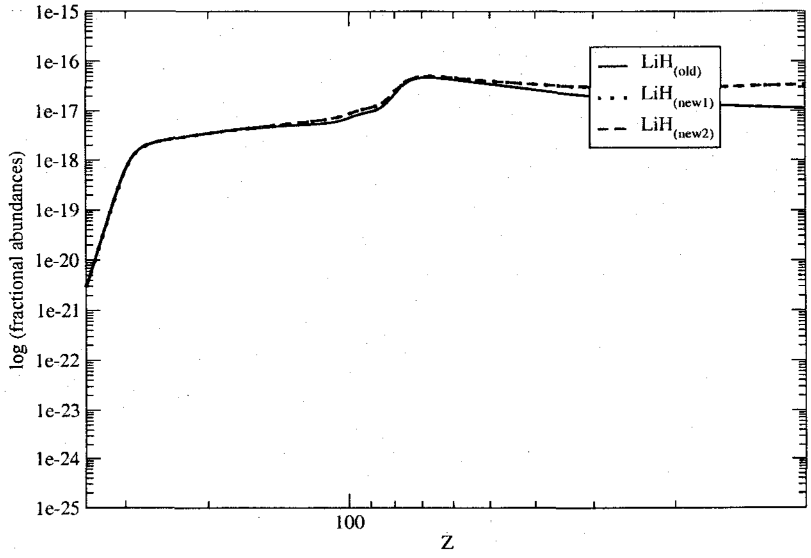

Figure 18 The old and new abundances of LiH

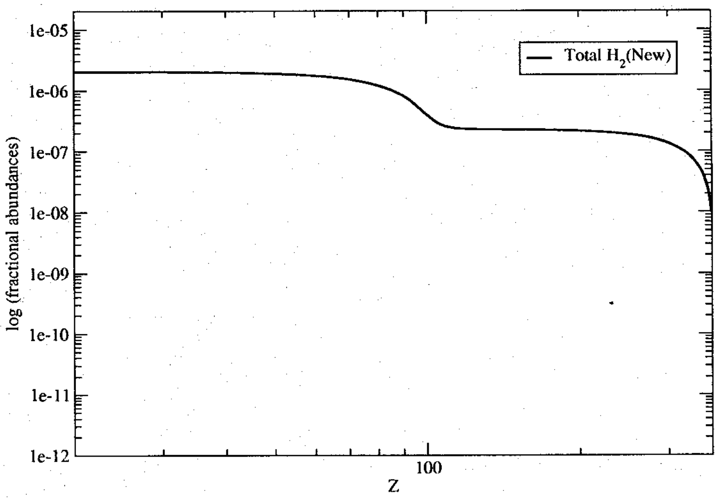

Figure 19 The total abundances of H_2 from this study

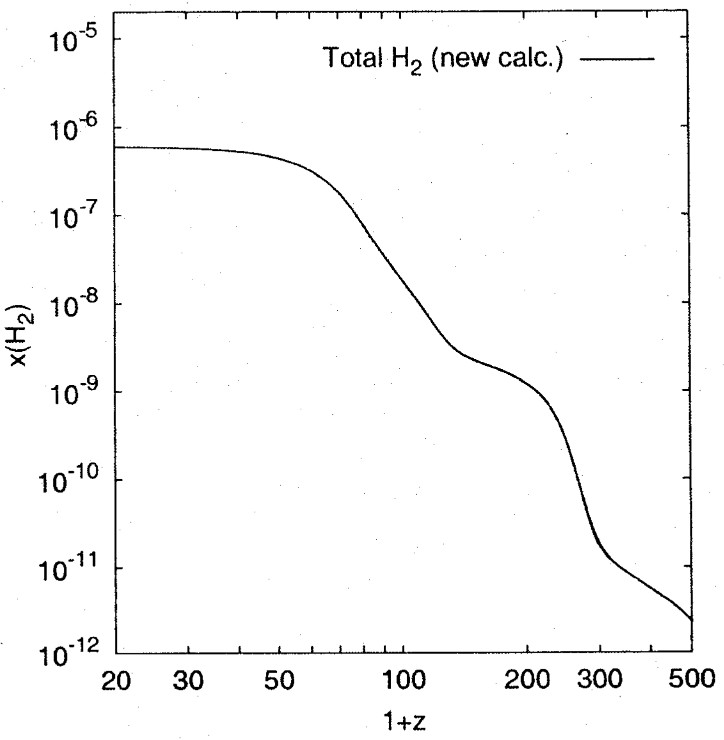

Figure 20 The total abundances of H_2 from Hirata and Padmanabhan, 2006

CHAPTER 7

CONCLUSIONS

I have discussed the contribution of H_2^+ between $11 \leq z \leq 365$. In comparison to previous calculations, I have resolved all 190 vibrational levels of H_2^+. The final results show that there were noticable but not significant changes in the abundances of 11 molecules and molecular ions.

I found that with all vibrational levels the photoassociation, photodissociation, and charge transfer contribute the most for creation and destruction of H_2, H_2^+, and most molecules and molecular ions. As I mentioned earlier, H_2^+ definitely can act as a medium to create and destroy molecules or molecular ions, and vibrational levels contribute to the amount of their final abundances.

Many parts of my present work can be improved. First, more precise calculations or mesurements of cross sections are needed for all levels. For instance, instead of using the rate coefficients for $v = 0$ for some of reactions one can resolve for all vibrational levels. Second, because H_2^+ is a molecular ion, there is not only a vibrational quantum number but a rotational quantum number as well. In this work I assumed that the rotational quantum number (J) is zero, but 423 levels of all ro-vibrational modes must be considered for better results.

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