Recombination efficiency of molecular hydrogen on interstellar grains and its effect on production of H_2

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Abstract. We study the efficiency of molecular hydrogen recombination on grain surfaces using both the rate equation (which tracks the average number of species) and the master equation (which tracks the expectation values of the species). We have incorporated Langmuir-Hinselwood rejection term in obtaining the efficiency. We use this result to compute H_2 production rates as a function of the grain temperature and accretion rate of atomic hydrogen. Our general conclusion is that the H_2 formation efficiency is very much dependent on the grain temperature and the accretion rate of the atomic hydrogen on grains. We provide tables of H_2 production rates which could be readily used for future calculation of production of more complex molecules in the gas phase.

Keywords : Molecular cloud – star formation – grain chemistry

1. Introduction

Over the last years several works have been carried out to investigate the formation of complex molecules in cool interstellar clouds (Prasad and Huntress 1980a, 1980b; Leung, Herbst and Hübner 1984; Hasegawa and Herbst 1993, Hasegawa, Herbst and Leung 1992). One of the stumbling blocks in this aspect has been to identify mechanisms to produce H_2 molecules. It has been long realized that purely gas phase reactions are very improbable and one needs to invoke the grain chemistry (e.g., Gould and Salpeter 1963; Hollenbach and Salpeter 1971; Hollenbach, Werner and Salpeter 1971). The steady state production

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rate of molecular hydrogen per unit volume is expressed according to (Hollenbach et al. 1971),

$$R_{H_2} = \frac{1}{2} n_h v_H \sigma \gamma N_g, \tag{1}$$

where, n_h and v_H are the number density and the speed of H atoms in the gas phase, respectively, σ is the average cross sectional area of a grain, and N_g is the number density of the grains. The parameter γ is the efficiency of formation of H_2 molecules i.e., the fraction of H atoms striking the grain that eventually forms a molecule. If the efficiency γ is assumed to be 1, then for a typical molecular cloud H_2 formation rate is $\sim 10^{-17}$ cm^{-3} sec^{-1} (see, e.g., Millar et al. 1997). In the present paper, we investigate the dependence of molecular hydrogen formation efficiency on external conditions such as the nature and the size of the grains and on grain temperature and accretion rate for each type of grain. We used three types of grains, namely, Olivine, amorphous carbon and one having a barrier energy which is the average of the above two types. The grain size distribution is taken from Weingartner and Draine (2001ab). The plan of the present paper is the following: In Section 2, we give a summary of the rate equation approach and the master equation approach (Biham et al. 2001) to calculate the time dependence of H and H_2 respectively. We also present the computational procedure of the accretion rate on a grain. In Section 3, we present our results. In Acharyya et al. (2005) we have already shown that for higher accretion rate of H, the rate equation approach is to be used. Here, we used this criterion to calculate the recombination efficiency and our code automatically uses the correct procedure depending on the hydrogen flux and the number of H and H_2 present in grains. Furthermore, we show that the Langmuir-Hinselwood rejection term in the rate equation is very important for higher flux values as well as for lower grain temperatures. At a high flux, a significant fraction of the grain surface is occupied by H or H_2 and only a fraction of the grain surface could be accessed by the freshly in-falling hydrogen. Since the thermal hopping is hindered at low temperatures, H would be practically immobile. Moreover, the desorption energy of H is higher than that of H_2. Thus the grain will be full of accreted H and some H_2, thereby blocking further accretion. In Section 4, we present a Table containing the H_2 formation rate for each type of grain as a function of the number density of H in the gas phase and grain temperature. These rates would be directly usable in obtaining abundances of more complex molecules.

2.   Formation of the molecular hydrogen

We first discuss very briefly two ways of computing the evolution of molecular hydrogen on grain surfaces. One of them deals with the evolution of the average number of each species and the other solves the problem probabilistically.

2.1 (a) Rate equation method

When the grains have a large number of reactant atoms or molecules, it is convenient to use the rate equation method. Here one deals with the average number of reactants. The basic equations which govern the evolutions of H and H_2 are discussed below.

Let us consider n_H to be the number of H atoms on a grain at time t and let n_{H2} be the number of H_2 molecules at that instant. The number density of H can be considered to change in the following way:

$$\frac{dn_H}{dt} = F_H(1 - f_{grh} - f_{grh2}) - W_H n_H - 2(A_H/S)n_H^2. \tag{2a}$$

Here, F_H is the accretion rate of H (measured in units of second^{-1}) which increases the number of H on a grain by sticking to it. The first multiplicative term $(1 - f_{grh} - f_{grh2})$ on the right hand side is called the Langmuir-Hinselwood rejection term (hereafter, referred to as LHRT). This term excludes the fraction of the grain surface already covered by H or H_2. The factors f_{grh} and f_{grh2} are fractions of grain occupied by atomic hydrogen and molecular hydrogen respectively. Clearly, this term is significant in the high accretion rate regime when a sizable fraction of grain is occupied. When the grains are at a low temperature, the desorption rate becomes relatively slower compared to the formation rate. In this case also the rejection term becomes significant. W_H is the desorption co-efficient of hydrogen $\nu \exp(-E_1/k_b T)$, where, E_1 is the activation barrier energy for desorption of H atom, k_b is the Boltzmann's constant and T is the temperature of the grain. The term containing W_H therefore causes a reduction of the number of hydrogen atoms on the grain. On the grain surface, mainly due to diffusive processes, two H atoms combine to form a single H_2 molecule. $A_H = \nu \exp(-E_0/k_b T)$, the hopping rate, gives the probability of this to happen. Here, ν is the vibrational frequency,

$$\nu = \frac{2sE_d}{\pi^2 m_H}, \tag{2b}$$

where, $s \sim 10^{14}$ is the surface density of sites on a grain (Biham et al., 2001), m_H is the mass of the H atom and E_d is the binding energy. This is normally taken to be 10^{12} - 10^{13} s^{-1}. E_0 is the activation barrier energy for diffusion of H atom. This term also reduces the number of H and hence the minus sign in the equation. The diffusion through tunneling has not been taken into account as it could be less important (Katz et al. 1999). S is the number of sites per grain:

$$S = 4\pi r^2 s. \tag{2c}$$

The following equation gives the rate at which the number of H_2 increases with time:

$$\frac{dn_{H2}}{dt} = \mu(A_H/S)n_H^2 - W_{H2}n_{H2}, \tag{2d}$$

where, W_{H2} is the desorption co-efficient of hydrogen molecule which is given by $\nu \exp(-E_2/k_bT)$, E_2 is the activation barrier energy for desorption of H_2 molecule. The parameter μ represents the fraction of H_2 molecule that remains on the surface upon formation while $(1-\mu)$ fraction is desorbed spontaneously due to the energy released in the recombination process. The H_2 production rate R_{H2} in the gas due to grain is then given by,

$$R_{H2} = (1-\mu)(A_H/S)n_H^2 + W_{H2}n_{H2}. \tag{3a}$$

The values for energy barriers E_0, E_1, E_2 and μ are taken from Katz et al. (1999). In our calculations, we used $E_0 = 24.7$ meV, $E_1 = 32.1$ meV, $E_2 = 27.1$ meV and $\mu = 0.33$ for Olivine, $E_0 = 44$ meV, $E_1 = 56.7$ meV, $E_2 = 46.7$ meV and $\mu = 0.413$ for amorphous carbon. We used a third model in which the intermediate activation barrier energies have been used. We gave 50 percent weight to each of the two types of grains. This gives the activation energies of these intermediate grains as $E_0 = 34.35$meV, $E_1 = 44.4$meV, $E_2 = 36.9$meV and $\mu = 0.37$. The recombination efficiency is defined as,

$$\eta = 2R_{H2}/F_H. \tag{3b}$$

Due to the difference in barrier energies, η of different types of grains become significant in completely different temperature ranges. For instance, for Olivine, the temperature range is around $7-13$ K, and for carbon this range is around $13-25$ K. For intermediate barrier energy case that we are considering, this range is around $10-18$ K. The grain size distributions have been taken from Table 1 of WD. Here, Case A parameters with $R_v^b = 5.5$ and $b_C = 3 \times 10^{-5}$ have been chosen. Fig. 1 shows the variation of the effective grain area (product of the number density of grains and the surface area of the grain) A_g as a function of the grain radius indicating that smaller grains have the highest contribution. The dashed curve is for amorphous carbon and the solid curve is for Olivine. In both the cases, we divided the grains into three classes depending on the size for simplicity after taking appropriate weighted average (see, Table 1 and Table 2). For intermediate types of grains, the activation barrier energies have been chosen to be the average of the energies for the above two types.

2.2 (b) Master equation method

It is convenient to use the master equation method (Biham et al. 2001) to study the formation process when the number of particles in each of the species on the grain is 'small'. This process accounts for both the discrete nature of the hydrogen and the fluctuations of its number and solves the problem probabilistically. For instance, its dynamical variables are the probability $P_H(N_H)$ that there are N_H atoms on a grain at a given time. One needs to study the time evolution of the probabilities through the same type of equations as in Eq. 2(a-b), except that the expectation values $< N_H >$ and $< N_{H2} >$ are to be used instead of the average number. The equations are:

$$\frac{d < N_H >}{dt} = F_H(1 - f_{grh} - f_{grh2}) - W_H < N_H > -2(A_H/S) < N_H(N_H - 1) >, \tag{4a}$$

and

$$\frac{d<N_{H2}>}{dt} = \mu(A_H/S) < N_H(N_H - 1) > -W_{H2} < N_{H2} > . \tag{4b}$$

Since $P_H(N_H)$ represents the probability that there are N_H hydrogen atoms on the grain, by sum rule on probabilities:

$$\Sigma_{N_H=0}^{\infty} P_H(N_H) = 1. \tag{5}$$

The time derivatives of these probabilities, $\dot{P}_H(N_H)$ are given by,

$$\begin{aligned}
\dot{P}_H(N_H) &= F_H(1 - f_{grh} - f_{grh2})[P_H(N_H - 1) - P_H(N_H)] \\
&\quad + W_H[(N_H + 1)P_H(N_H + 1) - N_H P_H(N_H)] \\
&\quad + (A_H/S)[(N_H + 2)(N_H + 1)P_H(N_H + 2) - N_H(N_H - 1)P_H(N_H)].
\end{aligned}$$
$$\tag{6a}$$

Similarly, the probability that there are N_{H2} hydrogen molecules on the grain is given by $P_{H2}(N_{H2})$. The time evolution of these probabilities is given by,

$$\dot{P}_{H2}(N_{H2}) = W_{H2}[(N_{H2} + 1)P_{H2}(N_{H2} + 1) - N_{H2}P_{H2}(N_{H2})]$$

$$+\mu(A_H/S) < N_H(N_H - 1 > [P_{H2}(N_{H2-1}) - P_{H2}(N_{H2})]. \tag{6b}$$

From these probabilities, one gets the expectation values for the number of H atoms on the grain as,

$$< N_H >= \Sigma_{N_H=0}^{\infty} N_H P_H(N_H), \tag{7a}$$

and the expectation value for the number of hydrogen molecules are,

$$< N_{H2} >= \Sigma_{N_{H2}=0}^{\infty} N_{H2} P_H(N_{H2}). \tag{7b}$$

The rate at which the number of hydrogen molecules which are released back into the gas is given by,

$$R_{H2} = (1 - \mu)(A_H/S) < N_H(N_H - 1) > +W_{H2} < N_{H2} > . \tag{8}$$

2.3 Computation of accretion rates

Before we study the molecular hydrogen formation efficiency we would like to compute the accretion rate of H on a grain surface. This will allow us to choose the upper and lower limits of the accretion rates within which the H_2 formation rates would be relevant. As in the kinetic theory of gas, the accretion rate is computed from the rate of H which a grain 'sees'. This is given by,

$$F_H = \alpha \pi r^2 v_H n_h, \tag{9}$$

where, α is the probability that an H atom will stick to a grain, v_H is the root-mean-square velocity of the hydrogen which is given by,

$$v_H = \sqrt{8k_b T_{gas}/\pi m_p}, \tag{10}$$

n_h is the number density of hydrogen, r is the mean radius of a grain $r = r_{grain}$. More accurately, it is the sum of the radii of the grain and the hydrogen atom. So we use, $r = r_{grain} + r_H$ ($r_H \sim 10^{-8}$ cm is taken to be the radius of a hydrogen atom). T_{gas} is the temperature which is taken to be $90^o K$. The sticking factor α may vary from 0.1 to 1. We use $\alpha = 0.5$ through out the paper (van Dishoeck et al. 1993). m_p is the mass of an hydrogen atom. We choose cloud the mass density to change from 10^{-24} gm/cm^3 to 10^{-17} gm/cm^3 and the corresponding number density changes from 0.6cm^{-3} - 0.6×10^7 cm^{-3}. Normally, in a diffused and in dense clouds the number density is around $1 - 10^3$ cm^{-3} and 10^{3-6} cm^{-3} respectively.
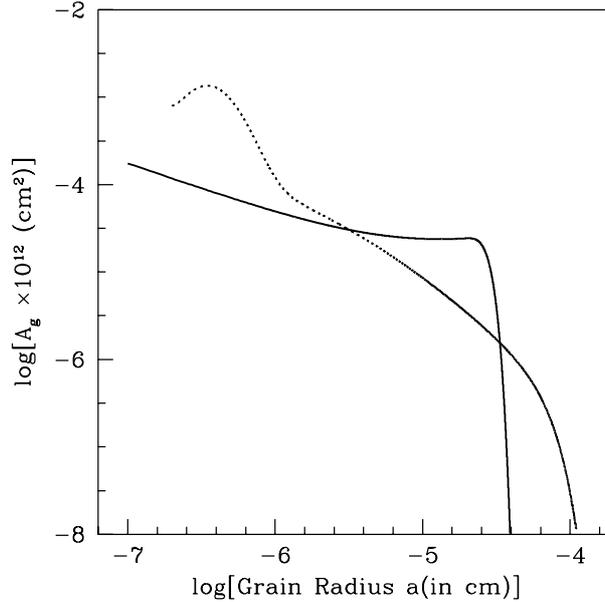
Figure 1. Variation of the effective grain area A_g as a function of the grain radius for the Olivine (solid) and carbon (dashed).

3.   Results

We now present the recombination efficiencies (Eq. 3b) as functions of accretion rates and the grain temperatures for different types of grains mentioned above. In Figs. 2(a-c) we plot η for (a) Olivine, (b) amorphous carbon and (c) intermediate type grains.

Table 1. Average Olivine grain parameters.

Radius (cm)	grain/gas number density ratio	sites
0.40E-06	0.30E-10	0.20E+03
0.36E-05	0.13E-11	0.16E+05
0.19E-04	0.74E-13	0.46E+06

Table 2. Average carbonaceous grain parameters.

Radius (cm)	grain/gas number density ratio	sites
0.36E-06	0.31E-09	0.16E+03
0.29E-05	0.14E-11	0.11E+05
0.21E-04	0.14E-13	0.54E+06

Temperatures of the grains (marked on each curve) are chosen according to the activation barrier energies of these grains in such a way that a significant production of H_2 may take place. The solid curves represent the results when the LHRT (Eq. 2a) is included and the dotted curves show results without this term taken into account. We clearly see that for each case, the LHRT plays an important role for higher accretion rates and must be incorporated in any further study of the grain chemistry. We wish to point out that while obtaining the results we used both the rate equations and the master equations in their respective regimes of importance. Since Olivine has the lower activation barrier energy, the range of temperatures in which the efficiencies are high is also lower.

In Figs. 3(a-c) we show the variation of η as a function of temperature for fixed accretion rates. The accretion rates are marked on the curves. The solid and the dotted curves represent cases with and without LHRT respectively. Note that for low temperature LHRT becomes important because the desorption rate is relatively lower and therefore the accreted H as well as H_2 which are formed remain on the grain surfaces thereby blocking the sites for further accretion.

In the literature, it is customary to use the same H_2 production rate and efficiency for all ranges of temperature and accretion rate. We show that this is far from accurate. For instance, in Figs. 4(a-b) we plot 3D diagrams containing the variation of η as a function of temperature and number density of H in the gas phase for (a) Olivine and (b) amorphous carbon. In this case, the smallest grains are chosen (see, Tables 1-2). Since at a given temperature of the ambient gas, the accretion rate is proportional to the number density alone, calculations are done using the number density. On the surface, contours of constant temperature and number density have been plotted. We note that over the entire range of number density that one would be interested in, the efficiency is high only in a narrow range of temperature – for Olivine, it is in the range of $6 - 10$ K and for carbon, it is in the range of $12 - 18$ K. Since it is expected that at different phases of the collapse of the interstellar matter, the grain temperature would be different, H_2 production would be 'turned on' only in certain phases and not through out its evolution.
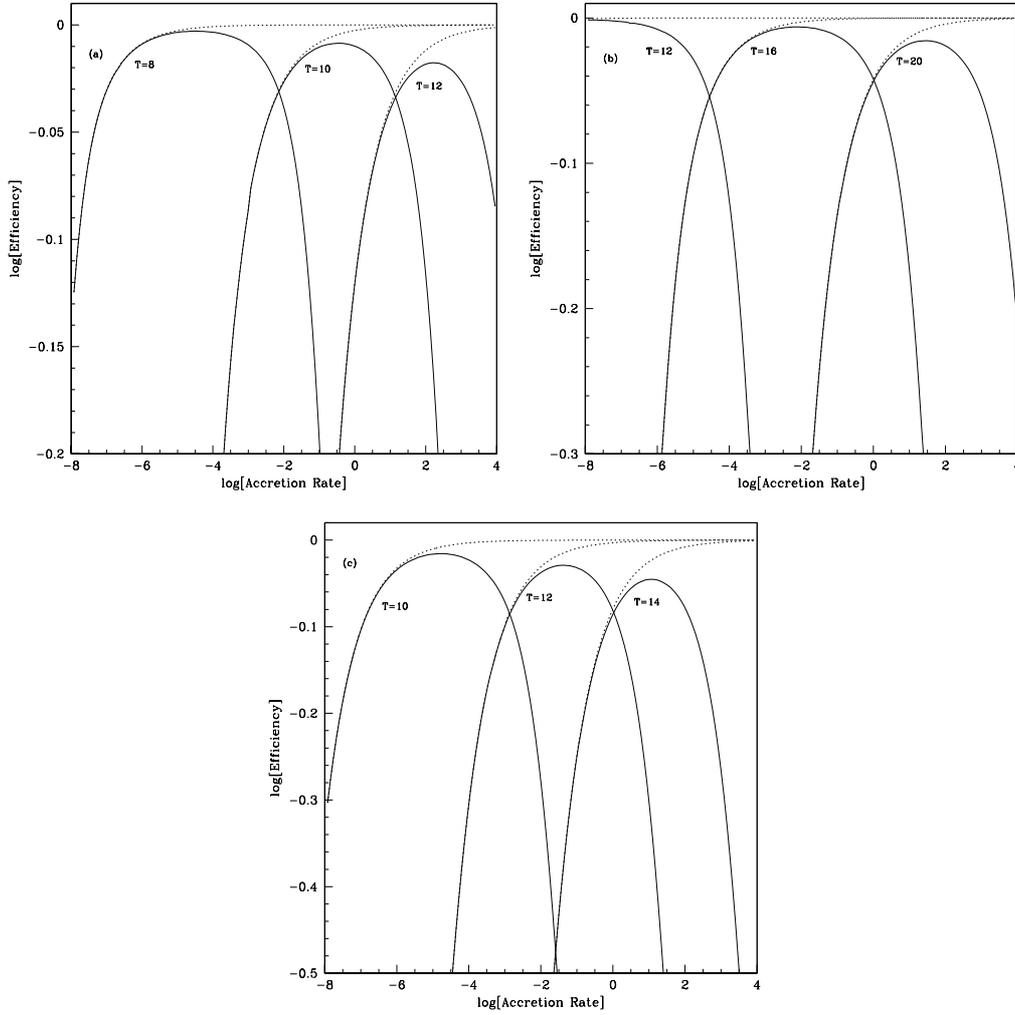
Figure 2a-c. Recombination efficiency η of H_2 for (a) Olivine (b) carbon and (c) intermediate type grains with (solid) and without (dashed) LHRT as a function of accretion rate for a fixed temperature. Curves are drawn for three different temperatures as marked.

The gas temperature for which the result is presented is $T_{gas} = 90$ K. Since the accretion rate depends on the mean velocity of the gas, which in turn is proportional to $T_{gas}^{1/2}$, the result is not too sensitive to the ambient gas temperature. We have verified this by explicit computation. We have also calculated η for intermediate type grains in which the activation barrier energies are intermediate between carbon and Olivine. The results lie in between the two extreme cases presented above.
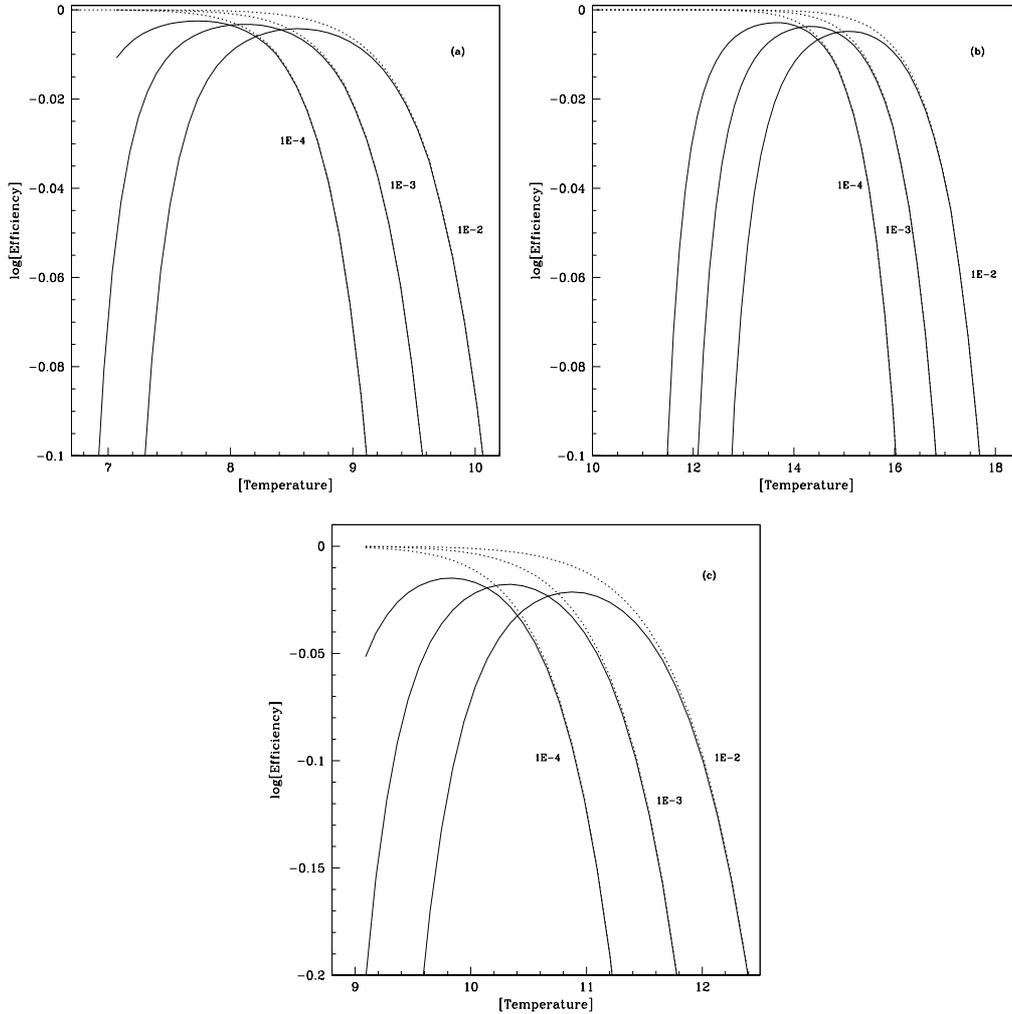
Figure 3a-c. Recombination efficiency η of H_2 for (a) Olivine (b) carbon and (c) intermediate type grains with (solid) and without (dashed) LHRT as a function of temperature for a fixed accretion rate. Curves are drawn for three different accretion rates as marked.

In Figs. 5(a-b), the same Figures are drawn with the largest grain size (see, Tables 1-2). In this case, the accretion rate is higher for a given number density, and therefore the 'turning on' phenomenon occurs at a slightly higher temperature.

In Tables (3-5) we give the rates at which the molecular hydrogen forms at various temperatures (rows) and at various gas densities (columns). Here the results from all the three grain sizes have been combined. Table 3 is for Olivine, Table 4 is for carbon and Table 5 is for intermediate type grains respectively. These numbers are to be compared
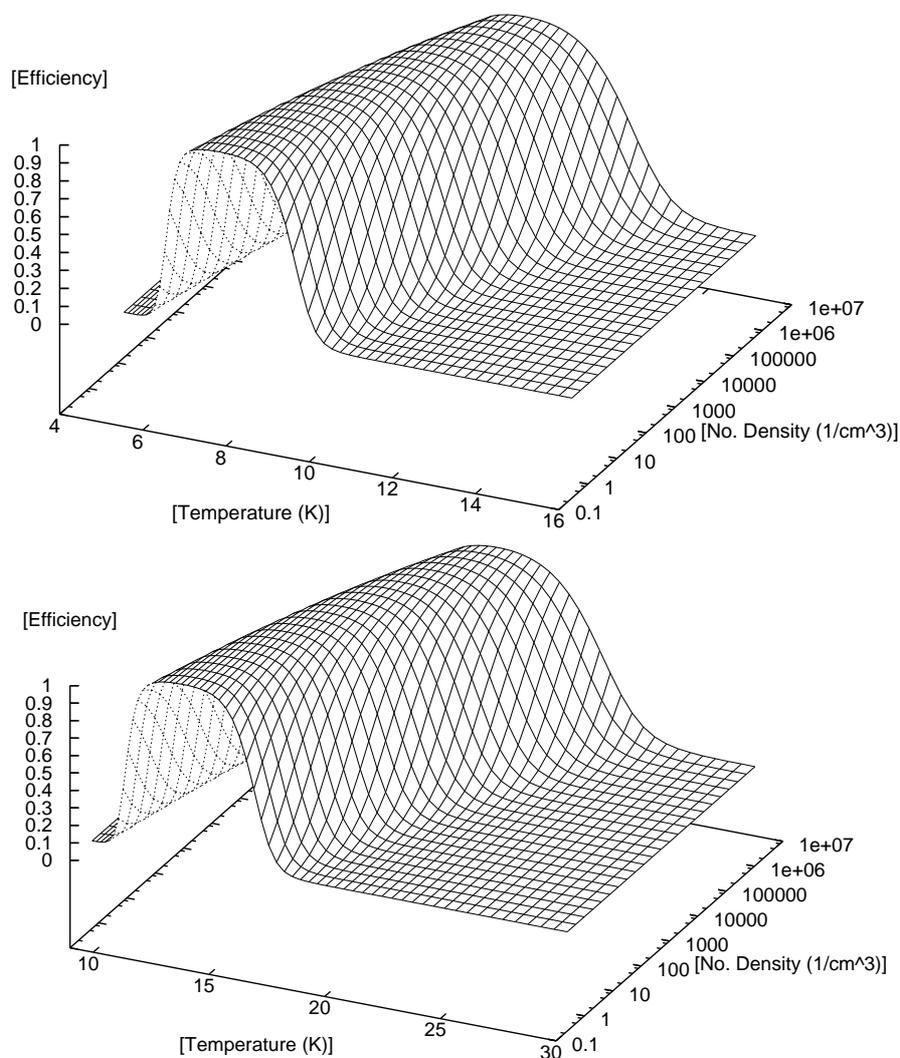
Figure 4a-b. Recombination efficiency η of H_2 for (a) Olivine and (b) carbon as a function of the grain temperature (T) and the number density n_h in the ambient gas of $T_{gas} = 90$K. Contours of constant T and n_h are shown on the surface. The smallest grain sizes of (a) 40 Å and (b) 36 Å have been chosen.

with the standard constant rate of a few times 10^{-18} rate used in the literature. We find that these rates are very strongly varying functions and recommended that these tables may be used to obtain more accurate results.

Table 3. Rates (cm^{-3} sec^{-1}) of H_2 formation for Olivine grains at representative temperatures and densities.

n(cm^{-3}) → T(K) ↓	1	10	10^2	10^3	10^4	10^5
10	0.259E-18	0.181E-15	0.546E-13	0.853E-11	0.100E-08	0.104E-06
12	0.129E-21	0.129E-18	0.129E-15	0.129E-12	0.106E-09	0.435E-07
14	0.569E-24	0.569E-21	0.569E-18	0.569E-15	0.569E-12	0.563E-09
16	0.974E-26	0.974E-23	0.974E-20	0.974E-17	0.974E-14	0.974E-11
18	0.411E-27	0.411E-24	0.411E-21	0.411E-18	0.411E-15	0.411E-12
20	0.325E-28	0.325E-25	0.325E-22	0.325E-19	0.325E-16	0.325E-13
22	0.408E-29	0.408E-26	0.408E-23	0.408E-20	0.408E-17	0.408E-14
24	0.722E-30	0.722E-27	0.722E-24	0.722E-21	0.722E-18	0.722E-15
26	0.167E-30	0.167E-27	0.167E-24	0.167E-21	0.167E-18	0.167E-15
28	0.474E-31	0.474E-28	0.474E-25	0.474E-22	0.474E-19	0.474E-16
30	0.159E-31	0.159E-28	0.159E-25	0.159E-22	0.159E-19	0.159E-16
32	0.614E-32	0.614E-29	0.614E-26	0.614E-23	0.614E-20	0.614E-17

Table 4. Rates (cm^{-3} sec^{-1}) of H_2 formation for Carbon grains at representative temperatures and densities.

n(cm^{-3}) → T(K) ↓	1	10	10^2	10^3	10^4	10^5
10	0.672E-18	0.711E-17	0.716E-16	0.716E-15	0.716E-14	0.716E-13
12	0.125E-16	0.119E-14	0.949E-13	0.363E-11	0.520E-10	0.544E-09
14	0.121E-16	0.127E-14	0.127E-12	0.124E-10	0.115E-08	0.822E-07
16	0.242E-17	0.579E-15	0.108E-12	0.124E-10	0.126E-08	0.124E-06
18	0.334E-19	0.302E-16	0.179E-13	0.542E-11	0.106E-08	0.122E-06
20	0.468E-21	0.468E-18	0.462E-15	0.411E-12	0.235E-09	0.727E-07
22	0.144E-22	0.144E-19	0.143E-16	0.143E-13	0.139E-10	0.111E-07
24	0.802E-24	0.802E-21	0.802E-18	0.801E-15	0.800E-12	0.789E-09
26	0.703E-25	0.703E-22	0.703E-19	0.703E-16	0.703E-13	0.702E-10
28	0.870E-26	0.870E-23	0.870E-20	0.870E-17	0.870E-14	0.870E-11
30	0.141E-26	0.141E-23	0.141E-20	0.141E-17	0.141E-14	0.141E-11
32	0.285E-27	0.285E-24	0.285E-21	0.285E-18	0.285E-15	0.285E-12
34	0.687E-28	0.687E-25	0.687E-22	0.687E-19	0.687E-16	0.687E-13
36	0.193E-28	0.193E-25	0.193E-22	0.193E-19	0.193E-16	0.193E-13
38	0.615E-29	0.615E-26	0.615E-23	0.615E-20	0.615E-17	0.615E-14
40	0.219E-29	0.219E-26	0.219E-23	0.219E-20	0.219E-17	0.219E-14

Table 5. Rates (cm^{-3} sec^{-1}) of H_2 formation for intermediate type grains at representative temperatures and densities.

n(cm^{-3}) → T(K) ↓	1	10	10^2	10^3	10^4	10^5
10	0.115E-16	0.120E-14	0.118E-12	0.106E-10	0.650E-09	0.154E-07
12	0.167E-18	0.133E-15	0.629E-13	0.997E-11	0.115E-08	0.116E-06
14	0.294E-21	0.294E-18	0.294E-15	0.282E-12	0.207E-09	0.709E-07
16	0.246E-23	0.246E-20	0.246E-17	0.246E-14	0.245E-11	0.237E-08
18	0.587E-25	0.587E-22	0.587E-19	0.587E-16	0.587E-13	0.586E-10
20	0.292E-26	0.292E-23	0.292E-20	0.292E-17	0.292E-14	0.292E-11
22	0.249E-27	0.249E-24	0.249E-21	0.249E-18	0.249E-15	0.249E-12
24	0.320E-28	0.320E-25	0.320E-22	0.320E-19	0.320E-16	0.320E-13
26	0.561E-29	0.561E-26	0.561E-23	0.561E-20	0.561E-17	0.561E-14
28	0.126E-29	0.126E-26	0.126E-23	0.126E-20	0.126E-17	0.126E-14
30	0.345E-30	0.345E-27	0.345E-24	0.345E-21	0.345E-18	0.345E-15
32	0.111E-30	0.111E-27	0.111E-24	0.111E-21	0.111E-18	0.111E-15
34	0.408E-31	0.408E-28	0.408E-25	0.408E-22	0.408E-19	0.408E-16
36	0.167E-31	0.167E-28	0.167E-25	0.167E-22	0.167E-19	0.167E-16
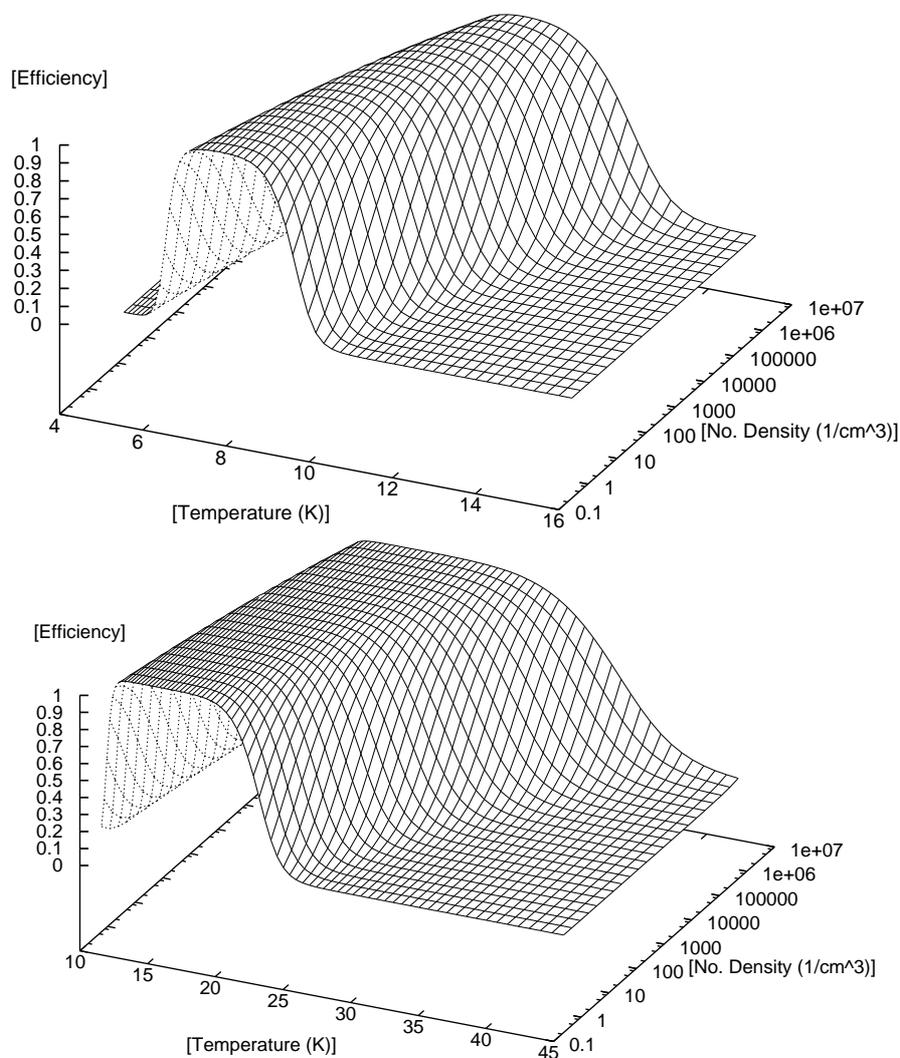
Figure 5a-b. Same as in Fig. 4a-b except that the larger grains of size (a) ∼1900 Å and (b) ∼2100 Å are chosen.

4.   Discussions

In this paper, we presented the detailed result of how the recombination efficiency depends on the activation barrier energy (type of the grain), the grain temperature, the number density of hydrogen in the gas phase (which together with temperature determines the flux of hydrogen on the grains) and finally, on the grain size. We showed that: (a) The Langmuir-Hinselwood rejection term is very important, especially when the accretion

rate is high or the temperature is lower. At high fluxes, a significant fraction of the grain surface is occupied by H or H_2 and only a fraction of the grain surface could be accessed by the incoming hydrogen. At low temperatures, the thermal hopping is hindered and H would be practically immobile. Moreover, the desorption energy of H is higher than that of H_2. Thus the grain will be full of accreted H and some H_2, thereby blocking further accretion. (b) The temperature dependence of the recombination efficiency is really strong, becoming important in only a narrow range. For instance, for Olivine, the temperature range is around $7-13$ K, for carbon this range is around $13-25$ K and for the intermediate barrier energy case that we are considering, this range is around $10-18$ K. We have provided the rate of H_2 formation under various circumstances in the form of tables. These numerical values may be used whenever accurate rates are required to obtain the chemical evolutions in interstellar clouds.

We wish to conclude by pointing out that the typical life-time of a molecular cloud is a few million years. Using the present experimentally obtained rates, we find that H_2 would be produced within the lifetime of the clouds in temperature range of 6-20K only when Olivine and amorphous carbon grains are present. Other mechanisms include tunneling and chemisorption of H_2 on grain surfaces. While the former one is possible at all temperatures, and is possibly faster than thermal hopping, the experimental results by Katz et al. (1999) do not show any evidence for tunneling. The later one is important only at high temperatures $\sim 200K$. Thus a complete understanding of H_2 formation requires more experimental work on various types of grain surfaces and at various temperatures.

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