Recombination Efficiency of Molecular Hydrogen on Interstellar Grains-II A Numerical Study

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2008 June 28

Abstract. A knowledge of the recombination time on the grain surfaces has been a major obstacle in deciding the production rate of molecular hydrogen and other molecules in the interstellar medium. We present a numerical study to compute this time for molecular hydrogen for various cloud and grain parameters. We also find the time dependence, particularly when a grain is freshly injected into the system. Apart from the fact that the recombination times seem to be functions of the grain parameters such as the activation barrier energy, temperature etc, our result also shows the dependence on the number of sites in the grain $S$ and the effective accretion rate per site $a_s$ of atomic hydrogen. Simply put, the average time that a pair of atomic hydrogens will take to produce one molecular hydrogen depends on how heavily the grain is already populated by atomic and molecular hydrogens and how fast the hopping and desorption times are. We show that if we write the average recombination time as $T_r \sim S^\alpha/A_H$, where, $A_H$ is the hopping rate, then $\alpha$ could be much greater than 1 for all astrophysically relevant accretion rates. Thus the average
formation rate of $H_2$ is also dependent on the grain parameters, temperature and the accretion rate. We believe that our result will affect the overall rate of the formation of complex molecules such as methanol which require successive hydrogenation on the grain surfaces in the interstellar medium.

Keywords: Molecular cloud – star formation – grain chemistry – numerical simulations

1. Introduction

It has long been suggested that the dust grains play a major role in the formation of molecular hydrogen in the interstellar medium (ISM) (Gould & Salpeter, 1963). Considerable studies were made since then to understand the real physical processes which are taking place both theoretically (e.g., Hollenbach, Werner & Salpeter, 1971; Takahashi, Matsuda & Nagaoka, 1999; Biham et al. 2001) as well as experimentally (e.g., Pirronello et al. 1997a,b, 1999). More recently, Biham et al. (2001), and Green et al. (2001) have computed $H_2$ production rate by physisorption. It was found that a significant production is possible in cooler ($\sim 10 – 25$K) clouds. Cazaux & Tielens (2002, 2004) use both physisorption and chemisorption, to demonstrate that $H_2$ production is possible at high temperatures ($\sim 200 – 400$K) also. The goal is to study the rate at which the $H$ atoms combine together on the surface of the grains to form $H_2$ and then they are desorbed into the gas phase to react with other atoms. When compared with the average mass fractions of various molecular species obtained through gas phase reactions (see, Chakrabarti & Chakrabarti, 2000ab; Das et al. 2006), it was found that the observed abundances of more complex species, such as methanol, are much higher. It is possible that methanol as well as its precursors also have to be formed on grain surfaces through successive hydrogenation. Our finding for molecular hydrogen has thus important bearings on the formation of more complex molecules on grains. These molecules would, in turn, desorb
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into the gas phase and would be expected to produce more complex species such as amino acids in due course.

One of the most challenging problems is to determine the average rate at which the recombination of atomic hydrogen takes place on a grain surface. In theoretical investigations which are prevalent in the subject (See, Acharyya and Chakrabarti, 2005; hereafter Paper I; Acharyya, Chakrabarti and Chakrabarti, 2005; hereafter ACC05), the diffusion rate $A_H$ (inverse of the diffusion time $T_d = 1/A_H$) is divided by $S$, the number of sites on the grain surface (e.g., Biham et al. 2001) to get the recombination rate. The argument for reducing the rate by a factor of $S$ is this: on an average, there are $S^{1/2}$ number of sites in each direction of the grain. Since the hopping is random, it would take square of this, i.e., $S$ number of hopping to reach a distance located at $S^{1/2}$ sites away, where, on an average, another $H$ is available. Thus, the effective recombination rate was chosen to be $A_H/S$. It is an empirical factor and needs more careful treatment. In our present paper, we replace $S$ by an 'unknown' quantity $S' = S^\alpha(t)$, where $\alpha(t)$ may be time dependent (if the grain and cloud parameters change) and it could also deviate from unity. Let $\alpha = \alpha_0$ when a steady state is reached. Higher the accretion rate, lesser should be the value of $\alpha_0$ as the effective surface area $S'(t \to \infty)$ gets smaller and smaller. The opposite is true for smaller accretion rates. In fact, in the limit, if the accretion rate is so low, that a lone $H$ sweeps around the grain several times to find another $H$, one would get $\alpha_0 > 1$ since the effective site number is higher than $S$. Using our simulation, we determine how the effective site number deviates from $S$, one way or the other when the accretion rate is varied. Our result is likely to have important consequences for the formation of other hydrogenated species, such as water, methanol on grain surfaces. This will be discussed elsewhere. Some preliminary results with steady state $\alpha_0$ have been presented in Das et al. (2005) and Chakrabarti et al. (2006). In the current paper, we discuss the time and temperature dependence of $\alpha(t)$ and studied the cases for more varied astrophysically important accretion rates.

In the next Section, we present the modified typical equations which govern the
molecular hydrogen production rate on a grain surface. Incorporating the physical aspects of these equations, we perform a numerical simulation to determine the numbers on the grains. In §2, we present the procedure for the simulation and in §3 we present the results for two types of commonly used grains, namely, olivine and amorphous carbon. We show how \( \alpha(t) \) depends on time and how it settles into a number (generally, \( > 1 \)) when steady state is reached. Finally, in §4, we present our concluding remarks.

2. Procedure of numerical simulation

The relevant equations which are generally solved on grain surfaces have been presented in Paper I (Eqs. 2a-d) and we do not repeat them here. However, for Monte-Carlo simulation we need to modify these equations. Since in our simulation we expect to get the rate of diffusion \( T_r(t) = S/A_H \) of H exactly, we can assume that the recombination time at any instant \( t \) could be written in the form:

\[
T_r(t) = \frac{S'}{A_H},
\]

(1)

where, \( S' \) is an ‘effective surface area’ which we may be written as \( S' = S^\alpha(t) \). Here, \( \phi_H = F_H(1 - f_{grh} - f_{grh2}) \). \( F_H \) is the accretion rate of \( H \) and \( F_H = A < v > N_H \), \( A \) being the area of a grain, \( < v > \) is the average velocity and \( N_H \) is the number density of \( H \) in the gas phase. Our goal would be to compute the steady state value \( \alpha_0 = \alpha(t \rightarrow \infty) \) for various grains (type and size) at various accretion rates and grain temperatures and to check if \( \alpha \sim 1 \). Thus, instead of Eqs. 2a of Paper I, the actual governing equation for atomic hydrogen should be,

\[
\frac{dn_H}{dt} = \phi_H - W_H n_H - 2(A_H/S^\alpha)n_H^2,
\]

(2a)

along with equation governing the rate of production of \( H_2 \) given by,

\[
\frac{dn_{H2}}{dt} = \mu(A_H/S^\alpha)n_H^2 - W_{H2}n_{H2},
\]

(2b)

where, \( A_H \) is the hopping rate given by \( \nu \exp(-E_0/k_B T) \), \( W_H \) is the desorption co-efficient of hydrogen atom given by, \( \nu \exp(-E_1/k_B T) \), \( W_{H2} \) is the desorption co-efficient of hydrogen molecule given by, \( \nu \exp(-E_2/k_B T) \). Here, \( E_0 \) is the activation barrier energy for
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diffusion of H atom, \(E_1\) is the activation barrier energy for desorption of H atom and \(E_2\) is the activation barrier energy for desorption of \(H_2\) molecule, \(\nu\) is the vibrational frequency given by \(\nu = \frac{2sE_d}{\pi^2 m_H}\), \(n_H\) be the number of H atoms, and \(n_{H_2}\) be the number of \(H_2\) on a grain at time \(t\), \(s \sim 10^{14-16}\) is the surface density of sites on a grain, \(m_H\) is the mass of the H atom and \(E_d\) is the binding energy. The parameter \(\mu\) represents the fraction of \(H_2\) molecules that remains on the surface upon formation while \((1-\mu)\) fraction is desorbed due to the energy released in the recombination process. The \(H_2\) production rate \(R_{H_2}\) in the gas due to grain is then given by,

\[
R_{H_2} = (1 - \mu)(A_H/S^\alpha)n_H^2 + W_{H_2}n_{H_2}.
\]

The values of the activation barrier energies \(E_0\), \(E_1\) and \(E_2\) are taken from Katz et al. (1999) and are given by, \(E_0 = 24.7\) meV, \(E_1 = 32.1\) meV and \(E_2 = 27.1\) meV for olivine and \(E_0 = 44\) meV, \(E_1 = 56.7\) meV and \(E_2 = 46.7\) meV for amorphous carbon grains. For olivine, \(\mu = 0.33\) and for amorphous carbon \(\mu = 0.413\) was used.

For the sake of simplicity, we assume each grain to be square in shape having \(S = n^2\) number of sites (square lattice). We use periodic boundary condition so that the lattice behaves like a closed surface. We anticipate that the result would be insensitive to the actual nature of the lattice when simulation is done for a long time. We use mono-layer on the grain surface. We choose the minimum time step to be \(t_h = 1/A_H\), the hopping time and advance the global time by this step. If \(\phi_H\) is the effective accretion rate (as defined above), after every time step, i.e., after every \(1/A_H\) seconds, \(\phi_H/A_H\) number of hydrogen atoms are dropped on the grain. If \(\phi_H\) is too low so that \(\phi_H/A_H < 1\), then, clearly, one H is dropped after every \(A_H/\phi_H\) steps. The exact site at which one atom is dropped is obtained by a pair of random numbers \((R_x, R_y, R_z, R_y < 1)\) obtained by a random number generator. This pair would place the incoming hydrogen at \((i, j)\)th grid, where, \(i\) and \(j\) are the nearest integers obtained using the Int function: \(i = \text{int}(R_x * n + 0.5)\) and \(j = \text{int}(R_y * n + 0.5)\). Each atom starts hopping with equal probability in all four directions. This was decided by another random number. When, during the hopping process, one atom enters a site which is already occupied by another atom, we assume
that a molecule has been formed and increase the number of \( H_2 \) by unity. However, when the atom enters a site occupied by an \( H_2 \), another random number is generated to decide which one of the other neatest sites it is going to occupy.

Thermal evaporation of \( H \) and \( H_2 \) from a grain surface are handled in the following way. Since \( W_H \) is the desorption rate for \( H \), one atom is supposed to be released to the gas phase after every \( 1/W_H \) seconds. We generate a random number \( R_t \) for every \( H \) present on the grain and release (at each time step, i.e., \( 1/A_H \) seconds) only those for which \( R_t < W_H/A_H \). Similar procedure is followed for the evaporation of \( H_2 \) for which the criterion for evaporation was \( R_t < W_{H_2}/A_H \).

Due to spontaneous desorption, a factor of \((1-\mu)\) of \( n_{H_2} \) is lost to the gas phase. Here too, a random number \( R_s \) is generated for each newly formed (within that time step) \( H \) present on the grain. Those which satisfy \( R_s < (1 - \mu) \) are removed to the gas phase.

We continue our simulation for more than \( 10^9 \) s. After an initial transient period, \( n_H \) and \( n_{H_2} \) reaches a quasi-steady state with some fluctuations. In a steady state, \( \alpha_0 \) can be calculated using Eq. 2a, i.e.,

\[
\alpha_0 = \log\left(\frac{2A_H n_H^2}{\phi_H - W_H n_H}\right)/\log(S).
\]

(4)

In this context, one important parameter \( \beta \) may be defined as the ‘catalytic capacity’ of a grain (Chakrabarti et al. 2006) which measures the efficiency of the formation of \( H_2 \) on that grain surface for a given pair of \( H \) residing on it. Let \( \delta N_{H_2} \) be the number of \( H_2 \) formed in \( \delta t \) time. Since two hydrogen atoms are required to create one \( H_2 \), the average rate of creation of one \( H_2 \) per pair of \( H \) atom would be given by,

\[
< A_{H1} > = \frac{1}{2n_H} \frac{\delta N_{H_2}}{\delta t}.
\]

(5a)

We identify the inverse of this rate with the average formation rate given by,

\[
T_f(t) = S^{\beta(t)}/A_H.
\]

(5b)

Thus,

\[
S^{\beta}(t) = A_H/ < A_{H1} > .
\]

(5c)
This yields $\beta(t)$ as a function of time as,

$$\beta = \log(A_H / < A_{H1} >)/\log(S).$$

(6)

Here too we can define $\beta_0 = \beta(t \to \infty)$. Our goal would be to see if $\beta_0$ thus obtained actually varies with grain parameters, accretion rate and temperatures. Intuitively, it should. This is because, when the accretion rate is very low, finding a second $H$ on the grain would be difficult and it can take several sweeps of the grain surface. Thus $\beta_0 > 1$ would be a possibility. On the other hand, when the rate is very high, many sites would be occupied and another $H$ would be met along any direction and $\beta_0$ could come down to $1/2$ or even less. Indeed, this is what we see as well. We have carried out the simulation with and without spontaneous desorption taken into account. In presence of the spontaneous desorption, we remove $H_2$ by generating a random number as soon as one $H_2$ is formed and checking if it is less or more compared to $\mu$. If less, $H_2$ remains on the grain, else it is taken out to the gas phase. The detailed results are discussed in the next Section.

3. Results and Discussions

Fig. 1 gives the variation of $n_H$ and $n_{H2}$ residing on the grain surface since the beginning of the simulation. We chose a grain with $10^4$ sites at 8K. For clarity, we plot average numbers in every $\sim 5.5 \times 10^6$s bin after the initial transient period of $\sim 2 \times 10^6$s is over. The simulation was carried out near about $10^{10}$s. The effective accretion rate is assumed to be $\phi_H = 7.98 \times 10^{-4}s^{-1}$. In this case, the steady state has clearly been reached by this time and we can compute $\alpha_0$ by using Eq. 4. This is done below.

3.1 Olivine grains

We start with the olivine grains which are kept at 8 K. The evaporation rate of $H_2$ is $W_{H_2} = 0.834844 \times 10^{-5}s^{-1}$ which corresponds to a time scale of $\sim 119782.8$s and similarly
Figure 1.: Variation of the number of H and $H_2$ on an olivine grain of $10^4$ sites kept at 8K and exposed to an effective accretion rate per site of $H$ $7.98 \times 10^{-8}$ s$^{-1}$. We carried out our simulation near about $10^{10}$s. For cleanliness, after the initial transient period of about $2 \times 10^6$s is over, we took time average at every $5.5 \times 10^6$s before plotting the numbers.

The evaporation rate of $H$ is $W_H = 0.59 \times 10^{-8}$s$^{-1}$ which corresponds to $\sim 169585908$s. The hopping time for hydrogen on this grain is $3680.58$s (data taken from Katz et al. 1999).

In Fig. 2a, we present the computed $\alpha_0$ (Eq. 4) as a function of $a_s$ – the effective accretion rate per site. The solid, dot-dashed and the dashed curves are for $S = 10^4$, $9 \times 10^4$ and for $10^6$ sites respectively. No spontaneous desorption has been included (i.e., $\mu = 1$). We extrapolated our curve to very low accretion rates which would have taken a very long computation time, just to show the trend of the result and extreme conditions. We note that $\alpha_0$ is generally higher than unity in the region of our interest. This is because $H$s are scattered few and far between and it takes a longer time (generally more than one sweeping) for one $H$ to locate another. $\alpha_0$ monotonically drops as the accretion rate goes up. In Fig. 2b, we show the variation of $\beta_0$ (Eq. 6) for the same case. Here too, we see that $\beta_0$ is very high compared to unity for low rates, but becomes $\sim 0.5$ or lower for higher rates as expected. Note that $\alpha_0$ and $\beta_0$ go down with increasing site number $S$ also. Since for a smaller grain, the possibility of getting it filled at a high rate is higher,
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Figure 2. (a-b): Variation of (a) $\alpha_0$ and (b) $\beta_0$ as a function of $a_s$, the effective accretion rate per site for various olivine grains kept at 8K. The dashed, dot-dashed and solid curves are for $S = 10^6$, $9 \times 10^4$, and $10^4$ respectively. $\alpha_0$ is clearly a function of the accretion rate. For rates relevant in molecular clouds $\alpha_0$ and $\beta_0$ are much larger than unity. For very high rates $\beta_0$ comes down to 0.5 or lower. The deviation is highlighted using dotted curves by extrapolating at very low accretion rates.

one would have expected an opposite result. However, it is to be remembered that for a larger grain, the accretion rate itself ($\phi_H = S a_s$) is also large. Hence the plots are to be compared carefully. For instance, the result of $a_s = 0.0005 \times 10^{-8}$s$^{-1}$ for $9 \times 10^4$ sites is to be compared with that of $a_s = 0.0045 \times 10^{-8}$s$^{-1}$ for $10^4$ sites in order to make a meaningful comparison. In any case, for reasonable $\phi_H$ values with number densities up to $10^6$ cm$^{-3}$, the relevant $a_s$ would be below $10^{-6}$ where $\alpha_0 > 1$ in general.
Figure 3. (a-d): In (a-b) snapshots of the grain surface with $H$ (hollow squares) and $H_2$ (filled squares) at two arbitrarily chosen times (a) $8 \times 10^8$s and at (b) $10^9$s. Here an olivine grain (at 8K) with 900 sites has been chosen. This is bombarded with an accretion rate per site of $H_{3.02 \times 10^{-7}}$ per sec. No spontaneous desorption has been assumed here. In (c-d) spontaneous desorption has been included and plotted for the same time as before. Thus, numbers of $H_2$ residing on the grain at any instant are lesser.

In Fig. 3(a-b), we present snapshots of the occupancy of $H$ (hollow squares) and $H_2$ (filled squares) at two instants of time on the grain containing only 900 sites at two arbitrarily chosen times (a) $t=8 \times 10^8$s (b) $t=10^9$s respectively. Here an olivine grain at
Figure 4. : Temperature dependence of $\alpha_0$ for the olivine grains at 10K (solid), 9K (dot-dashed) and 8K (dashed). The deviation is highlighted using dotted curves by extrapolating at very low accretion rates.

(8K) with 900 sites has been chosen. This grain is facing an accretion rate of $F_H/S$ of $3.02 \times 10^{-7} \text{s}^{-1}$ per site. No spontaneous desorption has been assumed here. This is to be compared with Fig. 3(c-d) for the same simulation and for the same time as before when the spontaneous desorption has been included. The numbers of $H_2$ are fewer since after formation of $H_2$ molecules some part of the $H_2$ are spontaneously desorbed in to the gas phase.

When temperatures of the grain is increased, all the rates go down exponentially. As a result, we expect $\alpha_0$ to rise with temperature for a given accretion rate. In Fig. 4 we show this behaviour for $T = 8, 9, 10$K respectively for olivine grains. We choose $S = 10^4$ in this case. This behaviour affects the recombination efficiency $\eta$ as defined by,

$$\eta = \frac{2R_{H_2}}{F_H}$$

itself. In Fig. 5, we compare the temperature dependence of $\eta$ as obtained from the rate equations (solid) curve with that obtained from our simulations. The accretion rate per site of $1.8 \times 10^{-9} \text{ sec}^{-1}$ was used (same in both the cases). We note that for $T \lesssim 7.5$K the simulation results are higher and for $T \gtrsim 7.5$K the simulation results are lower. This
Figure 5. A comparison between the recombination efficiency obtained from the rate equation (solid) and that obtained from our simulation (dashed). We use the accretion rate per site $1.8 \times 10^{-9}$ per second for a grain of diameter 0.1$\mu$m. The difference can be attributed to the temperature dependence of the $\alpha_0$ as shown in Fig. 4 above.

Figure 6. A comparison of the simulation results (dark circles) with those obtained from analytical considerations (dashed curves) when suitable modification of the average recombination rate is made. An Olivine grain of $10^4$ sites at a temperature of 8K has been chosen in this comparison. Dotted curves are drawn using analytical results for $\alpha_0$ extrapolated to very low accretion rates.
is because $\alpha_0$ itself is strongly temperature dependent as shown in Fig. 4 while the rate equation uses $S = S'$ (i.e., $\alpha_0 = 1$) for all temperatures.

In Fig. 6 we compare our results with the analytically obtained results from the rate equation method provided correct $S'$ was chosen (Eqs. 2ab). The simulation results are shown by the dark circles and those obtained from the analytical considerations are shown by the dashed curves. An Olivine grain of $10^4$ sites at a temperature of 8K has been chosen in this comparison. Dotted curves are drawn using analytical results for $\alpha_0$ extrapolated to very low accretion rates.

It is interesting to compare the results of our simulation with those obtained from the analytical considerations with and without our $\alpha_0$ factor. In Table 1, we present this comparison. We take an Olivine grain of $10^4$ sites at 8K and vary the accretion rates. In Column 1, we give the accretion rate per site of the grain. In Column 2 we present the coefficient $\alpha_0$ which we derive from our simulation. In Columns 3-5, we present the number of $H$ as obtained by our simulation and the modified equation (Eq. 2a) and the standard equations (Paper I) respectively. Columns 6-8, we present similar results for $H_2$. We find that our simulation matches more accurately with the analytical results provided $S'$ is chosen as the surface area. If the standard equation is used, the deviation is very significant. Indeed, the number of $H$ on the grain could be roughly half as much when simplistic analytical model is used. What observe is that on the grains we tend to have more $H$ and less $H_2$ than what analytical work suggests.

### 3.2 Amorphous carbon grains

Carbon grains produce significant $H_2$ at a higher temperature than olivine grains because all the barrier energies are higher. We plot in Fig. 7a the variation of $\alpha_0$ with $a_s$ at temperature 14K. The nature of variation of $\alpha_0$ remains the same, namely, $\alpha_0$ goes down with $a_s$. The solid, dot-dashed and the dashed curves are for $S = 10^6$, $9 \times 10^4$ and for $10^4$ sites respectively. In Fig. 7b, we show the variation of $\beta_0$ and as expected its value
can become as low as 0.5 for very large accretion rate. These results are representative as they are strongly temperature dependent as in the case of olivine (see, Fig. 4).

4. Concluding remarks

In this paper, we studied the behaviour of the average recombination time of atomic hydrogens on grain surfaces as a function of time, temperature, accretion rate and grain parameters. In the literature, it is simply assumed that the recombination time is grain site number divided by the diffusion rate. However, we find that this simplistic assumption is not valid especially when the accretion rate of $H$ on the grain is very low or very high. For very low rates, an atomic hydrogen may have to sweep a grain several times before meeting another atom to form a molecule. For very high rates, the grain surfaces could be

Table 1. Comparison of $H$ and $H_2$ abundances in various methods

| Accretion Rate per site $A_s (S^{-1})$ | $\alpha_0$ | $H$ with | $H_2$ with |
|--------------------------------------|----------|----------|----------|
|                                      |          | simulation $\alpha_0 \neq 1$ | $\alpha_0 = 1$ | simulation $\alpha_0 \neq 1$ | $\alpha_0 = 1$ |
| $6.79 \times 10^{-7}$                | 1.04     | 403.11   | 407.80   | 340.57   | 361.71 | 383.82 | 377.48 |
| $2.72 \times 10^{-7}$                | 1.05     | 275.78   | 278.02   | 219.31   | 149.96 | 158.16 | 156.53 |
| $2.72 \times 10^{-8}$                | 1.07     | 99.03    | 99.31    | 70.35    | 15.40  | 16.14  | 16.11  |
| $1.36 \times 10^{-8}$                | 1.08     | 72.27    | 72.42    | 49.80    | 7.71   | 8.08   | 8.07   |
| $5.43 \times 10^{-9}$                | 1.09     | 47.30    | 47.37    | 31.52    | 3.11   | 3.23   | 3.23   |
| $2.72 \times 10^{-10}$               | 1.11     | 11.62    | 11.62    | 7.01     | 1.49 $\times 10^{-1}$ | 1.59 $\times 10^{-1}$ | 1.60 $\times 10^{-1}$ |
| $1.09 \times 10^{-10}$               | 1.12     | 7.46     | 7.48     | 4.42     | 5.81 $\times 10^{-2}$ | 6.24 $\times 10^{-2}$ | 6.35 $\times 10^{-2}$ |
| $2.72 \times 10^{-11}$               | 1.13     | 3.86     | 3.82     | 2.18     | 1.31 $\times 10^{-2}$ | 1.49 $\times 10^{-2}$ | 1.55 $\times 10^{-2}$ |
| $*2.04 \times 10^{-11}$              | 1.13     | 3.36     | 3.33     | 1.89     | 9.7 $\times 10^{-3}$ | 1.11 $\times 10^{-2}$ | 1.17 $\times 10^{-2}$ |
| $*2.92 \times 10^{-12}$              | 1.14     | 1.32     | 1.30     | 0.70     | 1.3 $\times 10^{-3}$ | 1.5 $\times 10^{-3}$ | 1.6 $\times 10^{-3}$ |
| $*4.16 \times 10^{-13}$              | 1.16     | 0.52     | 0.51     | 0.26     | 2.00 $\times 10^{-4}$ | 2.00 $\times 10^{-4}$ | 2.00 $\times 10^{-4}$ |
| $*5.95 \times 10^{-14}$              | 1.17     | 0.20     | 0.20     | 0.10     | 2.11 $\times 10^{-5}$ | 2.81 $\times 10^{-5}$ | 3.13 $\times 10^{-5}$ |

* represents the extrapolated value.
Figure 7. (a-b): Variation of (a) $\alpha_0$ and (b) $\beta_0$ as a function of $a_s$, the effective accretion rate per site, for various amorphous carbon grains kept at 14K. The solid, dot-dashed and dashed curves are for $S = 10^4$, $9 \times 10^4$, $10^6$ respectively. The exponents $\alpha_0$ and $\beta_0$ are strong functions of the accretion rate. For low rates $\beta_0$ is higher than unity, while for higher rates it is close to 0.5 or even lower. The deviation is highlighted using dotted curves by extrapolating at very low accretion rates.

We found that on an average, $\alpha_0$, the index which determines the average recombination time, could be greater than 1 for very low rates. We also find that $\alpha_0$ depends very strongly on the nature of the grains as well as the temperature and grain site numbers. We show how the number of H and $H_2$ change with time and determine the time scales in partially filled with $H$ and $H_2$ and search for another $H$ need not take $S$ number of hops.
which quasi-equilibrium is reached. Thus the recombination time is a complex function of these parameters. We defined another index $\beta$ (Chakrabarti et al. 2006) which is a measure of the average formation rate of $H_2$. This index also is also a strong function of accretion rate per site. In fact, for very high rates the index may go down to 0.5 or even lower. A comparison of the recombination efficiency as obtained from our procedure with that obtained from the rate equation clearly shows a deviation easily attributable to the temperature dependence of $\alpha_0$ in a realistic case.

The results we obtained are likely to be astrophysically important because of several factors. The physical reason of the dependence of the average recombination time is so generic that one needs to revise all the abundances made on the grain surfaces. We find that even for $H$, we have more $H$ left over on grains, while less $H_2$ is produced and released. Thus, analytical considerations will always over produce molecules obtained on grain surfaces. Similarly, if, for example, methanols are produced through successive hydrogenation process on a grain surface, at each step such corrections would be required and the final abundance would be greatly affected. This will be done in near future.

Work of AD has been partly supported by a DST Project and the work of KA is partly supported by an ISRO project. SKC and AD also acknowledge Abdus Salam ICTP where a part of the work has been completed while they visited as Senior Associate and a conference participant respectively.

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