EVOLUTION OF MOLECULAR ABUNDANCE IN PROTOPLANETARY DISKS

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ABSTRACT

We investigate the evolution of molecular abundance in quiescent protoplanetary disks which are presumed to be around weak-line T Tauri stars. In the region of surface density less than 10^2 g cm^{-2} (distance from the star $\gtrsim$ 10 AU in the minimum-mass solar nebula), cosmic rays are barely attenuated even in the midplane of the disk and produce chemically active ions such as He$^+$ and H$_3^+$. Through reactions with these ions CO and N$_2$ are finally transformed into CO$_2$, NH$_3$, and HCN. In the region where the temperature is low enough for these products to freeze onto grains, considerable amount of carbon and nitrogen is locked up in the ice mantle and is depleted from the gas phase in a time scale $\lesssim 3 \times 10^6$ yr. Oxidized (CO$_2$) ice and reduced (NH$_3$ and hydrocarbon) ice naturally coexist in this part of the disk. The molecular abundance both in the gas phase and in ice mantle varies significantly with the distance from the central star.

Subject headings: circumstellar matter — ISM: molecules — stars: formation — stars: pre-main sequence — solar system: formation

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1. INTRODUCTION

Radio, infrared, and optical observations have recently revealed the existence of circumstellar disks around young stellar objects (Sargent & Beckwith 1994; O'dell & Wen Zheng 1994). Planet formation must be going on at least in some of them. Theoretical study on the evolution of molecular abundance in such " protoplanetary " disks is important from various points of view. First, it will directly show what material the bodies in the planetary systems are made from. Secondly, molecular abundance can be a useful probe in investigating the formation processes of planetary systems. For example, we may be able to reduce the processes, places, and epochs of the formation of primitive bodies, such as comets, by comparing their molecular composition with the theoretical results on the distribution and evolution of molecular abundance in the disk. Thirdly, study of the structure and evolution of the disk by observations of molecular lines should ask for a help of theoretical study on molecular evolution. For example, the amount of the gaseous component in the disk is estimated by observations of molecules other than the main component H_2 because H_2 can hardly emit photons except at very inner region of the disk. Knowledge on the abundance of the molecules relative to hydrogen is indispensable for such study.

Some theoretical works have been done on the molecular abundance in protoplanetary disks. Prinn and his colleagues (Prinn 1993, and references therein) investigated the molecular evolution in fully turbulent accretion disks and proposed the kinetic inhibition (KI) model. Their basic idea is that the molecular abundance in the matter flowing outwards is " quenched " when its temperature has decreased to a value below which the time scale for chemical reaction is larger than the dynamical time scale. Adopting the lifetime of the disk $\sim 10^{13}$ s, they concluded that the molecular abundance was quenched at $850 - 1500$K, and that CO and N_2 were the dominant component in the solar nebula. They considered neutral-neutral reactions which can be efficient in the region of $T \gtrsim$ several $\times 10^2$ K.

In this letter we investigate the evolution of molecular abundance in a relatively quiescent disk in the post-accretion phase, the so-called weak-line T Tauri (WTTS) phase and thereafter, in which transport and mixing of matter is not so efficient as in the earlier active phases mentioned above. We consider the disk regions where the column density is lower than the attenuation length of cosmic rays, 96 g cm^{-2} (Umebayashi & Nakano 1981). The minimum-mass solar nebula (Hayashi 1981) satisfies this condition in the region more than about 7AU away from the central star with the temperature $T \lesssim 10^2$ K. We take into account the ionization by cosmic rays and the subsequent ion-molecule reactions, which were not considered in the previous works.

2. DISK MODEL AND REACTION NETWORK

As the model of the protoplanetary disk, we adopt the so-called minimum-mass solar nebula (Hayashi 1981), which has the the distribution of the surface density $\Sigma(R) = 54 \ (R/10\mathrm{AU})^{-3/2}$ g cm^{-2} and temperature $T(R) = 89 \ (R/10\mathrm{AU})^{-1/2}$ K, where R is the distance from the central star. This model is consistent with the distribution of the temperature and the surface density estimated from the observations of dust continuum (Beckwith et al. 1990). Hydrostatic equilibrium determines the density distribution perpendicular to the midplane of the disk (e.g., Aikawa et al. 1996).

We consider the gas-phase reactions, adsorption onto grains, and thermal desorption from grains. The reaction network we use is essentially the same as the one described in Aikawa et al. (1996). We adopt the UMIST94 data base (Millar et al. 1991; Farquhar & Millar 1993) for the gas-phase reactions, and also take into account some three-body reactions referring to Brasseur & Solomon (1986). Table 1 shows all the atoms and molecules included in our network (except H, H_2, and He) and their adsorption energies. Because the attenuation of cosmic rays is inefficient, we adopt the ionization rate in the dark cloud, $\zeta \approx 10^{-17}$ s^{-1}. We neglect the ionization and dissociation by the interstellar and stellar ultraviolet radiation since it can be attenuated by grains in a thin surface layer of the disk (see § 4.3). We take the sticking probability $S = 0.3$ for the collision of a gas particle with a grain (Williams 1993). For simplicity, we assume that all grains are spherical with radius $a = 10^{-5}$ cm and that the dust-gas ratio is the same as that in the interstellar clouds. Although the dust-gas ratio near the midplane might be enhanced by sedimentation of dust, it does not affect much the results; we have obtained almost the same results with the dust-gas ratio higher by orders of magnitude.

Since our reaction network consists of one- and two-body reactions and contains only a small number of three-body reactions, we consider the region of the density by number of hydrogen nuclei, $n_H \lesssim 10^{12} \mathrm{cm}^{-3}$, which corresponds to $R \gtrsim 10$ AU for the minimum-mass solar nebula. With a typical rate coefficient $k \sim 10^{-30} \mathrm{cm}^6 \mathrm{s}^{-1}$ for the three-body reactions we have in this density range $kn(H_2) \lesssim 10^{-18} \mathrm{cm}^3 \mathrm{s}^{-1}$ even for the most abundant species H_2 as a third body. This is smaller than the characteristic rate coefficient $\sim 10^{-17} \mathrm{cm}^3 \mathrm{s}^{-1}$ for radiative association, which is the slowest among the two-body reactions. Thus the three-body reactions are not important in this density range.

For simplicity and clarity, we assume that the density and temperature do not change with time. Since we are mainly interested in the quiescent (WTTS) phase, we neglect the radial transport of matter and perform calculation up to $\sim 10^7$ yr. The initial molecular abundance is the same as in Aikawa et al. (1996), which assumed mostly the observed abundance in the dark cloud TMC-1. However, the molecular abundance may change during the active phase of the disk. To find out the influence of the initial condition, we also perform calculation with another set of the initial abundance; all carbon is in the form of CO, the remaining oxygen is locked up in water ice mantle, and nitrogen is in N_2.

3. NUMERICAL RESULTS

Since the result is found to be much more sensitive to the temperature than to the density, we show as the representative cases the results at $T = 30$ and 90K corresponding to the regions of $R = 87$ and 9.7AU with the density n_H at the midplane 2.9×10^9 and 1.2×10^{12} cm^{-3}, respectively.

Figures 1a and 1b show the results for the first set of the initial condition. The solid lines show the time variation of the abundance of carbon-bearing molecules relative to hydrogen. In the region of $T = 30$K (Figure 1a) the abundance of CO remains nearly constant at its initial value $n(CO)/n_H \approx 7 \times 10^{-5}$ up to 10^6yr. Thereafter CO decreases steeply, and CO_2 ice and HCN ice become dominant. The main process of forming CO_2 and HCN is as follows. Through the reaction with H_3^+, CO is transformed into HCO^+, some of which become HCO mainly through the grain surface recombination. Reactions of HCO with C

and N finally form CO_2 and HCN in the gas phase[2]. Once CO_2 and HCN are formed, they are adsorbed by grains in a time as short as ~ 10 yr (Aikawa et al. 1996). Since these molecules are hardly desorbed at $T = 30$K, they are locked up in the ice mantle, and as a result carbon is depleted from the gas phase. At somewhat higher temperatures (e.g., $T = 90$K as in Figure 1b), the thermal desorption is efficient enough to compensate the adsorption; although CO_2 becomes abundant, CO is also abundant on a time scale of 10^7 yr.

The dotted lines in Figures 1a and 1b show the time variation of the abundance of oxygen-bearing molecules. Oxygen is initially assumed to be mostly in the form of O atom and CO molecule. The abundance of O_2 in the gas phase and H_2O ice in the grain mantle increases extensively with time. The H_2O molecules form mainly in the following process. The reaction between O and H_3^+ produces OH^+, most of which are transformed into H_3O^+ through H atom-abstractions from H_2. Then H_3O^+ recombines to produce H_2O. In the later stages where O_2 becomes dominant, the main reaction of forming OH^+ is the H atom-abstraction by O^+, which is produced via destruction of O_2 by He^+. Since H_2O freezes onto grains at these temperatures while O_2 does not, most oxygen freezes out in the form of H_2O ice and the abundance of O_2 decreases in a time scale of several $\times 10^6$ yr.

The dashed lines in Figure 1 show the time variation of the abundance of nitrogen-bearing molecules. Initially most nitrogen is assumed to be in the form of N atoms. As time goes on, N_2, HCN ice, and NH_3 ice become dominant. The main formation process of NH_3 is as follows. The reaction of N_2 with He^+ forms N^+, which is transformed into NH_4^+ by repeating H atom-abstraction. Finally NH_4^+ is turned into NH_3 through dissociative recombination and grain-surface recombination. At temperatures below about 70K, NH_3 freezes onto grains and most nitrogen is depleted from the gas phase. At higher temperatures as in Figure 1b, NH_3 cannot freeze and N_2 is dominant even at later stages.

4. DISCUSSION

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[2]By recombination on grains HCO^+ is transformed into HCO radical or CO + H with unknown branching ratio. We assumed that the former branch is dominant. The time scale of the formation of CO_2 and HCN becomes longer if we assume otherwise.

4.1. Implications to Planetary Science

We review the main points of our results and discuss the implications to planetary science. First, we have found that CO and N_2 are transformed into CO_2 and NH_3. The main cause for this is in cosmic rays, which have not been taken into account in the previous works. Cosmic rays produce chemically active ions such as H_3^+ and He^+ which can destroy CO and N_2. This results in the depletion of CO in the gas phase and hence the faintness of its emission lines in the cold regions ($T \lesssim 70K$) of the disks at the age $\gtrsim$ several $\times 10^6$ yr. This also means that CO_2 ice and NH_3 ice will be detected in these regions. Secondly, our results show that oxidized (CO_2) ice and reduced (NH_3 and hydrocarbon) ice coexist in the protoplanetary disks. This coexistence has also been suggested by the KI model (Prinn 1993). This result is to be noted because their coexistence is one of the most important characteristics of comets (Yamamoto 1991). CO and N_2 would also coexist in ice mantle if they are physically trapped in water ice (Bar-Nun et al. 1985), although this effect is not included in our calculation. Finally, we have found that the molecular abundance in the gas and in ice mantle varies considerably with the distance from the central star. Comparison of this result with the molecular abundance of comets will enable us to deduce where comets formed, although quantitative discussion is out of the scope of this paper.

4.2. Dependence on the Initial Condition

The initial condition we have adopted so far is that considerable amount of carbon, oxygen, and nitrogen are atomic (see § 2 in Aikawa et al. 1996). In order to check the dependence on the initial condition, we have made calculation for another set of the initial abundance mentioned in § 2. Figure 2 shows the result for this case in the region of $T = 30K$. We can see that CO_2 ice becomes dominant in this case as well. Although there are no oxygen atoms initially, they are extracted from CO by the reaction with He^+. The remaining carbon is transformed into hydrocarbon. At higher temperatures ($T \gtrsim 70K$), CO_2 becomes abundant at later stages, although its abundance $n_{CO2}/n_H = 10^{-5}-10^{-6}$ is lower than that for the first case on the initial condition. Similarly, N_2 is destroyed by He^+ and is transformed into HCN ice and NH_3 ice.

4.3. Discussion on the Assumptions

Although we have neglected the radial transport of matter, our results are qualitatively applicable to the disks with radial transport such as the accretion disk and weakly-turbulent disk, because the chemical paths described in § 3 are always active and dominant in the reaction network as long as the matter is in the region of low temperature and low density ($R \gtrsim 10AU$ in the minimum-mass solar nebula). The molecular evolution in the accretion disks will be described in the forthcoming paper in more detail. On the other hand, our results are not applicable to the disks with efficient mixing where the strong turbulence or convection mixes matter between the inner hot ($T \gtrsim$ several$\times100K$) region and the outer cold region ($R \gtrsim 10AU$) in a time scale $\lesssim 10^6$yr, as investigated by Prinn (1993).

We have neglected the UV photolysis. Smaller grains sink more slowly toward the midplane of the disk (Nakagawa, Nakazawa, & Hayashi 1981). In addition, even a weak turbulence which cannot efficiently transport matter radially would be sufficient to prevent the sedimentation of small grains. Therefore, it would be possible that small grains shield the main part of the disk from the UV radiation. Mid- to far-infrared excesses observed in the spectra of WTTS strongly suggest the existence of small grains at $R \gtrsim 10AU$ even in the relatively quiescent disks (Strom et al. 1989).

If almost all grains sank to the midplane in less than about 10^6yr despite the above discussion and the mid- to far-infrared excesses in WTTS, our results were not applicable. The molecular abundance must then be affected by the photolysis because the line shielding is not efficient enough for some kinds of species.

TABLE 1

THE ADSORPTION ENERGIES OF ATOMS AND MOLECULES IN KELVIN [a]

Species	Adsorption Energy (K)	Species	Adsorption Energy (K)
C	800	C_2H	1460
N	800	C_3	2010
O	800	CCN	2010
Na	11800	CO_2	2690[b]
Mg	5300	NH_2	860
Si	2700	NO_2	2520
S	1100	OCN	2010
Fe	4200	OCS	3000
HS	1500	O_2H	1510
CH	650	O_3	2520
C_2	1210	SO_2	3460[b]
CN	1510	H_2CO	1760
CO	960[b]	H_2CS	2250
CS	2000	CH_3	1160
NH	600	C_2H_2	2400[c]
N_2	710[c]	C_3H	2270
NO	1210	C_3N	2720
NS	2000	NH_3	3080[b]
OH	1260	H_2C_3	2110
O_2	1210	HC_3N	2970
SiH	2940	CH_4	1080[c]
SiC	3500	CH_3O	1710
SiO	3500	C_3H_2	2110
SiS	3800	CH_3CN	2270
SO	2000	CH_3OH	4240[b]
H_2O	4820[b]	CH_3O_2	2370
H_2S	1800	C_3H_3	2220
HCN	4170[c]	H_3C_3N	3270
HCO	1510	C_3H_4	2470
CH_2	960	CH_3OOH	2620

[a]Allen & Robinson 1977 and Hasegawa & Herbst 1993 except for [b] and [c]

[b]Sandford & Allamandola 1993

[c]Yamamoto, Nakagawa, & Fukui 1983

Fig. 1.— Evolution of the molecular abundance in two representative regions of the disk, (a) $R = 87$AU ($n_H = 2.9 \times 10^9$ cm^{-3}, $T = 30$K) and (b) $R = 9.7$AU ($n_H = 1.2 \times 10^{12}$ cm^{-3}, $T = 90$K). The initial molecular abundance was determined referring to the abundance in dark clouds. The solid, dotted, and dashed lines represent the abundance of carbon-, oxygen-, and nitrogen-bearing molecules, respectively, relative to hydrogen.

Fig. 2.— Evolution of the molecular abundance at $R = 87$AU ($n_H = 2.9 \times 10^9$ cm^{-3}, $T = 30$K) with the initial condition that carbon is in the form of CO, nitrogen is in the form of N$_2$, and the remaining oxygen is locked up in water ice mantle. The other details are the same as in Fig. 1

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log n_i/n_H

log time [yr]

-10   -8   -6   -4

0   2   4   6   8   10

CO

O$_2$

N$_2$

HCNice

H$_2$O
ice

CH$_4$

NH$_3$

N$_2$

NH$_3$

CH$_4$

O$_3$

CO$_2$

HCNice

H$_2$Oice