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Chemical Models of Circumstellar Disks

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Abstract. We investigate the evolution of molecular abundances in circumstellar disks around young stars via numerical simulations. The results are compared with the composition of comets and radio observations of protoplanetary disks. First, we consider the molecular evolution in the midplane of the disk. Because of ionization by cosmic-rays or decay of radioactive nuclei, the molecular evolution in the region $R \gtrsim 10$ AU bears some similarity to that in molecular clouds. Considerable amounts of CO and N_2, which come from the cloud core, are transformed, however, into CO_2, CH_4, NH_3, and HCN. In regions where the temperature is low enough for these products to freeze onto grains, they accumulate in ice mantles. In the inner warmer regions of the disk, these molecules are desorbed from the mantles and transformed by gas-phase reactions into less volatile molecules, such as larger hydrocarbons, which then freeze out. Molecular abundances both in the gas phase and in ice mantles crucially depend on the temperature and thus vary significantly with the distance from the central star. Molecular abundances in ice mantles show reasonable agreement with the composition of comets. Our model suggests that comets formed in different regions of the disk having different molecular compositions.

Secondly, we report two-dimensional (R, Z) distributions of molecules in circumstellar disks. In the Z-direction, which is perpendicular to the midplane, there is a steep gradient of density and radiation field. Since the density is lower in the regions removed from the midplane, there are significant amounts of gas-phase species in these regions, while most species are adsorbed onto grains in the midplane. Chemistry in the surface regions is also affected by the X-rays and UV radiation from the central star, and UV radiation from the interstellar field. The molecular abundances in these regions differ significantly from those in the midplane. Radicals such as CN are especially abundant near the disk surface. We obtain radial distributions of molecular column densities and averaged molecular abundances, which show reasonable agreement with the observational data at millimeter wavelengths.

1. Introduction

Planetary systems are formed in protoplanetary disks around young stars, while star-disk systems are formed by the gravitational collapse of precursor molecular clouds. The study of the molecular evolution in protoplanetary disks is important because it can reveal the chemical connection between planetary matter and interstellar matter, and eventually help determine from what material the bodies in planetary systems are made.

Disk chemistry has been investigated since the 1970's. In their early work, Lewis and colleagues investigated the composition in the disk assuming thermo-chemical equilibrium (Lewis, Barshay, & Noyes 1979). For a gas with solar elemental abundances and for pressures appropriate to the solar nebula, they obtained that the disk should be CO- and N_2-rich at $R \lesssim 1$ AU and CH_4- and NH_3- rich at $R \gtrsim 1$ AU. It was pointed out, however, that in the region of low temperatures the reaction rates are so low that thermo-chemical equilibrium cannot be achieved within the time scale of the disk. Instead of the chemical equilibrium model, Prinn (1993, and references therein) proposed the "kinetic inhibition model" (hereafter KI model), assuming that matter at different radii is well-mixed by turbulence. Their basic idea is that the molecular abundances in the matter flowing outward are "quenched" when the temperature has decreased to a value below which the time scale for chemical reaction is larger than the dynamical time scale. Adopting a dynamical time scale for the disk of $\sim 10^{13}$ s, they concluded that molecular abundances are quenched at 850–1500 K ($R < 1$ AU) and that CO and N_2 were the dominant components in the solar nebula.

In recent years, there have been some major improvements in the theoretical study of disk chemistry (Aikawa et al. 1997, 1998, 1999; Finocchi & Gail 1997; Willacy et al. 1998). Firstly, it is found that ionization of the gas by cosmic rays and subsequent ion-molecule reactions have significant effects on molecular evolution in the disk, which are not included in the KI model. Since the attenuation length of the cosmic-ray ionization is about 96 g cm^{-2}, the disk is partially ionized by cosmic rays at $R \gtrsim 7$ AU in the minimum-mass solar nebula (Umebayashi & Nakano 1981). The reaction rate coefficients of ion-molecule reactions are larger than those of neutral-neutral reactions especially at low temperatures. Thus, ion-molecule reactions can be efficient even in the outer regions of the disk, which were regarded as chemically inactive in the KI model. Secondly, in recent papers the standard accretion-disk model (Lynden-Bell & Pringle 1974) has been adopted, in which most of the matter loses its angular momentum due to viscosity and migrates toward the central star. Indeed, observations at ultraviolet, optical, and infrared wavelengths suggest that there are accretion flows in protoplanetary disks (Basri & Bertout 1993, and references therein). Thirdly, recent models include interaction between the gas phase and the solid phase, such as formation of ice mantles. In §2 of this paper we review some important features of the chemistry in the midplane, based on Aikawa et al. (1999) and Aikawa & Herbst (1999*a*).

Recent radio observations are making great progress in the study of molecular abundances in protoplanetary disks. Emission lines of the CO molecule have been detected for T Tauri stars (Handa et al. 1995), while aperture-synthesis images have directly revealed the distribution of CO around some T Tauri stars in the Taurus molecular cloud with a spatial resolution of a few hundred AU

(Guilloteau & Dutrey 1998). In addition to the CO studies, Dutrey et al. (1997) have surveyed other molecular lines in the disks around DM Tau and GG Tau. These stars, with ages 1×10^6 yr and 3×10^5 yr respectively (Beckwith et al. 1990; Handa et al. 1995), have large gaseous disks with radii ~ 800 AU. Dutrey et al. (1997) reported average fractional abundances of CO, CN, CS, HCN, HNC, H_2CO, C_2H, and HCO^+, and found that the abundances of these molecules are lower than those in molecular clouds by a factor of 10–100. These are the first observational data suggesting that molecular evolution occurs in protoplanetary disks. Such an interpretation of the abundances is controversial, however, and raises a variety of questions. What, for example, causes the different molecular abundances between disks and clouds? Are the distributions of molecular abundances really homogeneous throughout disks? Can we use detected molecular emission lines as indicators of physical conditions in disks?

The answers to these questions require chemical models. Because there are steep gradients of density and radiation field in the direction perpendicular to the midplane, molecular abundances must depend on distance from the midplane. Since the observational data yield only the column densities of molecules, it is important to calculate not only molecular abundances in the midplane, but also the two-dimensional distribution of molecules in the disk, which is described in §3 of this paper (Aikawa & Herbst 1999*b*).

2. Molecular Evolution in the Midplane

2.1. Model

Because the density and temperature are not high enough for chemical equilibrium to be achieved within the evolutionary time scale of a protoplanetary disk, we solve time-dependent chemical equations in order to determine molecular abundances. We have adopted the so-called "new standard model" network of chemical reactions for the gas-phase chemistry with updated rate coefficients. In addition to reactions in the gas phase, we take into account the formation of H_2 molecules and the recombination of ions and electrons on grain surfaces. The formation of ice mantles due to adsorption of molecules and the thermal desorption of molecules from ice mantles are also explicitly followed. For simplicity and clarity, we do not consider other chemical reactions on grain surfaces because the reaction rates are still uncertain and because the whole concept of grain reaction rates is still controversial (Herbst, this volume).

2.2. Temporal evolution

In this subsection, we describe the molecular evolution of matter as it accretes toward the central star. We consider a disk with an initial radius $R \sim 1000$ AU. The matter at each radius slowly migrates inward with velocity $v_{\rm R} \sim 10^{-4}$ AU yr^{-1}. The density $n_{\rm H}$ and the temperature T of the matter change with time as the matter migrates. We compute the molecular evolution along the accretion flow. The calculation is performed for a period of 3×10^6 yr, which is a typical duration time for the accretion phase (Strom et al. 1989).

As an example we consider the molecular evolution in matter which migrates from R=395 AU to R=10 AU in 3×10^6 yr. The carbon evolution for $t \geq 2.4 \times 10^6$

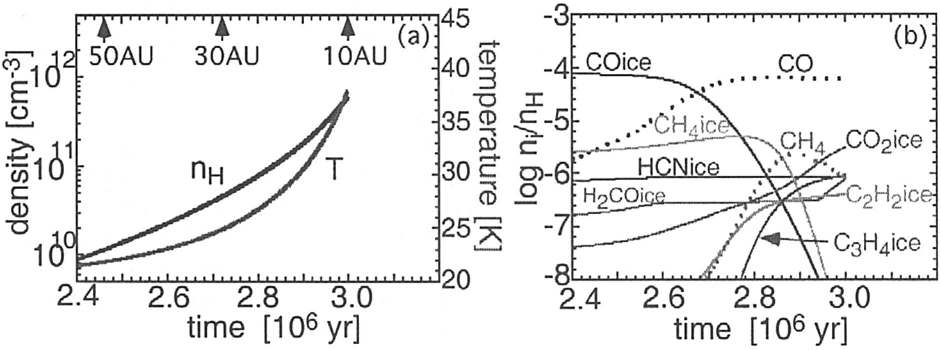

Figure 1. Evolution of molecular abundances in matter that migrates from $R = 54$ AU to $R = 10$ AU in the period between $t = 2.4 \times 10^6$ yr and 3×10^6 yr. (*a*) The temperature T and the density of matter $n_{\rm H}$ as functions of time. (*b*) Evolution of C-bearing molecules. The solid lines show ice components, and the dotted lines show gaseous molecules.

yr is shown in Figure 1. Figure 1*a* shows the density and the temperature of the matter as functions of time. In this period the matter migrates from 54 AU to 10 AU, and the temperature rises to ≈ 38 K. Because of the high density and low temperature, most of the molecules are adsorbed onto grains. Although we put all carbon in the form of CO initially, various kinds of molecules are already formed by the time the matter reaches these regions, and the molecular composition in the ice mantle is consistent with that in comets. We performed calculations with several different sets of initial molecular abundances, and found that the final molecular abundances at $t \sim 3 \times 10^6$ yr do not sensitively depend on the initial conditions. As the matter moves to warmer regions, some ices sublimate. For example, CH_4 is desorbed around $t \sim 2.9 \times 10^6$ yr ($R \sim 20$ AU) when the temperature rises to its sublimation temperature ~ 28 K. Then CH_4 is transformed into larger hydrocarbons such as C_2H_2 and C_3H_4 by the gas phase reactions; these are subsequently adsorbed onto grains.

2.3. Radial distribution of molecules in the disk

In order to find out the spatial distribution of molecular abundances at the end of the accretion phase, we perform similar calculations as described above for matter that starts migration at various initial positions, moving in 3.0×10^6 yr from $R = 426$ AU to 20 AU, 456 AU to 30 AU, 486 AU to 40 AU, 514 AU to 50 AU, 541 AU to 60 AU, 568 AU to 70 AU, and 619 AU to 90 AU.

Figure 2 shows the spatial distribution of carbon-bearing molecules at $t = 3.0 \times 10^6$ yr. The molecular abundances do not change much at $R \gtrsim 50$ AU, where the temperature is nearly constant at ~ 20 K. At $R \lesssim 50$ AU, where the temperature rises considerably as R decreases, the molecular abundances vary with radius. For example, CH_4 ice is much less abundant at $R \leq 20$ AU than in the

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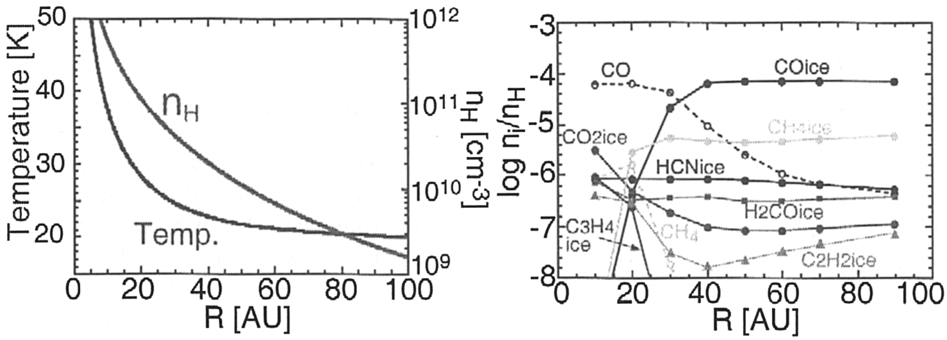

Figure 2. Distribution of density and temperature (*left*), and abundances of carbon-bearing molecules at $t = 3 \times 10^6$ yr (*right*) in the accretion disk.

outer regions. Instead, larger hydrocarbons such as C_3H_4 ice, CO_2 and H_2CO are more abundant at $R \leq 20$ AU than in the outer regions.

This result indicates that comets formed in different regions of the disk have different chemical compositions; for example, comets formed in inner regions will have higher abundances of large hydrocarbons. This is consistent with the observational data of A'Hearn et al. (1995), who found that comets in different orbital groups tend to have different chemical compositions, and that carbon-chain molecules are less abundant in comets formed in the outer region of the disk. It should be noted that if there are no active reactions in the disk, comets formed in the inner region of the disk will have generally lower molecular abundances than comets formed in the outer region.

2.4. Deuterium fractionation in protoplanetary disks

In addition to the molecular abundances, we have investigated the evolution of abundance ratios between singly deuterated isotopomers and normal species, and found that the molecules in the disk have higher D/H ratios than the protosolar value (2×10^{-5}) (Aikawa & Herbst 1999*a*). In previous studies on comets, a high D/H ratio had been interpreted in terms of unprocessed interstellar matter in comets. Our work, however, shows that deuterium fractionation and other chemical processes are occurring while matter is collapsing to form protoplanetary disks and during the disk phase itself. Both the absolute chemical abundances of gas-phase and condensed-phase species and the D/H ratios among these species thus reflect a continuous evolution as physical conditions change. Our results on both molecular abundances and D/H ratios of molecules are in reasonable agreement with recent observations of comets if we choose a radius of ~ 30 AU for comparison with cometary data, which suggests that cometary matter is not necessarily unprocessed interstellar matter.

3. Two-dimensional Distributions and Column Densities of Gaseous Molecules

3.1. Model

In this section we report two-dimensional distributions and column densities of various molecules in protoplanetary disks, and compare these with observational data at radio wavelengths. Here we adopt one of the simplest models for the disk structure – the static minimum-mass solar nebula of Hayashi (1981). Although it would be better if we could solve for the two-dimensional molecular evolution together with physical evolution in the disk, it is useful, as a first step, to comprehend the essential characteristics of disk chemistry using a simple static disk model. The effect of diffusion or hydrodynamic evolution in the disk can be estimated by comparing the dynamical timescale with the chemical timescale obtained in our model. Although the original minimum-mass model extends only through a radius $R_{\rm out} = 36$ AU, we extend the model to an outer radius of about $R_{\rm out} \sim 10^3$ AU, and investigate the region of radius $100 \leq R \leq 700$ AU, because in a survey of gaseous disks, several were found to have outer radii at the upper limit.

The chemical model is basically the same as in §2, except for the following three points. First, we include the effect of non-thermal desorption by adopting a low sticking probability. We estimate the effective sticking probability from the intensity of the CO emission lines observed towards GG Tau. According to Aikawa et al. (1996), the column density of gaseous CO at $R \gtrsim 200$ AU depends mainly on the sticking probability and age of the disk. Following Aikawa et al. (1996), we calculated the CO J=2→1 emission line for three isotopomers assuming various values of the sticking probability and found that the case with S=0.03 shows the best agreement with the observed spectra. Secondly, we take into account the effect of X-rays from the central star. At R=700 AU, for example, X-rays cause an ionization rate as high as $\zeta \sim 10^{-15}$ s^{-1} at the disk surface, while $\zeta \sim 10^{-17}$ s^{-1} in the midplane where it is caused mainly by cosmic rays (Glassgold et al. 1997). Our model also includes the photo-chemistry caused by the X-ray induced UV radiation. Thirdly, we include the photo-chemistry caused by the UV radiation from the central star and the interstellar field. Although the UV radiation is mainly attenuated by dust, self- and mutual-shielding are important for H_2 and CO. For these molecules, we solve for the molecular abundances and the UV attenuation self-consistently, adopting a one-dimensional slab model at each radius R (van Dishoeck & Black 1988; Lee et al. 1996).

3.2. Vertical distribution

Figure 3 shows the vertical distribution of various kinds of molecules at R=700 AU and at $t = 3 \times 10^5$ yr, which is a typical age of a T Tauri star. The solid lines are for the case with X-ray luminosity 1×10^{31} erg s^{-1}, while the dotted lines are for the case without X-rays. At the midplane, most of the molecules are adsorbed onto grains by the time depicted owing to the high density. At or near the surface, molecules tend to be dissociated by UV radiation. Hence the molecular abundances have their peak values at some intermediate region. The height at which a given molecular abundance reaches its peak value varies with

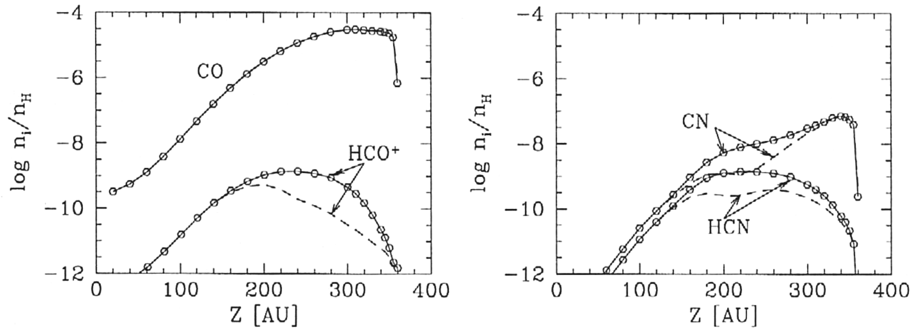

Figure 3. Vertical distribution of molecular abundances at R=700 AU and $t = 3 \times 10^5$ yr. The solid lines show the case with X-rays, and the dashed lines show the other case.

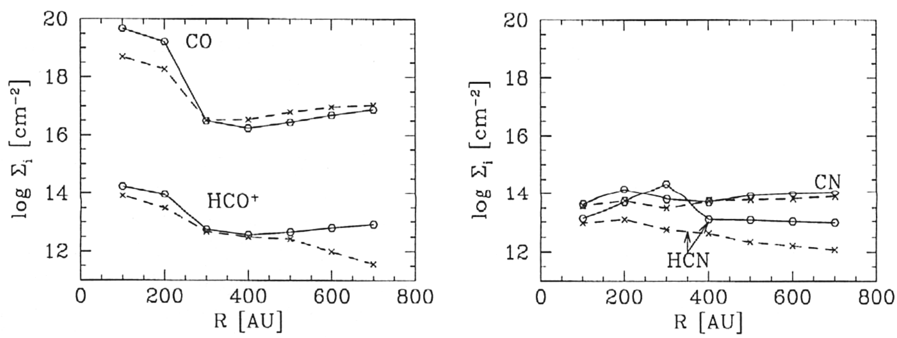

Figure 4. Radial distribution of molecular column density at $t = 3 \times 10^5$ yr. A minimum-mass disk model is assumed for the solid lines. For dashed lines, the total column density of the disk is lower than in the minimum-mass model by an order of magnitude.

species. Radicals, such as CN, have their peak abundances at larger heights Z compared with more stable species such as HCN. The abundances of most molecules are higher when X-rays are included, because more carbon is made available by the destruction of CO.

3.3. Column densities

By integrating the vertical distributions of molecular abundances, we obtain molecular column densities as functions of disk radius, which can be directly compared with the interferometric data. Among several hundreds of species included in our model, those detected in Dutrey et al. (1997) have the largest column densities. Figure 4 shows selected radial distributions of molecular column densities for assorted molecules in a disk irradiated by X-rays. The thick lines show column densities for the minimum-mass disk, and the thin lines for a less massive disk model with a total column density 10% of the "minimum-mass" model. The disk age is assumed to be $t = 3 \times 10^5$ yr. At radii greater than 300 AU, the column density of gas-phase CO is almost independent of radius, with

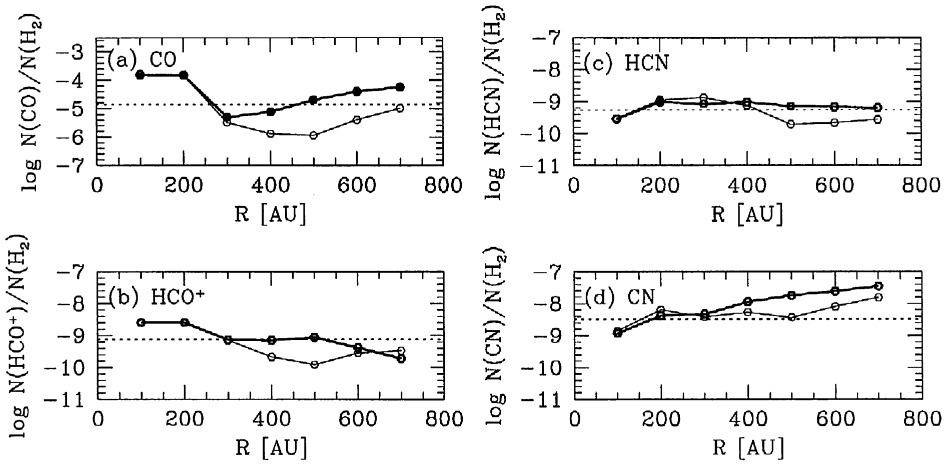

Figure 5. Radial distribution of averaged molecular abundances at $t = 3 \times 10^5$ yr (thick lines) and $t = 9.5 \times 10^5$ yr (thin lines).

only a weak increase with increasing radius. At these radii, gaseous CO exists only in regions removed from the midplane, and the amount of gas contained in these regions weakly increases with increasing radius, because the disk is more compressed by stellar gravity at smaller radii. At a radius near 200 AU, however, the temperature warms to the sublimation temperature of CO ($T \sim 20$ K). Hence the column density of gas-phase CO becomes much higher at $R \leq 200$ AU (Aikawa et al. 1996). The radial distributions of other carbon-bearing molecules also weakly increase with increasing radius beyond 300 AU for the same reason as for CO. Since the sublimation temperatures of HCN and CN are much higher than that of CO, the column densities of these species do not show a steep gradient at $R \leq 200$ AU. Interferometric data of the disk around LkCa15 shows that emission from CO and HCO^+ peaks at the center of the disk, while HCN and CN show central holes (Qi et al., this symposium), which is consistent with our model. However, CN emission from the DM Tau disk has a peak intensity at the center (Dutrey et al., this volume).

The dependence of the molecular column densities on the total (H_2) column density can also be seen in Figure 4. The column densities of HCN and HCO^+ are quite noticeably affected by the change in mass at regions of radius $R \gtrsim 500$ AU. These species can be used as probes to estimate the total column density of the disk.

3.4. Averaged abundances and comparison with observational data

In Figure 5 we show the averaged fractional abundances using our less massive disk model obtained by dividing the molecular column densities shown in Figure 4 by the column density of H_2 at each radius. The thick lines are for $t = 3 \times 10^5$ yr, and the thin lines for 9.5×10^5 yr. The dotted lines show the averaged abundances estimated from the observation of DM Tau by Dutrey et al. (1997). Considering that the age of DM Tau is 1×10^6 yr, we can see reasonable agreement between the model results and the observational data.

3.5. D/H ratios in gaseous molecules

In chemical models of molecular clouds, it is well known that D/H ratios in gaseous molecules are enhanced as the depletion of heavy elements proceeds. We found a similar effect in disks; in the "minimum-mass" disk the D/H ratio is typically higher than in our less massive disk model, where molecular depletion proceeds more slowly. For example, the column density ratio of DCN/HCN in the gas phase is 0.1 at $t = 3 \times 10^5$ yr and R=700 AU in the "minimum-mass" disk, while it is 0.01 in our less massive disk.

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Discussion

T. Velusamy: Do you have the vertical and radial distribution for methanol (CH_3OH) from your 2D model? We have detected methanol in the disk of L1157 and our data are consistent with gas phase CH_3OH from the warm surface layer of a flared disk at > 100 AU, similar to what your model shows for CN.

Y. Aikawa: Methanol is included in our models. Since CH_3OH is considered to be formed efficiently on grain surfaces, I think we have to include the grain surface chemistry to have a reliable conclusion.

J. M. Greenberg: When you state the significant effect of grain size on UV penetration what sizes did you use? Did you use the average interstellar extinction law? There is a reason to expect that where ices adsorb so will the small particles which give the UV extinction.

Y. Aikawa: We adopt the average interstellar extinction law assuming that the grain size in the disk is the same as that of interstellar grains. Our model shows that the column densities of some species depend sensitively on the UV radiation field, and thus on the grain size. It is interesting if we can get information on grain sizes from molecular observations.

J. Rawlings: You emphasized the importance of the ionization rate in the early part of your talk. What value(s) of ζ have you used in your models? The magnetic fields in the vicinity of a protostar are highly twisted and the cosmic ray flux may be very different from that in intersteller clouds.

Y. Aikawa: As a standard case we adopt $\zeta = 1.3 \times 10^{-17}$ s^{-1}, and we also performed the calculation with $\zeta = 1.3 \times 10^{-18}$ s^{-1}. The ionization rate by cosmic rays depends on initial energy spectrum of cosmic rays, and strength and structure of magnetic fields in the vicinity of a protostar. According to Umebayashi & Nakano (1981), who investigated the propagation of cosmic rays, $\zeta = 10^{-18}$–10^{-17} s^{-1} is reasonable at $R \gtrsim 10$ AU. It should be noted that decay of radio active elements also causes ionization with rates $\zeta \sim 10^{-18}$ s^{-1}.

M. Kress: CO_2 is a very oxidized species and NH_3 is a very reduced species, yet the model results show that they coexist at ~ 10 AU. Is this because they form in the gas at separate times and then freeze out as ices?

Y. Aikawa: Since the molecular evolution is caused by ion-molecule reactions, both oxidized and reduced species are formed at the same time in the gas phase.

R. Y. Shah: Could you comment on D/H ratios in the ice and gas, particularly on the influences of interstellar sources of deuteration?

Y. Aikawa: We calculated the molecular evolution from the molecular cloud phase (including cloud collapse) through the accretion disk phase. Our model shows that most of the interstellar ices, which have a high D/H ratio, survive and are incorporated into comets. But we also found that a significant amount of molecules is formed in the disk and incorporated into comets. Because of deuterium exchange through ion-molecule reactions, the molecules formed in the disk have a higher D/H ratio than the cosmic elemental abundance.