

Disk Chemistry and Cometary Composition

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Abstract. We describe a theoretical study of protoplanetary disk chemistry. By considering physical conditions similar to that of the protosolar nebula, we attempt to assess the contribution made by material from the cooler nebular regions to cometary composition. Calculations are presented which determine the spatial and temporal chemistry of the gas and dust within the 5-40 AU comet-forming region of the nebula. We show that there is little radial variation in the solid-state distribution of some molecules which could potentially be parents of the carbon-chain species observed in comets. We conclude that the apparent variation in abundance of C_2 and C_3 between long- and short-period comets is the result of chemical processing during their lifetimes and not differences in composition at the time of formation.

1. Introduction

Short-period comets formed in the nebula roughly where they reside today ($\sim 30-1000$ AU) and comprise the Kuiper Belt. On the other hand, long-period comets formed closer to the protosun ($\sim 5-40$ AU), but dynamical effects led them to be ejected from there into the Oort Cloud (radii $\sim 10^3-10^5$ AU). There is an apparent variation in the coma abundances of C_2 and C_3 between each comet population, with the short-period comets being more depleted in these molecules (A'Hearn et al. 1995). As C_2 and C_3 are coma photoproducts (Helbert et al. 2000), any differentiation between the comet families must be due to chemical differences in the nuclear ices of the two populations. Possible nuclear parents are C_2H_2 (acetylene) and CH_3CCH (methyl acetylene). The origin of this differentiation could lie either in the protostellar disk chemistry which occurred during their formation (nature), or in the chemical-processing histories (photolysis, radiolysis, heating) of each family (nurture). Using a model of the chemistry in the protostellar disk, we might hope to discriminate between these two possibilities.

2. The Model

The model we have developed is constructed in two stages. First, the physical structure (density, temperature) of the disk is computed. This calculation includes the combined heating effects of viscous dissipation and irradiation by the central object, as well as a 2D treatment of the radiative transfer (Nomura 2002). The structure ($0 < r < 100$ AU) of a steady α -disk is produced for a central solar-mass object with mass accretion rate 10^{-7} solar masses per year.

Figure 1 shows the associated temperature and density distributions. These results are then used as input for a comprehensive chemical model, described in Markwick et al. (2002). Briefly, the reaction network comprises around 250 species and 2500 reactions of various types including photoprocesses and gas-grain interaction. The latter allows molecules to freeze out onto dust particles and be thermally evaporated as conditions allow. Note that this model does not include any reactions between species on the grain surfaces, except the formation of molecular hydrogen and some ion-grain recombination reactions. This is because there are conceptual problems in attempting to treat surface reactions in such a deterministic model. The model integrates the chemical rate equations at each point for which physical structure is available, and so 2D gas-phase molecular distributions can be produced (see Millar et al. 2003). In this work, we consider only the mid-plane abundances of solid-phase species, which we assume will be incorporated directly into cometary ices as they form.

3. Results and Discussion

Figure 2 shows the variation of some solid-phase carbonaceous species in the mid-plane of the disk. The region between 10 and 40 AU is a significant fraction of the comet-forming region and, encouragingly, we see that, due to the temperature structure of the mid-plane, molecules in the ice are abundant there. If we are to adopt the ‘nature’ perspective described above, then we might expect to see a difference in the carbon-chain abundances between 10 and 40 AU. However, Figure 2 shows that there is no variation in the abundances of these species in the region of interest. The same result is true for all species with 2 and 3 carbon atoms in the model: there is no variation between 10 and 40 AU. The reason for this is quite straightforward. The gas-grain interaction in the model is described by ‘freeze-out’. This is a balance between sticking collisions between molecules and grains, and the return of these molecules by evaporation from grain surfaces. Thermal desorption depends on the nebular dust (and gas) temperature, T , and on the binding energy of the molecule to the dust grain, E_b , a material property. The temperature structure in the mid plane is such that the thermal desorption rate ($\propto \exp[-E_b/kT]$) effectively switches the solid-state abundances between negligible and significant: binding energies are simply not low enough to allow a variation across the comet-forming region, where the temperature varies by only about 10 K. Hence, using the model described here, we conclude that any differences in carbon-chain composition between long- and short-period comets arise due to their different processing histories (see Stern 2003).

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References

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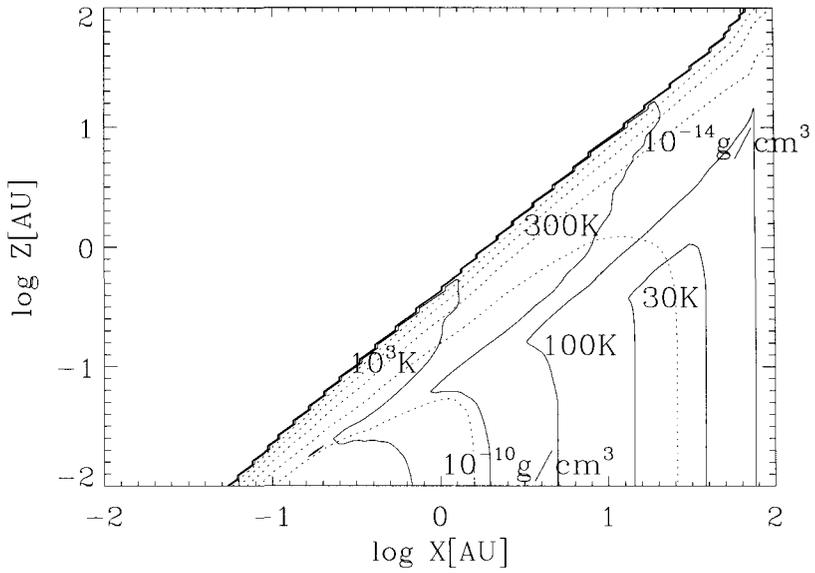


Figure 1. The two-dimensional structure of the disk for $r < 100$ A.U.

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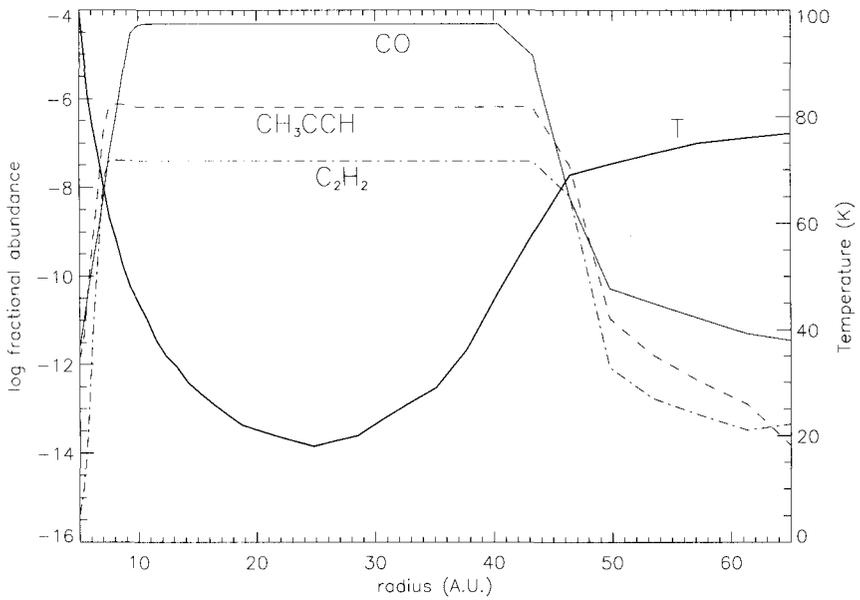


Figure 2. The mid-plane variation of the relative solid-phase abundances of C_2H_2 and CH_3CCH . The abundances are scaled to be the fractional abundance relative to gas-phase H_2 . Also shown is the temperature structure of the mid plane.