

# Chemistry of Ionization

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**Abstract.** We discuss the chemical evolution of the fractional ionization in a protoplanetary disk in detail. To calculate the ionization structure, we use a 2D flared disk model, a gas-grain chemical network with surface reactions, and take into account stellar X-rays, stellar and interstellar UV radiation, cosmic rays, and short-living radionuclides. Applying our reduction techniques, we find small subsets of chemical reactions reproducing the evolution of the ionization degree at representative disk locations with an accuracy of 50%–100%. It is found that the disk can be divided into three chemically distinct layers. In the dense and cold midplane the ionization degree is low and sustained by cosmic rays and radionuclides only. It can be accurately represented by very small chemical networks consisting of tens of species and reactions only. In the intermediate layer the ionization chemistry is driven mainly by the attenuated stellar X-rays and thus very complicated. For the first time, we argue that surface hydrogenation of long carbon chains can be of crucial importance. Consequently, in the intermediate layer reduced networks consist of more than 100 species and reactions. Finally, in the unshielded disk surface layer the ionization chemistry is regulated by a small set of photo-processes. The reduced networks contain a few tens of species and reactions. The relevance of these results to the MHD disk modeling is briefly discussed.

**Keywords.** accretion disks, astrochemistry, MHD, molecular processes, stars: formation, planetary systems: protoplanetary disks

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## 1. Introduction

During the last decade an efficient mechanism for the global angular momentum transport in protoplanetary disks has been proposed by Balbus & Hawley (1991), where an anomalous effective viscosity is produced by MHD turbulence driven by the magnetorotational instability (MRI). The value of the disk ionization degree is a key factor in determining the efficiency of MRI and accretion in general. A typical young protoplanetary disk covers a wide range of physical conditions, which results in the well-known layered structure: (1) An “active” surface subject to high-energy stellar radiation and thus being unstable to MRI, and (2) a “quiescent” midplane (“dead” zone) where the ionization degree is very low and MRI is not operative (e.g., Gammie (1996)). Despite the complexity of the involved physical and chemical processes, in MHD studies of accretion disks a simplified chemical equilibrium model is mainly used. Obviously, such a simple approach may not be applicable everywhere in the disk. In this contribution we present the ionization structure of a protoplanetary disk, summarize chemical processes that dominate the ionization degree in various disk regions, and discuss the applicability of the chemical equilibrium approach (see also Semenov, Wiebe, & Henning (2004)).

## 2. Model

We adopt the steady-state flared disk model of D’Alessio et al. (1999) with a central T Tauri star producing high X-ray and UV fluxes. Cosmic rays and interstellar UV radiation field are considered to be the other ionizing factors. The disk ranges from 1 to about 400 AU in radial direction and  $\sim 0.01$ –700 AU in vertical direction. With this model in hand, we calculate the evolution of the disk fractional ionization over 1 Myr, using a gas-grain chemical model based on the UMIST 95 database (Millar et al. (1997)) and the set of surface reactions of Hasegawa et al. (1992). The photodesorption of mantle species is taken into account along with thermal and cosmic ray-induced desorption. As initial abundances, we utilize those calculated for a dark cloud model. Using the reduction techniques described in Wiebe et al. (2003), we analyze which chemical processes govern the evolution of the ionization degree in several representative disk locations.

## 3. Results

We find that in the midplane and surface layer the ionization chemistry is controlled by several tens of reactions. In the inner warm midplane region the key reactions are the ionization of molecular hydrogen by cosmic rays, followed by the formation of  $\text{H}_3^+$  ions which rapidly react with metals and electrons. The metal ions are slowly neutralized by recombination with electrons and thus become the dominant charged species. In the outer midplane region, metals are irreversibly depleted onto dust grains and therefore ion-molecule reactions of  $\text{H}_3^+$  with simple neutrals like CO and  $\text{N}_2$  are important. Finally, these molecular ions recombine with dust grains and electrons. The dominant ions at 1 Myr are  $\text{HCO}^+$ ,  $\text{H}_3^+$ , and  $\text{N}_2\text{H}^+$ . In the surface layer the life cycle of the free electrons includes the photoionization of carbon atoms and simple radicals, like OH and CO, as well as X-ray ionization of atomic and molecular hydrogen. Then hydrogen ions and  $\text{H}_3^+$  react with oxygen, water, hydroxyl, and CO, resulting in the formation of  $\text{HCO}^+$ ,  $\text{H}_3\text{O}^+$ , and  $\text{OH}^+$ . These molecular ions further react with either their neutral analogs or electrons, thus closing the chemical cycle. The chemical equilibrium of the fractional ionization in these regions is achieved after 100 – 1000 years.

It is in contrast to the intermediate layer, where the ionization equilibrium is not reached during 1 Myr. The following chemical processes regulate the evolution of the ionization degree there. Initially abundant  $\text{HCO}^+$  and  $\text{H}_3^+$  recombine very rapidly, while metal ions are neutralized and stick to dust grains. Then, few equilibrium states are reached with  $\text{NH}_4^+$ ,  $\text{H}_3\text{CO}^+$ , and  $\text{HCO}^+$  as the dominant ions, where their abundances increase in this sequence. After the initial decline, the evolution of the fractional ionization shows a step-like behavior. Consequently, one needs a reduced network that includes a few tens of species involved in cycles of synthesis and destruction of the above ions. However, at  $3 < R < 30$  AU the situation is more complicated because the density is high and the temperature is low enough to allow efficient gas-grain interactions. The simple step-like evolutionary trend does not work anymore since the incorporation of carbon atoms into long carbon chains becomes important. This process leads to decrease of the  $\text{CH}_4$  abundance, which regulates the amount of ionized sulfur in the gas-phase. Therefore,  $\text{S}^+$  rapidly becomes a dominant ion at  $t \sim 3 \cdot 10^{3-5}$  years. However, oxidation slowly destroys long carbon chains and the methane abundance in the gas-phase grows again, restoring the  $\text{CH}_4$ - $\text{S}^+$  equilibrium cycle. Thus, the reduced network must incorporate almost all species with up to 6 carbon atoms and some *surface reactions*. This is the first indication that the surface chemistry may have a great impact on the evolution of fractional ionization in protoplanetary disks.

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