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Cosmic Rays and the Origin of Volatiles in Protoplanetary Disks

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Abstract. The origin of water and other volatiles in protoplanetary disks can be either interstellar or due to chemical processing during the protoplanetary disk phase. Depending on the strength of the ionization field present during this stage, an active chemical evolution in the protoplanetary disk midplane can lead to formation of complex volatiles on timescales shorter than the disk dissipation timescale. For this reason, we investigate the effects of cosmic rays and the usually neglected cosmic ray induced UV ionization field in time dependent chemical models of protoplanetary disks. These results are benchmarked against our current knowledge of the chemical composition of cometary ices. We conclude that water and other, more complex volatiles can be preserved in the ice mantles of dust grains. This ice mantle growth can also have a significant impact on the dust opacity and hence on the temperature profile of the disk midplane. This effect will be observable in the near future with ALMA.

Keywords. Astrochemistry, Comets: General, Protoplanetary Disks, (ISM:) Cosmic Rays

1. Introduction

Observations of comets present to date a fairly inhomogeneous dataset, with comets from different families (Jupiter family, Oort cloud) and observations taken at different orbital times before and after aphelion. Bockelee-Morvan (2010) summarize the abundance pattern emerging from those measurements. Water is the dominant species (∼80%), followed by CO, CO_2, CH_3OH, CH_4, NH_3, and H_2CO (in order of decreasing abundance). There are about two orders of magnitude spread in CO/water abundance and about one order of magnitude for other species. The reason can be different evolutionary tracks, formation histories, formation locations or different orbital phases at which the data was taken (Ferrín 2013). However, if no important sources of ionization are present in the disk midplane, we cannot expect primordial material to be chemically processed into the more complex species found in comets. For this reason, we propose that cosmic ray induced processes can be a significant source of ionization in comet-forming regions.

Cosmic rays can penetrate down into the midplane of a typical T Tauri protoplanetary disk (PPD) beyond ∼1 AU (depending on the surface density power law). This is where planetesimals are expected to form from small, bare and ice-coated dust grains. The composition of the ices that form during the protoplanetary disk stage can be strongly influenced by cosmic ray driven chemistry. This includes secondary ionization processes that can be enhanced up to an order of magnitude, in the case of the cosmic ray induced UV field (Chaparro Molano & Kamp 2012).

2. Model predictions for ices

We use the thermo-chemical disk modeling code ProDiMo (Woitke *et al.* 2009). The gas thermal balance and chemistry are solved consistently using a network of 90 species

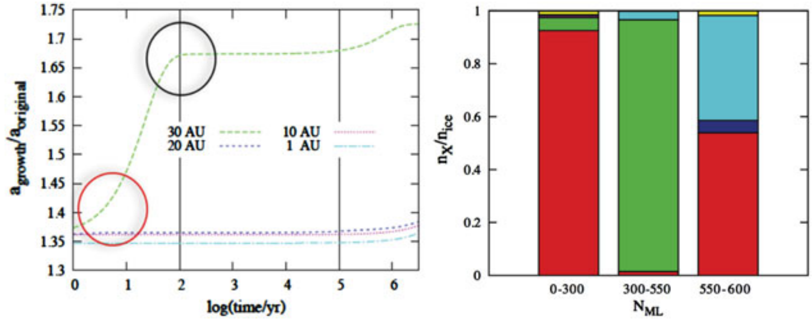

Figure 1. *Left*: Growth factor evolution of a 0.2 μm dust grain due to ice mantle deposition. Red: original ISM mantle. Black: PPD mantle. *Right*: Composition of ice mantles at 30 AU.

(gas and ice) and 1100 reactions (mostly UMIST, Woodall *et al.* 2007). In this first assessment, we neglect surface chemistry. After solving the disk thermal balance, we run a time-dependent chemistry solver using molecular cloud abundances as initial conditions.

Cosmic ray induced photoprocesses favor CO_2 ice formation at the expense of water, CH_4 and CO. Reactions with He^+ (created by cosmic rays) destroy CO, releasing oxygen to form CO_2 and water. After 1 Myr, cosmic ray induced UV photons ionize CH_3, leading to CH_5^+ and subsequent recombinations that form stable CH_4.

Acharyya *et al.* (2011) found that ice mantles can increase the grain size by ~30% in cold molecular clouds. We account here for grain growth in two ways: (1) PPD>ISM size distribution (2) ice mantle growth. The first ~300 ML of mostly water ice form during the first 10 Myr (ISM dust, 20 K, 10^6 cm^{-3}). The remaining ~600 ML build up in the PPD model (PPD grains, 20 K, 7×10^{10} cm^{-3}). A 0.2 μm grain grows by a factor ~1.8 due to ice mantle deposition (Fig. 1).

3. Conclusions

We thus propose a possible scenario for the formation of ice mantles on the surface of dust grains: (1) The first ice mantles form during the lifetime of molecular clouds, typically a few Myr (e.g. Tielens & Hagen 1982, Chang *et al.* 2007). In this stage, surface chemistry can already lead to the formation of more complex organic species such as methanol. (2) These ices are processed during the formation of a star+disk system, which takes less than 1 Myr (e.g. Visser *et al.* 2009). (3) During the protoplanetary disk stage, a second ice mantle forms. Evolutionary timescales in this stage can be up to a few Myrs. These ice mantles are formed in layers whose composition strongly depends on the distance to the proto-Sun and on the strength of the local ionization field. This effect also leads to a shift in the grain size distribution function, which will affect the disk midplane temperature profile.

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