The molecular composition of the protoplanetary disk midplanes with shadow structures beyond the H_2O snowline

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Understanding the chemical structures in protoplanentary disks are important to explain the observational results of disks, planetary atmospheres, and small objects in the solar systems, such as comets and asteroids. Recently, Ohno & Ueda (2021) found that the vicinity of the current Jupiter orbit could be lower than 30 K because of the shadow structure if the small-dust surface density varies by a factor of 30 across the H_2O snowline in the T Tauri disk (the protosolar disk), and that the shadow can cause the condensation of most volatile substances, namely N_2 and noble gas.

In our study, we adopted a detailed gas-grain chemical reaction network, and investigated the radial abundance distributions of dominant carbon-, oxygen-, and nitrogen-bearing molecules and the radial profiles of the elemental ratios in the gas and ice of the same T Tauri disks with shadow structures.

According to our calculations, the shadowed disks have significant amounts of molecules such as HCN, CH_4, and H_2CO, which were not included in the previous study (Ohno & Ueda 2021). In the shadowed disks, molecules such as CO_2, CH_4, and C_2H_6 absorbed onto dust grains outside 2 au, and the gas-phase C/O ratios are around unity in most cases, although gas-phase N/O ratios are >>1 in the shadowed region and show spatial variations which are much larger than those of the C/O ratios, and thus the N/O ratios would be an useful tracer of the disk shadowed region.

In addition, in the shadowed region, the abundances of saturated complex organic molecules such as H_2CO, CH_3OH, and NH_2CHO increase, whereas those of unsaturated complex organic molecules such as C_2H_2, C_3H_2, $HCOOCH_3$ decrease. We consider that the sequential hydrogenerations of especially CO on cold dust-grains play the dominant role in the formation of former saturated organic molecules, whereas the radical-radical reactions on the warm dust-grains and gas-phase reactions are important for the formation ot the latter unsaturated organic molecules. We also investigated the dependance of the disk chemical structures on ionisation rates and initial abundances.

In this presentation, we introduce these results of our chemical modeling in detail, and we discuss the implication for molecular line observations in disks with e.g., ALMA and relations with the molecular abundances of small bodies such as comets and asteroids.

Keywords: Protoplanetary disks, Snowlines, Organic molecules, Dust grains, Chemical evolution, Planetary Atmospheres

