Multiple Paths of Deuterium Fractionation in Protoplanetary Disks

*Yuri Aikawa[1], Kenji Furuya[2]

1. Department of Astronomy, Graduate School of Science, University of Tokyo, 2. Center for Computational Sciences, University of Tsukuba

At low temperatures, molecular D/H ratios become higher than the elemental D/H ratio. Such a deuterium enrichment is caused by several exothermic exchange reactions. In recent years, spatial distributions of various deuterated species have been investigated using ALMA. In TW Hya, for example, DCN emission is centrally peaked, while DCO^+ emission is ring like. It has been interpreted in terms of main deuteration paths of each species; deuteration of HCN is caused by an exchange reaction, the exothermicity of which is higher than that for HCO^+. The spatial distributions of deuterated species, however, also vary among disks. We revisit deuterium chemistry in protoplanetary disks using an updated gas-grain chemical reaction network, in order to clarify the deuteration pathways in disks and to investigate the dependence of deuterium chemistry on various disk parameters. We found multiple paths of deuterium fractionation; exchange reactions with D atoms are effective, as well as those with HD. Radial distributions of molecular column density depends on grain sizes in disks. In a disk model with grain sizes appropriate for dark clouds, the freeze-out of molecules is severe in the outer midplane, while the disk surface is shielded from UV radiation and becomes molecule-rich, which tends to make their column density distribution relatively flat. When the dust grains have grown to millimeter size, the freeze-out rate of neutral species is reduced, and the abundances of gaseous molecules (e.g. DCO^+) are enhanced in the cold midplane. The effects of turbulence on chemistry are thus multifold; turbulent diffusion transports D atoms and radicals at the disk surface to the midplane, and stable ice species in the midplane to the disk surface. HCN and DCN in the gas and ice are much reduced at the innermost radii, compared with the model without turbulence, while other species show more complicated dependence. As water-ice bearing grains sediment and migrate to inner radii, the C/O ratio could increase in the outer radius. While HCN and DCN abundances increase with C/O ratio, the radial distributions of deuterated species are not much affected.

Keywords: protoplanetary disks, Deuterium fractionation