Model Prediction of Complex Organic Molecules in Protoplanetary Disks

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Protoplanetary disks are the natal place of planets. Understanding chemical components of gas, dust and ice in the disks is essential to investigate the origins of materials in our Solar system and other planetary systems. We investigate the synthesis of complex organic molecules (COMs) in protoplanetary disks using a large gas-grain chemical network including COMs together with a 2D steady-state physical model of a disk irradiated by UV and X-rays from the central star. COMs are efficiently formed on cold and warm grains in the disk midplane via hydrogen adding as well as radical-radical reactions on grain surface. Radiation processing on ice forms reactive radicals and helps build further complexity. Part of the icy molecules are photodesorbed into gas and their transition lines become observable. Actually, ALMA observations have detected CH3CN and CH3OH from protoplanetary disks. The line emitting region of these molecules are the outer relatively cold disk, which suggests that the molecules are non-thermally desorbed from grains following the formation on dust garains. Based on our model calculations, we perform ray-tracing calculations to predict line spectra of complex organic molecules observable with SPICA. Also, we discuss possible connection of COMs in protoplanetary disks to those in the Solar system objects, such as comets.

Keywords: protoplanetary disks, astrochemistry, radiative transfer