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Molecular Evolution in Collapsing Prestellar Cores II: The Effect of Grain-surface Reactions

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Stars are formed by gravitational collapse of molecular cloud cores. Molecular abundances in such cores are important, because cores are mainly observed by molecular lines. It also tells us about molecular evolution during the formation of stars and planetary systems. We investigate molecular evolution that occurs in collapsing prestellar cores by numerical calculation. To model the dynamics, we adopt the Larson-Penston solution and analogues with slower rates of collapse. For the chemistry, we utilize the new standard model (NSM) with the addition of deuterium fractionation and grain-surface reactions treated via the modified rate approach. The use of surface reactions distinguishes the present work from our previous model.

We find that grain-surface reactions efficiently produce H2O, CO2, H2CO, CH3OH, N2, and NH3 ices. In addition, the surface chemistry influences the gas-phase abundances in a variety of ways. For example, formation of molecular nitrogen on grain surfaces followed by desorption into the gas enhances the abundance of this gas-phase species and its daughter products N2H+ and NH3. Formation of H2O ice on grain surfaces reduces O atom abundance in the gas phase. Hence the early-phase species such as CCS survive for a longer time scale compared with the previous model without grain-surface reactions.

The current reaction network along with the Larson-Penston solution allows us to reproduce satisfactorily most of the molecular column densities and their radial distributions observed in L1544; CO and CCS are depleted at the core center, while N2H+ emission is centrally peaked. The agreement tends to worsen with models that include strongly delayed collapse rates.

In all of our models, the column density of N2H+ monotonically increases as the central density of the core increases during collapse from 3 10^5 cm-3 to 3 10^7 cm-3. Thus, the abundance of this ion can be a probe of evolutionary stage.

Theoretical model predicts that molecular D/H ratios increase as molecular depletion proceeds in dense cores. We find that observed D/H ratio is indeed higher in cores with high N2H+ column density, i.e. in more evolved cores. D/H ratios in assorted cores are best reproduced in the Larson-Penston picture with the conventional rate coefficients for fractionation reactions given by Millar, Bennet, & Herbst (1989). If we adopt the newly measured and calculated rate coefficients (Gerlich, Roeff, & Herbst 2002), the D/H ratios, especially N2D+/N2H+, become significantly lower than the observed values.