MONTE CARLO MODELING OF GAS-GRAIN CHEMISTRY IN STAR-FORMING REGIONS

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An understanding of the complex grain-surface chemistry responsible for the formation of organic molecules in regions of star and planet formation requires the details of the structure of icy grain mantles to be included into astrochemical models.
Here, we present a new macroscopic gas-grain Monte Carlo model with an icy grain mantle treated as a chemically reactive surface and a chemically inert bulk consisting of multiple molecular layers. The model allows us to track the chemical history of ice during its build-up in cold protostellar cores. Desorption processes important in the transition to the hot core stage of star formation are also included. The model is computationally efficient, which allows us to simulate a realistically complex chemistry based on the OSU.2008 network of gas-phase reactions and an extended set of grain-surface reactions, including the chemistry of complex organic species. The model is applied to simulate the chemistry that occurs during the evolution of protostellar matter from a cold core to a hot core phase. The results of modeling and their key differences from results obtained with traditional two-phase (gas-surface) astrochemical models will be presented.