A Unified Monte Carlo Treatment of Gas-Grain Chemistry in Clouds and Disks

A.I. Vasyunin (e-mail: vasyunin@mpia.de) (1), R.T. Garrod (2), D.S. Wiebe (3), D.A. Semenov (1), and Th. Henning (1)

(1) Max-Planck-Institute for Astronomy, Germany
(2) Cornell University, USA
(3) Institute of Astronomy of Russian academy of sciences, Russia

From the synthesis of H_2 in molecular clouds, to the formation of complex organic molecules in star-forming regions, a full understanding of interstellar chemistry requires the consideration of both gas-phase and dust grain-surface processes. However, the lack of accurate computational tools for the modeling of coupled gas-grain chemical systems presents a major obstacle to the achievement of this goal, as has long been realized.

Accurate simulation of gas-phase chemistry alone may be achieved using rate equations (RE), and this method is frequently extended to the simulation of the grain-surface chemistry. However, the discreteness of surface processes in some situations (when the number of reacting particles per grain is less than 1) can invalidate the use of rate equations. To avoid this problem, one have to either solve a full chemical master equation directly (e.g., with a Monte Carlo algorithm) or introduce modifications to the rate equations (MRE).

We build a realistic astrochemical model using a Monte Carlo approach to all gas phase and grain surface chemical processes, which is the first time this has been done. This allows us to properly take into account the stochastic nature of grain surface chemical reactions, which are of essential importance for the formation of organic molecules -- i.e., the precursors of life as we know it.

We found that stochastic effects are significantly affect modeled abundances of observationally important species and must be taken into account in many cases. Previously developed rate equations approaches fail to reproduce stochastic effects correctly. The recent modified rate approach (MRE) of Garrod et al. (2008) is shown to be the most accurate fast approach of accounting for stochastic effects in astrochemical modeling. Using this new MRE approach we asses the importance of stochastic effects in protoplanetary disks.