CONTROL ID: 2254986

TITLE: Monte Carlo kinetics simulations of ice-mantle formation on interstellar grains

ABSTRACT BODY:

Abstract Body: The majority of interstellar dust-grain chemical kinetics models use rate equations, or alternative population-based simulation methods, to trace the time-dependent formation of grain-surface molecules and ice mantles. Such methods are efficient, but are incapable of considering explicitly the morphologies of the dust grains, the structure of the ices formed thereon, or the influence of local surface composition on the chemistry.

A new Monte Carlo chemical kinetics model, *MIMICK*, is presented here, whose prototype results were published recently (Garrod 2013, ApJ, 778, 158). The model calculates the strengths and positions of the potential mimima on the surface, on the fly, according to the individual pair-wise (van der Waals) bonds between surface species, allowing the structure of the ice to build up naturally as surface diffusion and chemistry occur. The prototype model considered contributions to a surface particle's potential only from contiguous (or "bonded") neighbors; the full model considers contributions from surface constituents from short to long range. Simulations are conducted on a fully 3-D user-generated dust-grain with amorphous surface characteristics. The chemical network has also been extended from the simple water system previously published, and now includes 33 chemical species and 55 reactions. This allows the major interstellar ice components to be simulated, such as water, methane, ammonia and methanol, as well as a small selection of more complex molecules, including methyl formate ($HCOOCH_3$).

The new model results indicate that the porosity of interstellar ices are dependent on multiple variables, including gas density, the dust temperature, and the relative accretion rates of key gas-phase species. The results presented also have implications for the formation of complex organic molecules on dust-grain surfaces at very low temperatures.

CONTACT (NAME ONLY): Robin Garrod

CONTACT (E-MAIL ONLY): rgarrod@virginia.edu

AUTHORS/INSTITUTIONS: R. Garrod, University of Virginia, Charlottesville, Virginia, UNITED STATES|

PRESENTATION TYPE: Poster