Diffusion-limited reactivity in interstellar ice

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Interstellar grains are thought to play an important role in the formation of complex molecules in the interstellar medium[1]. However, the low temperature and scarcity of reactants present in their ice mantle strongly limit the formation of complex molecules. Whether or not long time scale can counterbalance this diffusion-limited solid-state reactivity at low-temperature depends on both the reaction rate constant and the diffusion coefficients of the reactants, whether they are neutrals or radicals.

I will present our combined experimental and theoretical study undertaken in order to better understand the importance of such a diffusion limited reactivity mechanism. As a model system the two reactants CO_2 and NH_3 are chosen. They are abundant in interstellar ices and have been shown to react thermally in ices[2] to give NH_2COOH and $NH_4^+NH_2COO^-$. The reaction rate constant of the NH_3 + CO_2 reaction in a water free environment is measured and the reaction mechanism rationalized on the basis of *ab-initio* calculations mimicking this reaction in both an ammonia and a water-ammonia cluster. This reaction is also studied in a more realistic water ice model using *ab-initio* molecular dynamic technics. The diffusion coefficients of CO_2 and NH_3 in the ice are determined using both laboratory experiments, classical and *ab-initio* molecular dynamics simulations. Our goal with this study is to use our determined diffusion coefficients and rate constant for the NH_3 + CO_2 reaction in a water ice model to develop a diffusion-reaction formalism to account for the slowing down induced by an increasing dilution of the reactants in the water ice mantle. The diffusion-limited reaction rate may be extrapolated to lower temperature and longer time scale to set a limit to the production of complex molecules in interstellar ice.

[1] **Tielens A.G.G.M. and Hagen W., *Astron. Astrophys.* 1982, 114, 245**
[2] **Bossa J.B. et al. *Astron. Astrophys.* 2008, 492, 719**