Grain surface chemistry in PDRs

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With the advent of the new generation of mm and sub-mm detectors (ALMA, NOEMA), molecules are detected in a large variety of galactic and extra-galactic interstellar environments. These molecules are unique probes to investigate the physical processes in interstellar gas and on grains. Theoretical models and laboratory experiments show that many of these molecules are efficiently formed on grains (H_2O, H_2CO, CH_3OH, CO_2, ...) and released in the gas. State-of-the-art astrochemical models have to take into account consistently both gas phase and surface chemistry to interpret observations and, to do so, they must rely on theoretical and laboratory experiments results. However, surface processes are complex to implement in astrophysical codes in which grain models are necessarily simplified.

We have implemented surface chemistry in a new version of the Meudon PDR code [1, 2], one of the state-of-the-art public astrochemical code (http://ism.obspm.fr). In the Meudon PDR code, grains are represented by distributions of amorphous carbonate, silicates and PAHs that contribute to the radiation field absorption, photo-electric effect, continuum emission and surface reactions. The grain surface model takes into account adsorption, formation of mantles, reactions as well as several desorption processes: thermal, photo-desorption, chemical desorption, cosmic rays desorption. Because the Meudon PDR code is a 1D code that solves in a coupled way the radiative transfer from far UV to sub-mm, thermal balance and chemistry for several hundred chemical species in the gas and on grains, it is possible to have access to grain mantle compositions and to efficiencies of the various surface processes as a function of depth taking into account the grain temperature and the intensity of the radiation field at each position.

In this talk, I will present this new model of grain surface chemistry. I will show how uncertainties on surface chemical reaction thresholds affect grain mantle composition and chemical abundances in PDRs. I will highlight the effect of competitive desorption processes (thermal, photon, chemistry, cosmic rays), in different environments to the light of new laboratory experiment results. Indeed, the latest photo-desorption experiments show this process may be less efficient on H_2O ices by one order of magnitude than commonly thought. This is a new challenge for astrochemical models since the common picture was that molecules such as CH_3OH is formed on grains and release in the gas by photo-desorption due to primary or secondary UV photons [3]. The role of cosmic rays on grains [4] and exothermicity of chemical reaction in grain mantles will be investigated to determine if they can be competitive enough to reach an agreement between astrochemical models, observations and laboratory experiments results.

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[3] V. Guzman et al. *The IRAM-30 m line survey of the Horsehead PDR. IV. Comparative chemistry of H2CO and CH3OH*, A&A. **560**, 73 (2013)

[4] E. Dartois et al. *Heavy ion irradiation of crystalline water ice. Cosmic ray amorphisation cross-section and sputtering yield*, A&A. **576**, 125 (2015)