MOLECULAR HYDROGEN FORMATION : EFFECT OF DUST GRAIN TEMPERATURE FLUCTUATIONS

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H_2 formation is a hot topic in astrochemistry. Thanks to Copernicus and FUSE satellites, its formation rate on dust grains in diffuse interstellar gas has been inferred (Jura 1974, Gry et al. 2002). Nevertheless, detection of H_2 emission in PDRs by ISO and Spitzer (Habart et al., 2004, 2005, 2011) showed that its formation mechanism can be efficient on warm grains (warmer than 30K), whereas experimental studies showed that Langmuir-Hinshelwood mechanism is only efficient in a narrow window of grain temperatures (typically between 10-20 K). The Eley-Rideal mechanism, in which H atoms are chemically bound to grains surfaces could explain such a formation rate in PDRs (Le Bourlot et al. 2012).
Usual dust size distributions (e.g. Mathis et al. 1977) favor smaller grains in a way that makes most of the available grain surface belong to small grains. As small grains are subject to large temperature fluctuations due to UV-photons absorption, calculations at a fixed temperature give incorrect results under strong UV-fields.

Here, we present a comprehensive study of the influence of this stochastic effect on H_2 formation by Langmuir-Hinshelwood and Eley-Rideal mechanisms. We use a master equation approach to calculate the statistics of coupled fluctuations of the temperature and adsorbed H population of a grain. Doing so, we are able to calculate the formation rate on a grain under a given radiation field and given gas conditions. We find that the Eley-Rideal mechanism remains an efficient mechanism in PDRs, and that the Langmuir-Hinshelwood mechanism is more efficient than expected on warm grains.
This procedure is then coupled to full cloud simulations with the Meudon PDR code. We compare the new results with more classical evaluations of the formation rate, and present the differences in terms of chemical structure of the cloud and observable line intensities. We will also highlight the influence of some microphysical parameters on the results.