Dust temperature fluctuations and surface chemistry: H_2 formation.

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Among dust grains, very small grains and PAHs are known to be of dominating importance for various processes. Indeed, big grains contain most of the dust mass, but the smallest grains dominate the total dust surface. Small grains are thus also the principal substrate for surface reactions, the most important of which is the formation of H_2.

However, models of H_2 formation must take dust temperature fluctuations into account. Small grains are sensitive to individual UV photons and undergo temperature spikes. Yet surface chemistry models almost always assume a non-fluctuating grain temperature. While this assumption is reasonable for the surface chemistry in dark cloud cores, it is much less justified for H_2 formation in UV-rich environments (e.g., diffuse gas or bright PDRs).

Various mechanisms can contribute to H_2 formation. The Langmuir-Hinshelwood mechanism involves physisorbed atoms migrating on the surface, and was experimentally found to have a limited temperature range of efficiency (10-20K) [1], while ISO and Spitzer observations of PDRs show efficient formation despite warmer dust [2]. Other mechanisms were proposed such as the Eley-Rideal mechanism [3], involving direct reaction between a chemisorbed atom and a gas atom, and insensitive to grain temperature.

We present the first complete analytical treatment of the statistical problem of surface chemistry with fluctuating temperatures, using a master equation approach to follow exactly both the temperature and the population of adsorbed atoms. We apply this treatment to the Langmuir-Hinshelwood mechanism and find it to be much more efficient than expected in unshielded environments under moderate UV fields, as the grain spends most of its time at temperatures lower than its average temperature. Another mechanism is still necessary to account for formation under strong UV fields, and the Eley-Rideal mechanism is found to retain most of its efficiency. Fast approximations of the exact results are constructed.

The effects of this new formalism on full cloud simulations are explored using the Meudon PDR code [4]. Effects are found in tracers of the cloud edge (H_2, CH^+) but remain limited. The increase in Langmuir-Hinshelwood efficiency nevertheless allows more flexibility in the choice of the poorly known microphysical parameters of the Eley-Rideal mechanism, as will be demonstrated using the constraints of the observations of a few well-known PDRs.

References:

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