H_2 formation from photodissociated PAH cations

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In interstellar conditions H_2 formation from gas-phase reactions involving hydrogen atoms are highly inefficient, hence H_2 formation models mostly rely on catalytic reactions on the surface of dust grains [1]. Additionally, molecular hydrogen formation in polycyclic aromatic hydrocarbons (PAHs) through the Eley–Rideal mechanism has been considered as well, although it has been found to have low efficiency in PDR fronts [2]. In a previous work [3], we have described the possibility of efficient H_2 release from medium to large sized PAHs upon photodissociation, with the exact branching between H-/H2-loss reactions being molecule dependent. Here, we investigate the astrophysical relevance of this process, by using a model for the photofragmentation of PAHs under interstellar conditions [4]. We focus on three PAHs cations (coronene, ovalene, and circumcoronene), which represent three possibilities in the branching of atomic and molecular hydrogen losses. We find that, for ovalene (H_2-loss dominated) the rate coefficient for H_2 formation reaches values of the same order as H_2 formation in dust grains. This result suggests that this hitherto disregarded mechanism can account, at least partly, for the high level of molecular hydrogen formation in dense PDRs.

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