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Interstellar Catalysis of Molecular Hydrogen through Superhydrogenation of Polycyclic Aromatic Hydrocarbons

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In the field of astrochemistry and surface science a primary objective is to identify and characterize effective catalysts which have a plausible existence in the interstellar medium (ISM). Molecular hydrogen (H_2) is the most abundant molecule in the ISM with well-established and efficient catalytic formation routes in many regions of interstellar space. However, in certain regions of the ISM, discrepancies between formation rates and dissociations rates have been found [1]. Specifically, in Photodissociation regions (PDRs), the dissociation rate is so high that prevailing formation routes may not be efficient enough to explain the observed abundancies of H_2 and needed formation rates. Here we examine a group of planar nanosized molecules called polycyclic aromatic hydrocarbons (PAHs) as possible catalysts of H_2 formation. Significant abundancies of PAHs have been observed to spatially overlap with regions of high H_2 formation rates [2].

We have used temperature programmed desorption (TPD) and scanning tunneling microscopy (STM) to examine a template PAH, coronene ($C_{24}H_{12}$). Density functional theory (DFT) reveals that coronene and possibly other PAHs will have 0eV energy barriers for both Hydrogen (H) addition and H_2 abstraction even at low super-hydrogenation degrees (4 adatoms) [3]. The state of hydrogenation will therefore depend on these competing processes and their relative cross sections for addition, σ_{add}, and abstraction, σ_{abs}.
Monolayers of neutral PAH molecules are deposited on a highly oriented pyrolytic graphite (HOPG) surface and exposed to different fluences of D or H atoms. The atomic beam is estimated to have a temperature of approximately 1000K. Fully deuterated coronene ($C_{24}D_{36}$) is observed, indicating formation of HD via an exchange process between H and D [4].
First addition cross sections, $\sigma_{add}(0)$ for D/H addition can be found experimentally from the exponential decay in pristine coronene as a function of D/H fluence. Cross sections of $\sigma_{add,H}(0) = 0.25 \pm {}^{0.14}_{0.05}\,\text{Å}^2$ for H addition and $\sigma_{add,D}(0) = 0.065 \pm {}^{0.10}_{0.05}\,\text{Å}^2$ for D addition are best fits to data. Determination of sequential addition and abstraction cross sections, however, require further modelling and will here be determined through comparisons to Kinetic Monte-Carlo (KMC) simulations.
Also observed from TPD is indications of preferred D/H-PAH configurations with high stability and increased barriers against further D/H addition. Experimental data points towards a barrier preventing addition to the center ring. These barriers are not detected when a high temperature atomic beam is used (T≈2000K) [5].

References:

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