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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 abundances 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 abundances 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,  $\sigma_{add}$ , and abstraction,  $\sigma_{abs}$ .

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  $\sigma_{add,H}(0) = 0.25 \pm 0.05 \text{ \AA}^2$  for H addition and  $\sigma_{add,D}(0) = 0.065 \pm 0.05 \text{ \AA}^2$  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 ( $T \approx 2000\text{K}$ ) [5].

### References:

- [1] Tielens, A., *Reviews of Modern Physics*, 85 (2013) 1021-1081.
- [2] Habart, E.; et. al., *Astronomy and Astrophysics* 397 (2003) 623-634.
- [3] Rauls, E.; and Hornekær L., *The Astrophysical Journal* 679 (2008) 531.
- [4] Mennella, Vito, et al *The Astrophysical Journal Letters* 745.1 (2011): L2.
- [5] Thrower, J. D., et al *The Astrophysical Journal* 752.1 (2012): 3.

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