Investigation of the role of oxygen functionalized PAHs in small molecule formation

R. Jaganathan[1*], J. Thrower[1], F. D. S. Simonsen[1], L. Hornekær[1]

[1]*Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark*

[*]*Corresponding author e-mail address: rijutha@phys.au.dk*

Polycyclic aromatic hydrocarbons (PAHs) contain up to 20% of the carbon in the galaxy and form an important component of interstellar dust. They have been detected along sight lines to a variety of interstellar objects through their infrared absorption bands in the range 3 – 20 micron characteristic of C-H, C-C stretching and bending modes and are expected to contain 20 – 100 C atoms. In cold regions of the interstellar medium (ISM) siliceous and carbonaceous dust grains are covered by an icy mantle with the most dominant component of the ice being H_2O. PAH molecules along with other simple and complex molecules are also expected to be condensed. Laboratory processing of water ice and PAH mixtures with energetic radiation such as UV light or protons show that superhydrogenated PAHs are produced alongside PAHs with alcohol and ketone functional groups indicating that such species are formed in the ISM on icy grains [1, 2]. Interstellar ices could contain neutral and ionized PAHs, alcohols, ketones and quinones at the 2% - 4% level relative to water [3].

In photodissociation regions of the ISM where UV photons dissociate molecules and grain surface reactions are inefficient, PAHs were postulated as catalysts in molecular hydrogen formation. Experiments and theoretical calculations indicate that PAHs play a role as catalysts for H_2 formation through the formation of superhydrogenated PAHs [4, 5]. The impact of the presence of other functional groups on the catalytic formation of small molecules remains unclear. I will present laboratory studies on the catalytic activity of 6,13 – pentacenedione (PQ) when exposed to atomic hydrogen.

A monolayer of PQ was prepared under ultra-high vacuum conditions on a HOPG surface mimicking a carbonaceous dust grain, and then exposed to a controlled fluence of hydrogen atoms. Temperature programmed desorption was then used to study the products formed on the surface. The first species to form even at very short H atom exposures has a mass 294 amu indicating the loss of an oxygen atom from PQ, potentially through the formation of H_2O, OH or CHO. Magic numbers are seen for intermediate H atom exposures indicating barriers to addition The cross section for addition of the first H atom was determined and is at least 10 times higher than that for coronene and pentacene studied previously.

Acknowledgments: We acknowledge the European Union (EU) and Horizon 2020 funding award under the Marie Skłodowska-Curie action to the EUROPAH consortium, grant number 722346.

References

[1] Bernstein, M. P., et al., Advances in Space Research 30.6 (2002): 1501-1508.
[2] Gudipati, M. S. and Yang, R., The Astrophysical Journal Letters 756.1 (2012): L24.
[3] Bernstein, M. P., et al., Science 283.5405 (1999): 1135-1138.
[4] Rauls, E., and Hornekær, L., The Astrophysical Journal 679.1 (2008): 531.
[5] Thrower, J. D., et al., The Astrophysical Journal 752.1 (2012): 3.