Formation of Superhydrogenated PAHs and their Role in Interstellar H_2 Formation

J. D. Thrower[1], B. Jørgensen[1], E. E. Friis[1], A. Skov[1], H. Lemaître[1], P. A. Jensen[1], A. M. Cassidy[1], S. Baouche[1], A. C. Luntz[1], R. Balog[1], M. Andersen[1], B. Hammer[1], V. Mennella[2], L. Hornekær[1]

[1]*Aarhus University, Department of Physics and Astronomy, Aarhus, 8000, Denmark*
[2]*INAF, Osservatorio Astronomico di Capodimonte, Napoli, 80131, Italy*
thrower@phys.au.dk

Polycyclic aromatic hydrocarbon molecules (PAHs) account for several per cent of the carbon in the galaxy, with observations revealing infrared emission attributable to such species in a wide range of environments. PAHs are therefore thought to play an important role in many interstellar chemical processes. The observed correlation between H_2 and PAH emission in PDRs has led to the suggestion that PAHs may play a role in H_2 formation in such environments [1]. We have demonstrated that PAH molecules are able to catalyse the formation of H_2 through the formation of superhydrogenated PAH molecules.

Density functional theory (DFT) calculations [2] considered the addition of H atoms to the coronene molecule and showed that (i) addition to all three distinct sites on the coronene molecule is possible and (ii) abstraction reactions involving superhydrogenated coronene can form H_2. We have combined infrared spectroscopy (IR), mass spectrometry and scanning tunneling microscopy (STM) to confirm these predictions. These measurements show the formation of superhydrogenated species upon exposure to H(D) atoms, as evidenced by the conversion of aromatic to aliphatic carbon centres [3], through addition of H(D) atoms to all sites on the molecule [4]. We also see evidence for the formation of H_2 and HD molecules as a result of abstraction reactions involving these species. STM measurements provide additional insight into the formation of species with different hydrogen configurations.

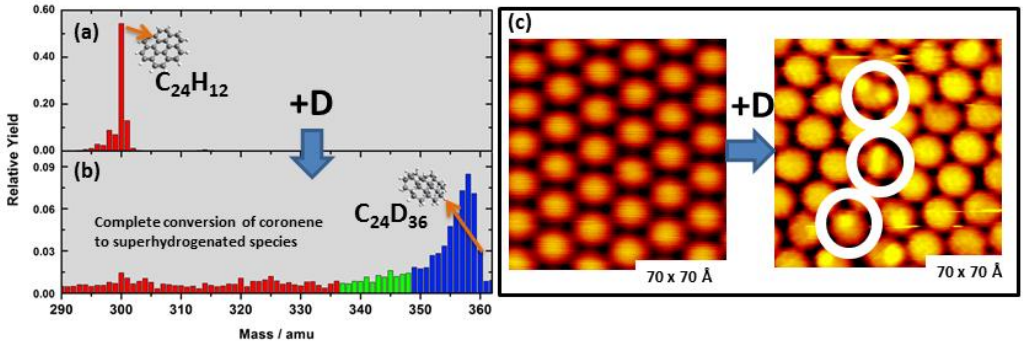

Figure 1: Mass spectra revealing the conversion of (a) coronene to (b) higher mass superhydrogenated coronene fragments following exposure to D atoms. (c) STM measurements reveal the formation of several distict adsorption structures following exposure to coronene to atomic hydrogen.

References:
[1] E. Habart et al., Astron.Astrophys., **397**, 623 (2003).
[2] E. Rauls & L. Hornekær, Astrophys. J., **679**, 531 (2008).
[3] V. Mennella, et al., Astrophys. J., **745**, L2 (2012).
[4] J. D. Thrower et al., Astrophys. J., **752**, 3 (2012).