

H₂ catalysis through superhydrogenation of interstellar polycyclic aromatic hydrocarbons

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Abstract. Experimental data showing superhydrogenation of neutral polycyclic aromatic hydrocarbons (PAHs) coronene, pentacene and pentacenequinone is presented. PAH monolayers were prepared on a highly oriented pyrolytic graphite surface and subsequently exposed to a beam of atomic hydrogen. The superhydrogenated PAH species were examined via temperature programmed desorption measurements. Stable intermediate superhydrogenation degrees as well as fully superhydrogenated species are observed and the initial reaction cross section for coronene has been determined.

Keywords. Astrochemistry, laboratory, ISM, molecules, clouds

1. Introduction

Polycyclic aromatic hydrocarbons (PAHs) can be detected almost everywhere in the interstellar medium (ISM) from their characteristic vibrational features in the infra-red and are believed to harbour 5-10% of the available carbon in the ISM (Tielens 2013). PAHs have been speculated to take part in molecular hydrogen (H₂) formation in the ISM and may contribute significantly in photodissociation regions (PDRs) as spatial overlap between regions of high H₂ formation and PAH emission have been observed (Habart *et al.* 2003). PAHs can in the presence of H atoms become superhydrogenated (H-PAH) (Thrower 2012) and calculations presented by Rauls & Hornekær 2008 reveal zero-energy barriers towards H₂ formation via H-H abstraction even at low superhydrogenation degrees. Here we use thermal desorption experiments to examine superhydrogenation of the neutral PAH species, coronene (C₂₄H₁₂), pentacene (C₂₂H₁₄) and pentacenequinone, PQ, (C₂₂H₁₂O₂), and their possible catalytic effect on H₂ formation.

2. Experimental method

The H-PAH species were investigated using the temperature programmed desorption (TPD) technique under ultra high vacuum (UHV) conditions with a base pressure of low 10⁻¹⁰ mbar. A home-built Knudsen-type effusion cell, kept at temperatures ranging from 115-150 °C depending on species, was used to deposit multilayers of PAHs onto highly oriented pyrolytic graphite (HOPG). 2-3 multilayers were obtained after 2 minutes of deposition. Monolayers were consistently produced by heating the HOPG sample to 330-370 K depending on species, hereby removing only the multilayers. The monolayers

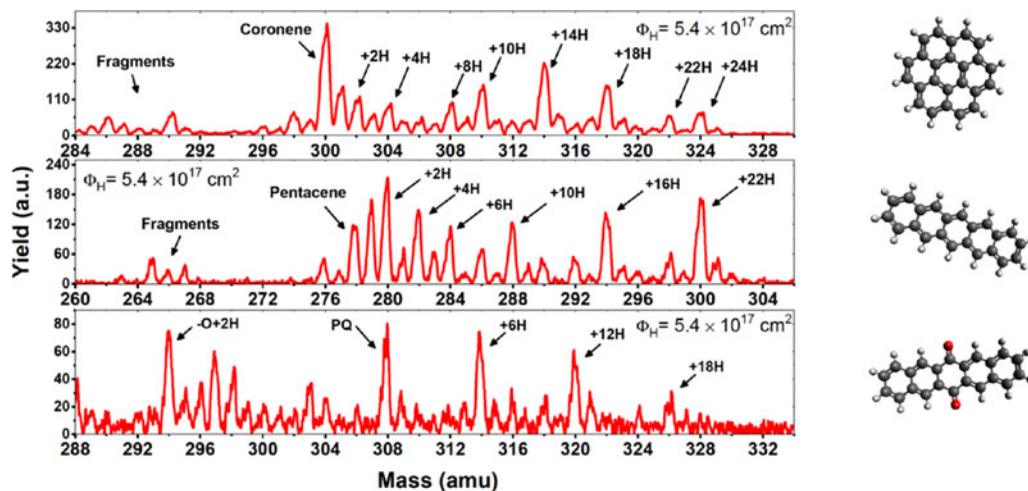


Figure 1. Three panels showing mass distributions of the PAHs coronene (top), pentacene (middle) and pentacenequinone/PQ (bottom) after being exposed to equal fluences of atomic hydrogen.

were then exposed to different fluences of atomic hydrogen (H) produced in a 2200 K hot hydrogen atomic beam source (HABS). The 2200 K hot H-atom beam is funnelled through a quartz nozzle which collisionally cools the beam to an estimated temperature of ≈ 1000 K. The TPD measurement was performed by heating the HOPG with a linear ramp of 1 K s^{-1} in front of a quadrupole mass spectrometer (QMS) (Extrel CMS LLC).

3. Results and Discussion

Figure 1 shows three mass spectra of the examined PAH species, coronene (top), pentacene (middle) and PQ (bottom) after being exposed to equal fluences of H-atoms. The mass spectra are obtained by integration of the TPD spectra within the given mass range over the relevant desorption temperature range. All three species exhibit high superhydrogenation degrees with both coronene and pentacene showing fully superhydrogenated product species at masses 324 ($\text{C}_{24}\text{H}_{36}$) and 300 ($\text{C}_{24}\text{H}_{36}$), respectively. The PQ does not become fully superhydrogenated ($\text{C}_{22}\text{H}_{34}\text{O}_2$, mass 330) and the H-PQ ends as H-pentacene. This result is consistent with the observed oxygen abstraction. Generally, species with even mass are more prominent than species with odd mass. This too is consistent with the expectations as the odd mass species have an open shell and hence behave as radicals. Furthermore, the breaking of conjugated rings in the PAH molecule by the addition of an H-atom seems to have a higher barrier and is observed in the mass spectra as 6 amu peak separations (Jensen *et al.* 2019).

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