Interaction of oxygen functionalised PAHs with H atoms

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AARHUS UNIVERSITET

europAH
the extensive and ubiquitous role of polycyclic aromatic hydrocarbons in space

Horizon2020, Grant number 722346

Introduction



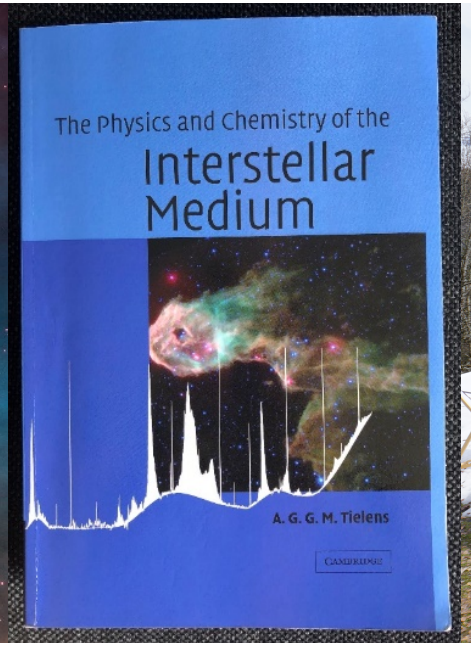
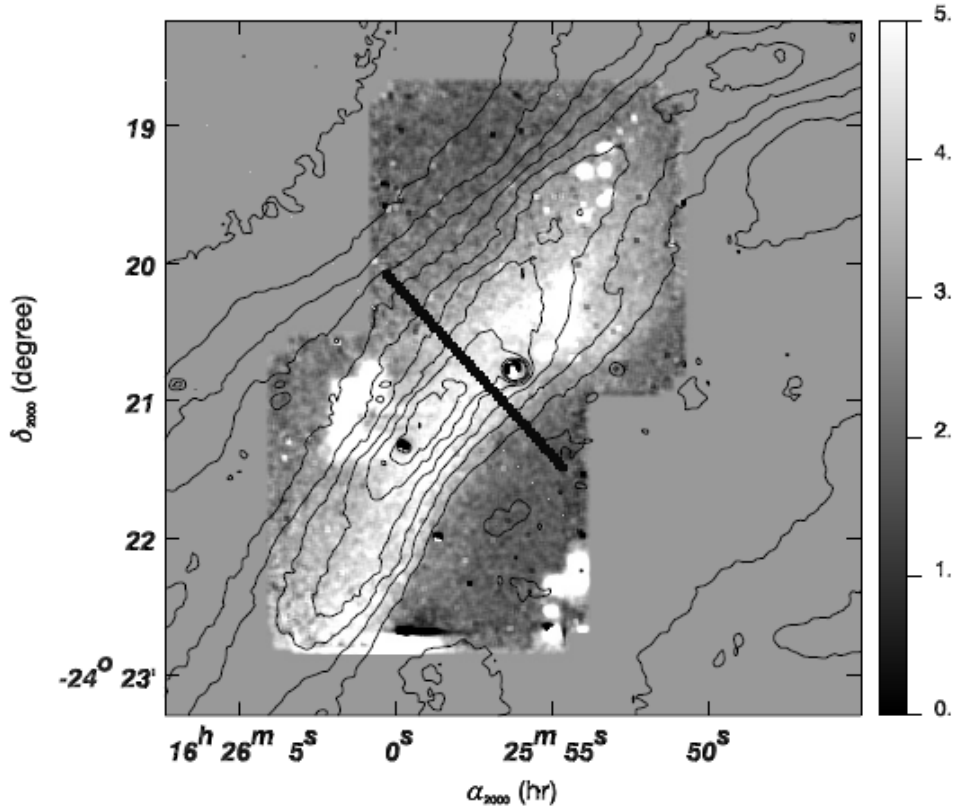






Image Credit & Copyright: Mario Zauner

PAHs as catalysts in PDRs



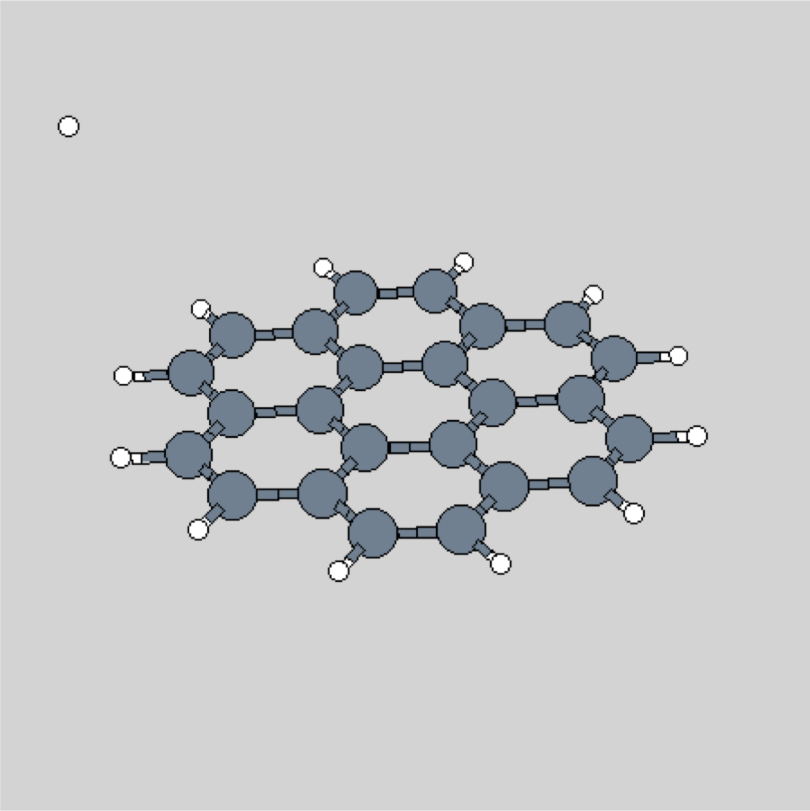
H_2 emission – grey scale
PAH emission – contours

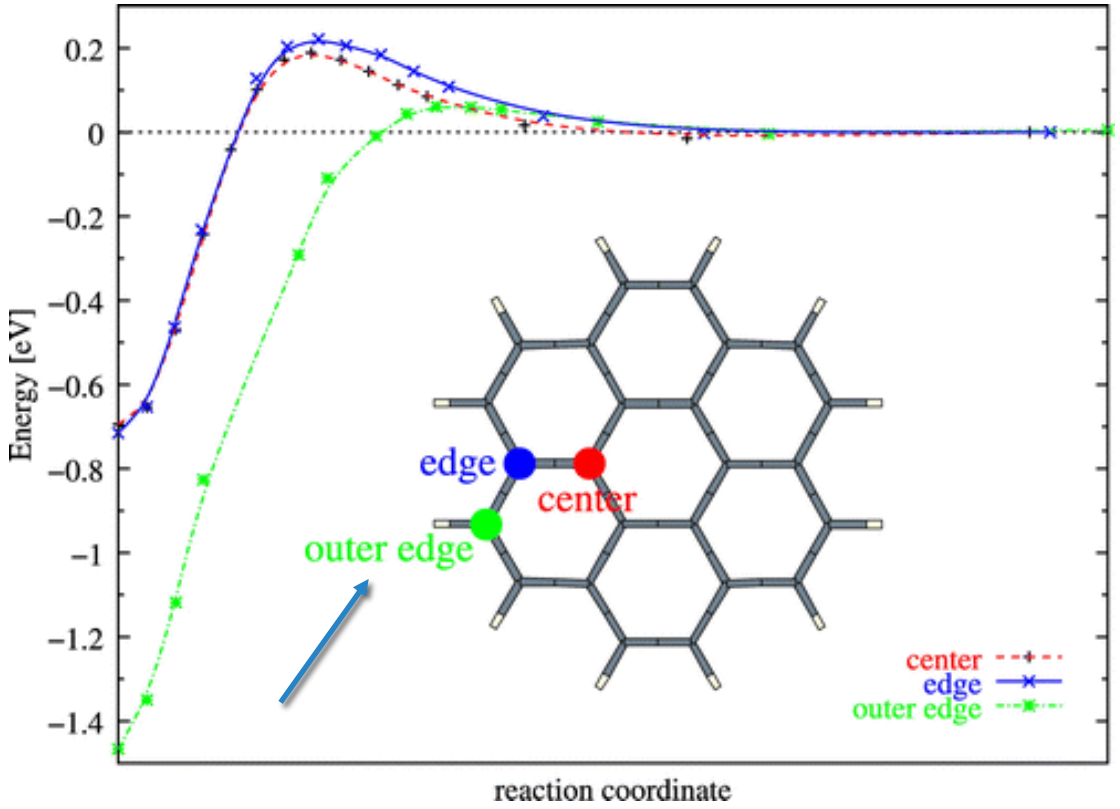
Correlation between PAH emission and high H_2 formation rates in PDRs with low UV flux

PAHs as catalysts for H_2 formation ?

Habart et al., 2004, Habart et al., 2003

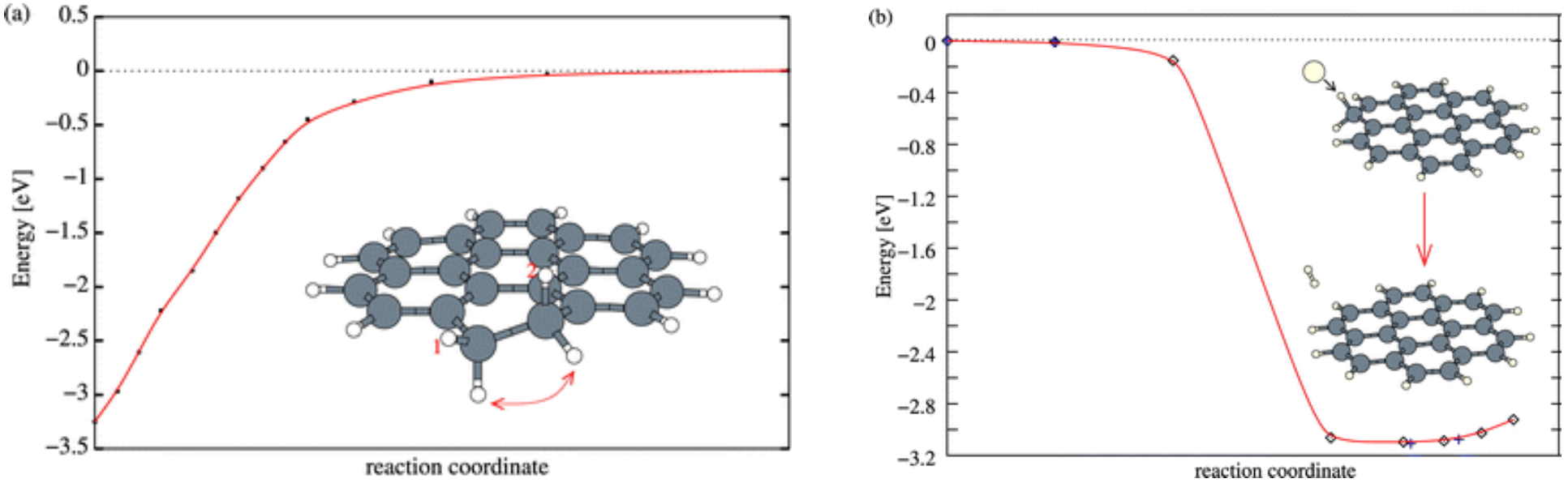
Neutral PAHs as catalysts





Rauls and Hornekær 2008, Pauzat & Ellinger 1994; Bauschlicher et al. 1998; Le Page et al. 2009;

Neutral PAHs as catalysts

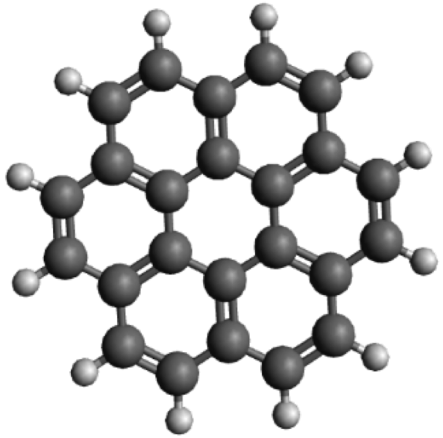


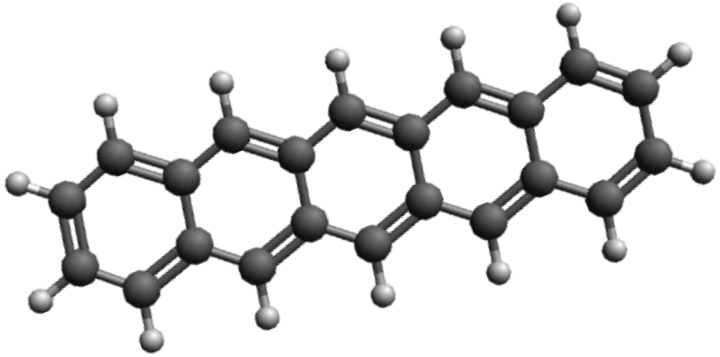
At higher superhydrogenation levels Density Functional Theory (DFT) calculations reveal low or zero barrier routes to nH-PAH formation and nH-PAH catalyzed H_2 formation

Rauls and Hornekær 2008

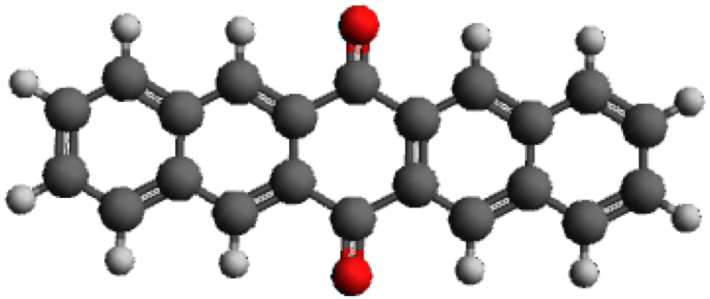
PAHs of interest

Coronene
- Mass 300 amu
- Arm chair edges



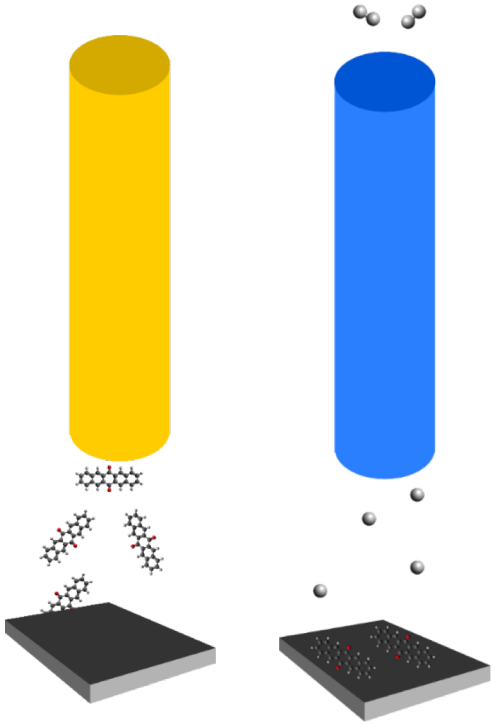


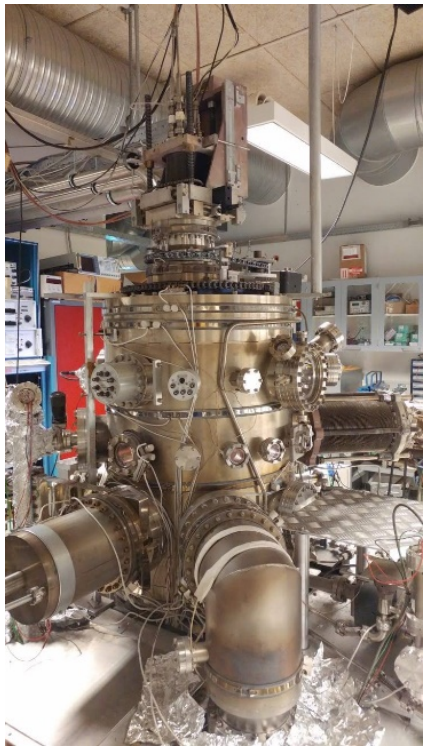
Pentacene
- Mass 278 amu
- Linear
- Zig-zag edges



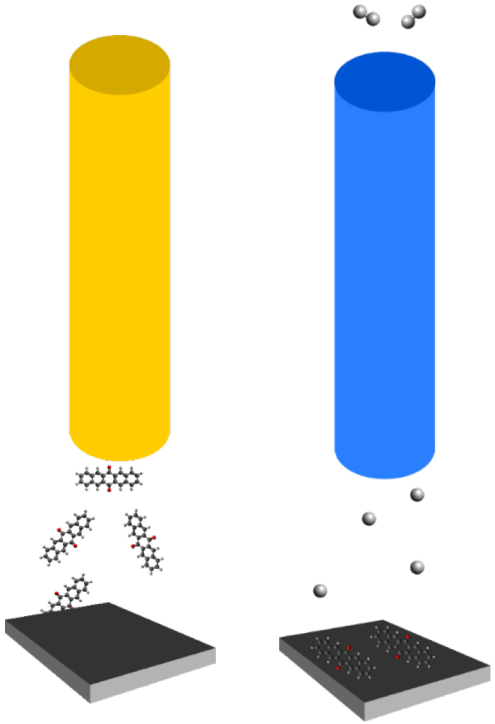
Pentacenequinone (PQ)
Mass 308 amu

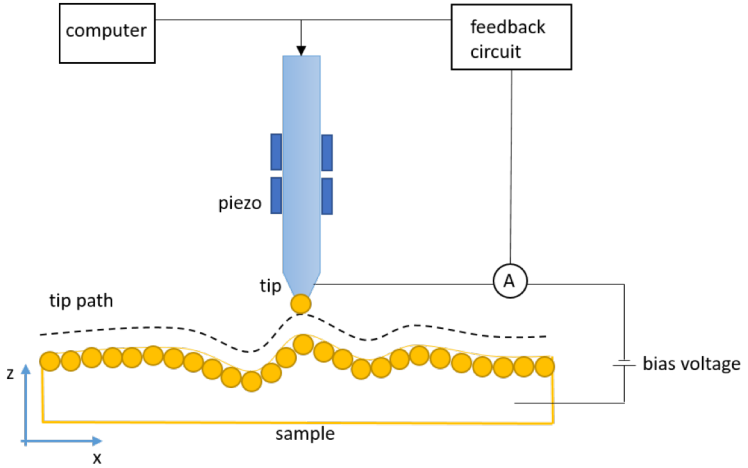
Studying Neutral PAHs in the Lab

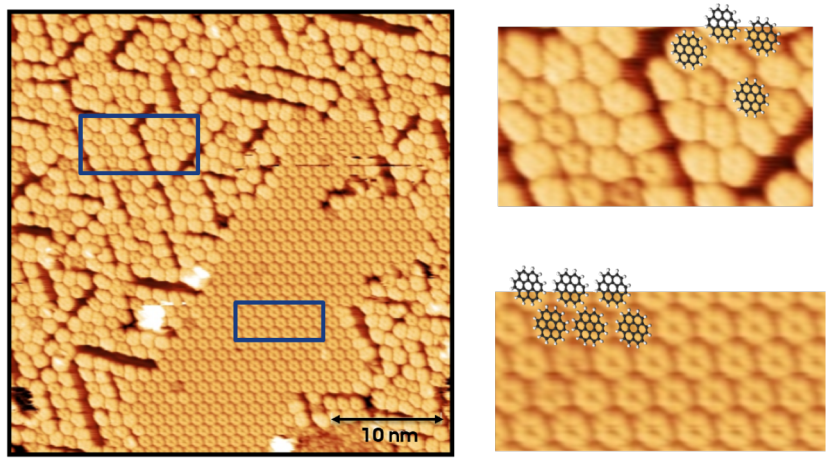




Studying Neutral PAHs in the Lab

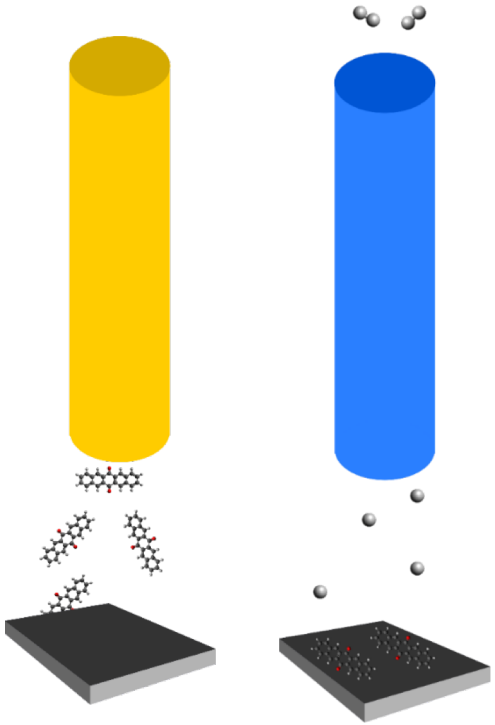


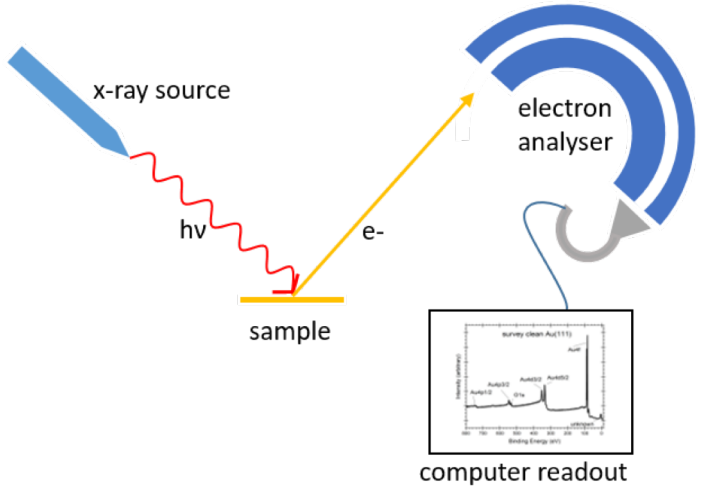


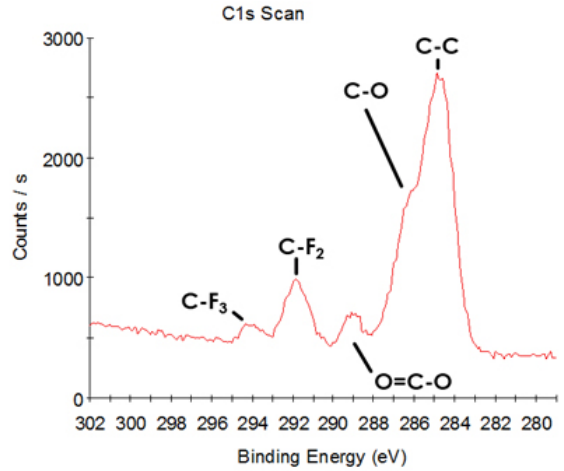


STM Image Credit: F D S Simonsen

Studying Neutral PAHs in the Lab

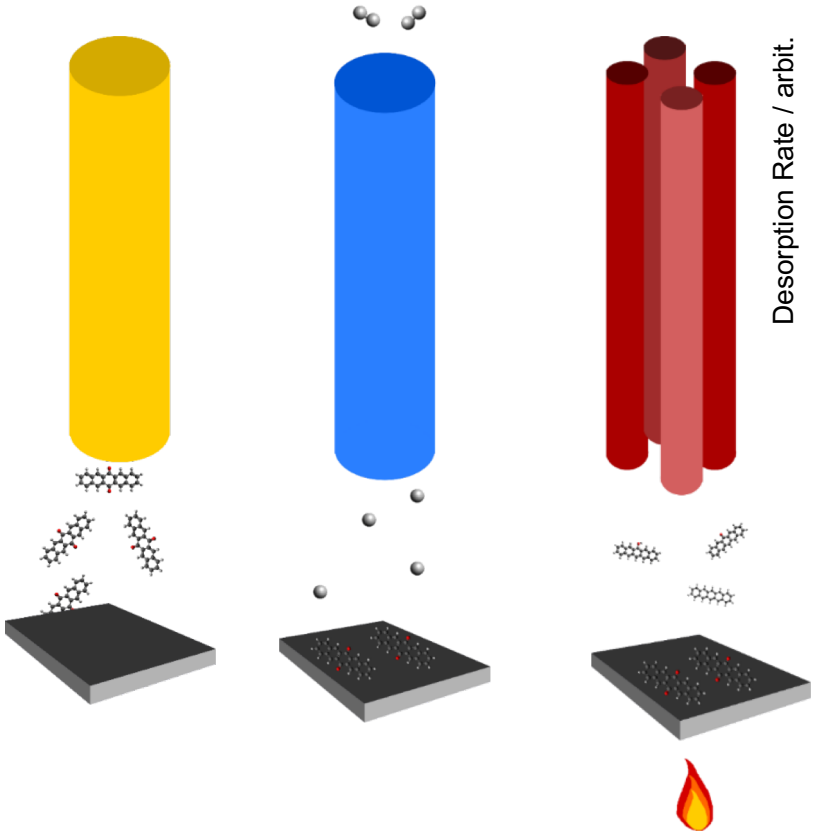


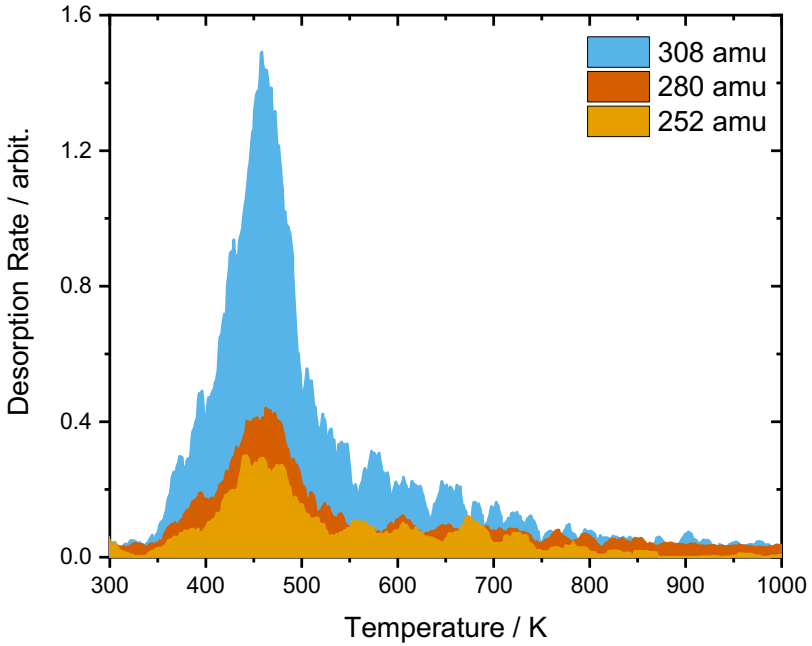




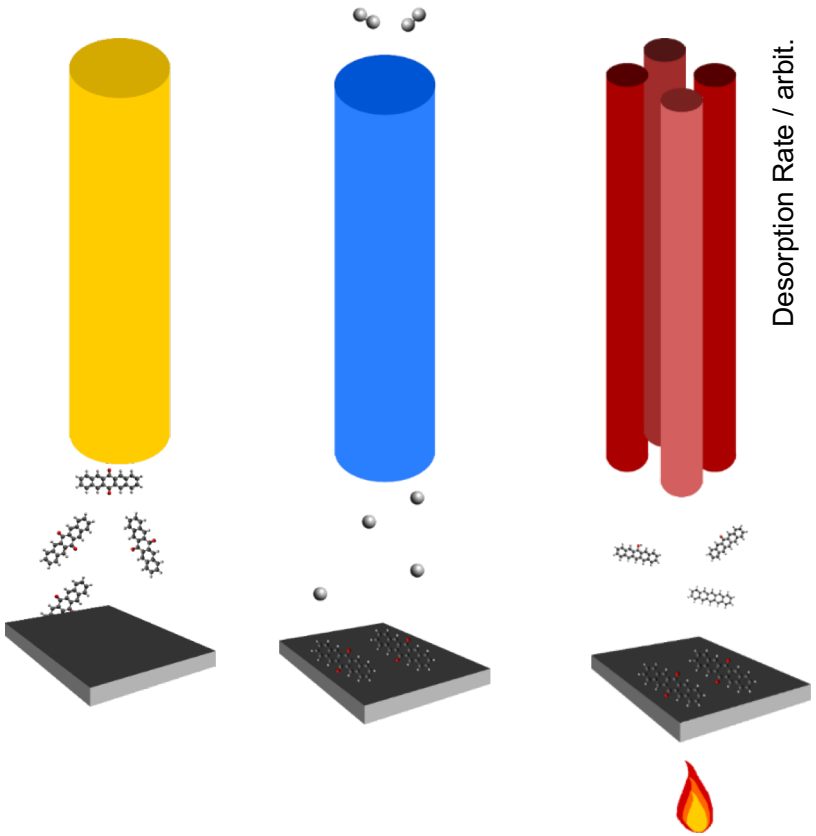
XPS Image Credit: CovalentMetrology

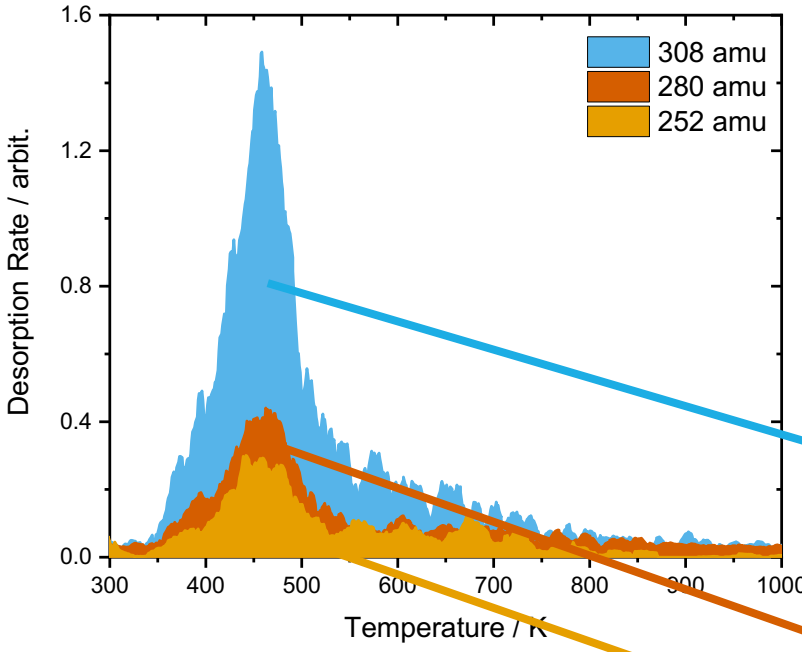
Studying Neutral PAHs in the Lab

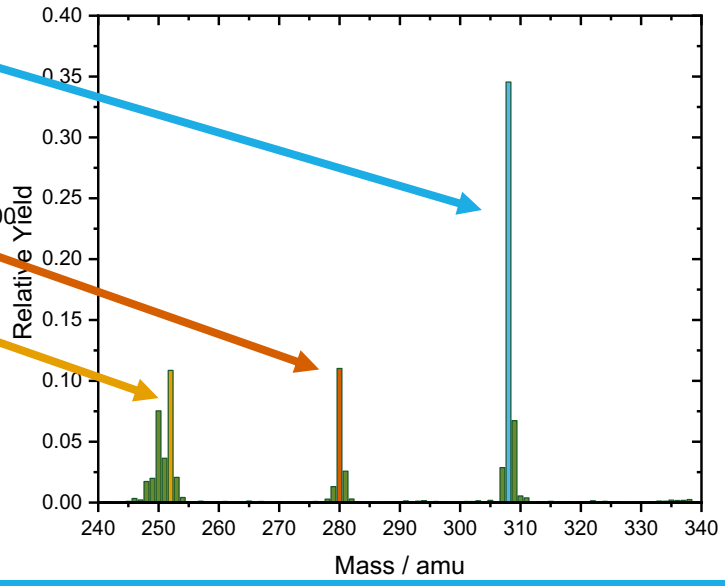




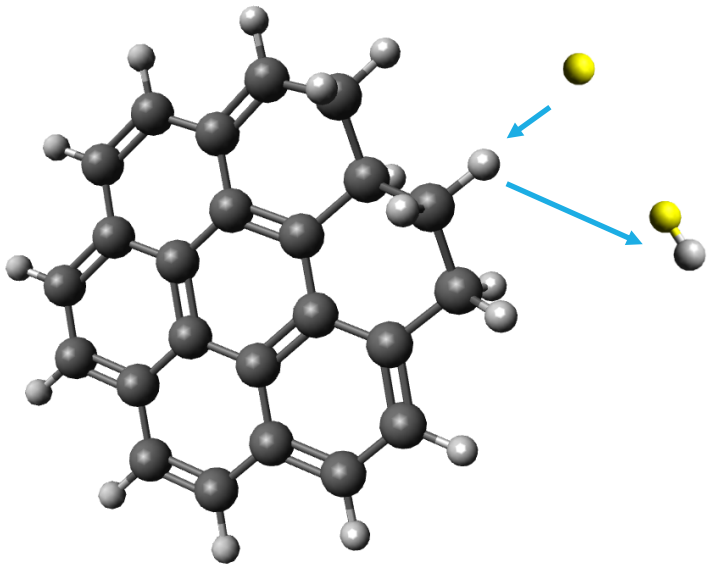
Studying Neutral PAHs in the Lab



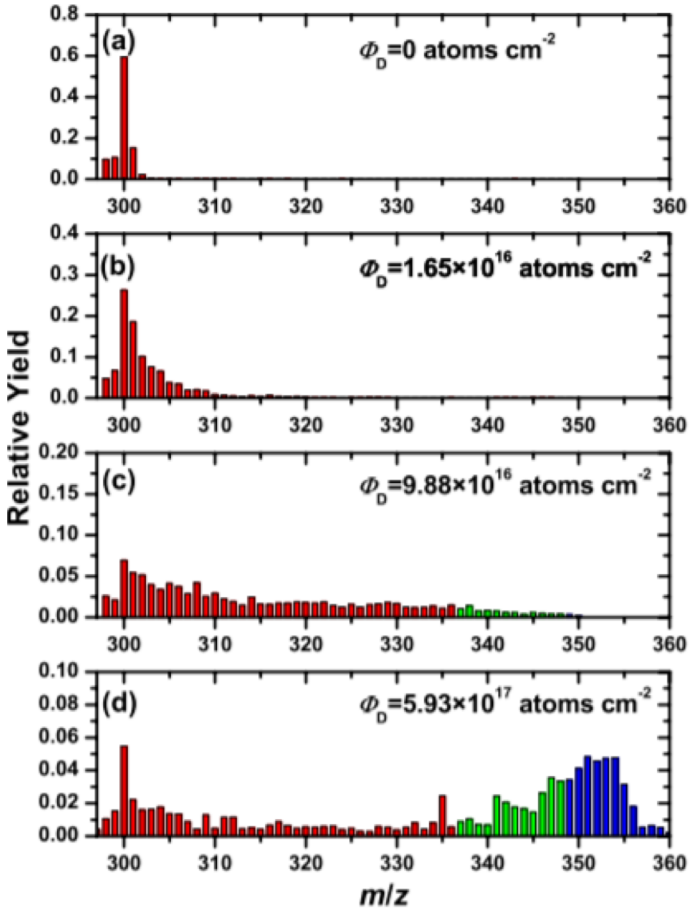




Coronene as catalyst in H_2 formation



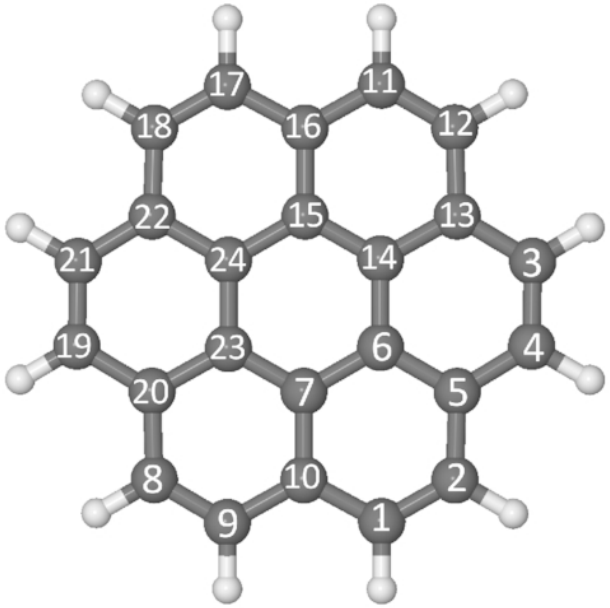
- Superhydrogenated coronene can be formed
- Evidence for formation of H_2 by abstraction

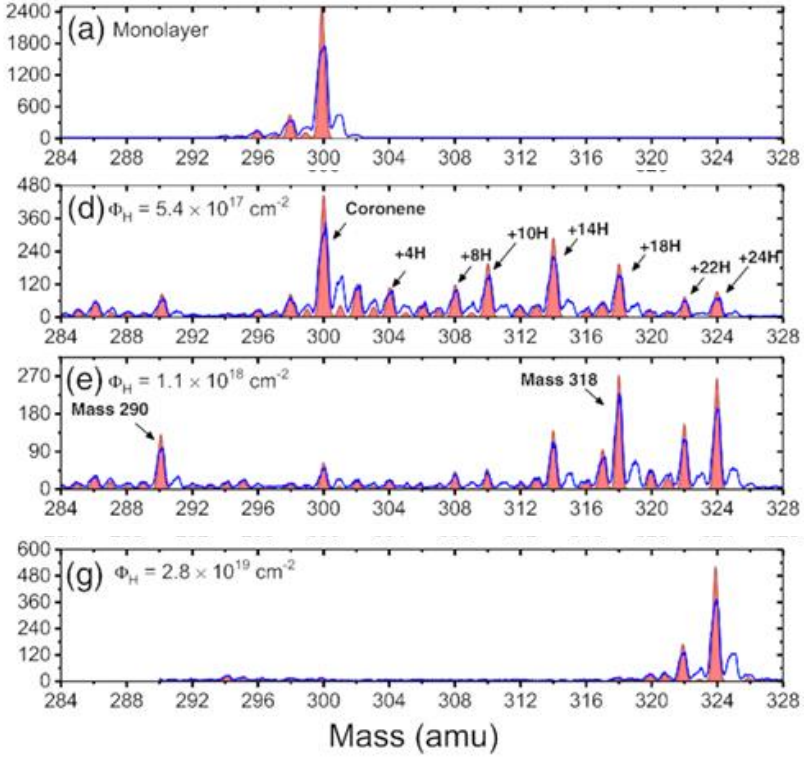


Thrower et al., 2012
Skov et al., 2014
Skov et al., 2016
Jensen et al. 2019

Interaction of Coronene with H

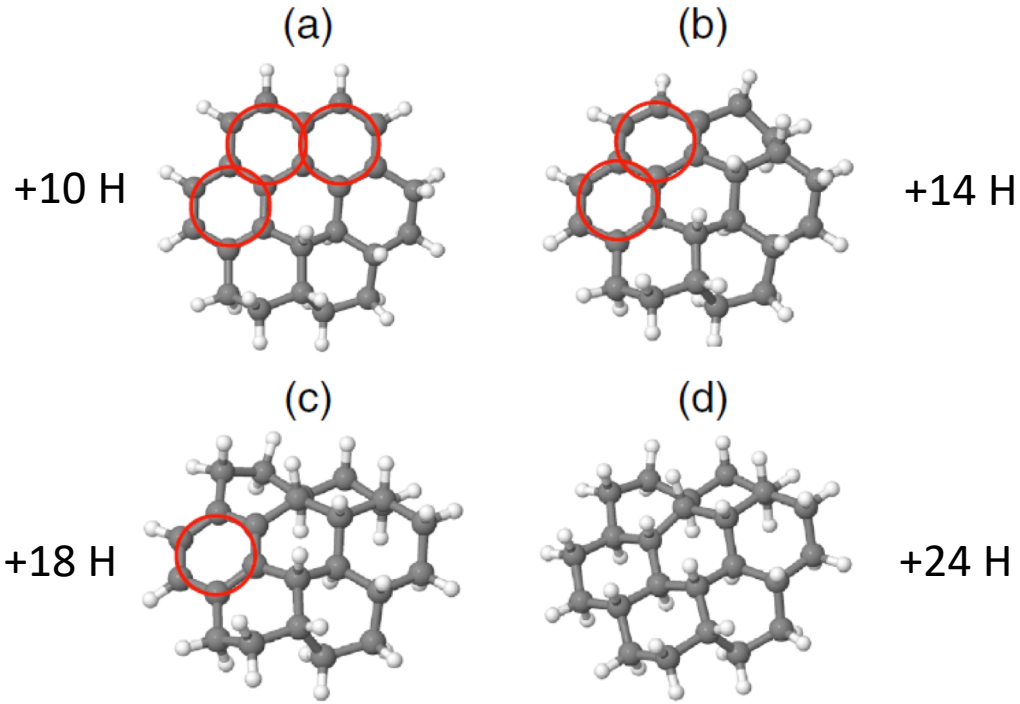
Peaks at specific masses indicate
1) Certain nH-PAH configurations are more stable than others
2) Sizeable barriers for further additions exist



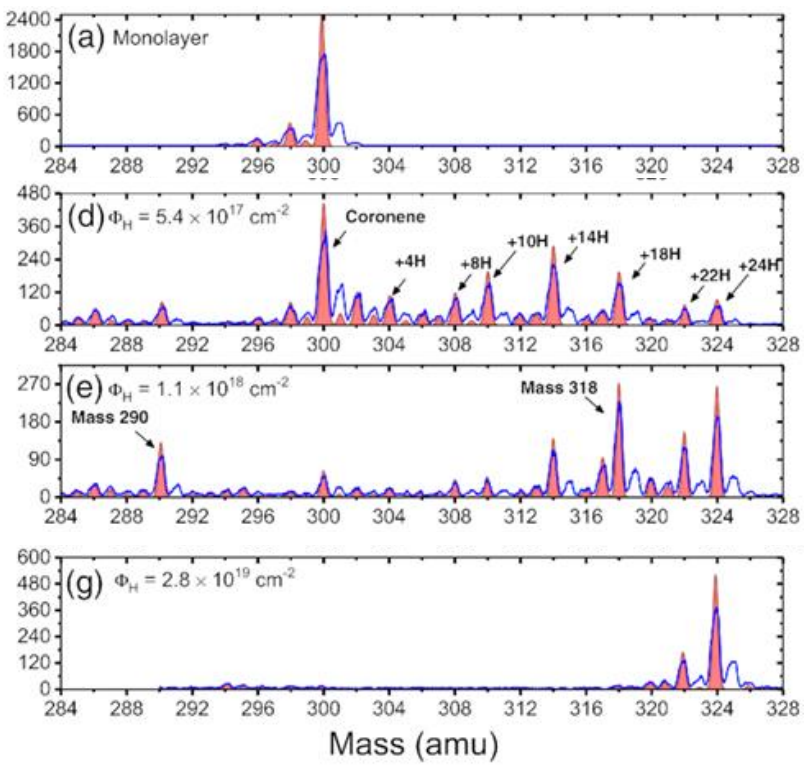


Jensen et al. 2019

Interaction of Coronene with H

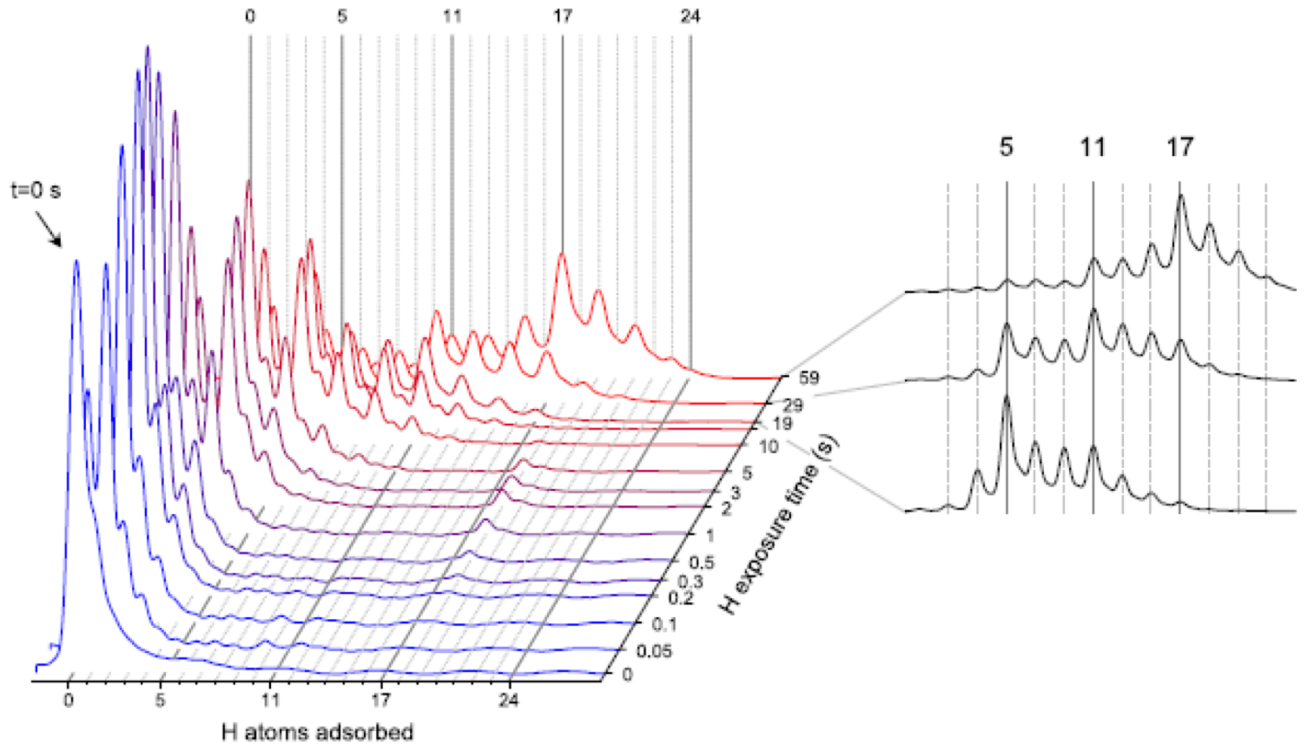


Residual aromaticity



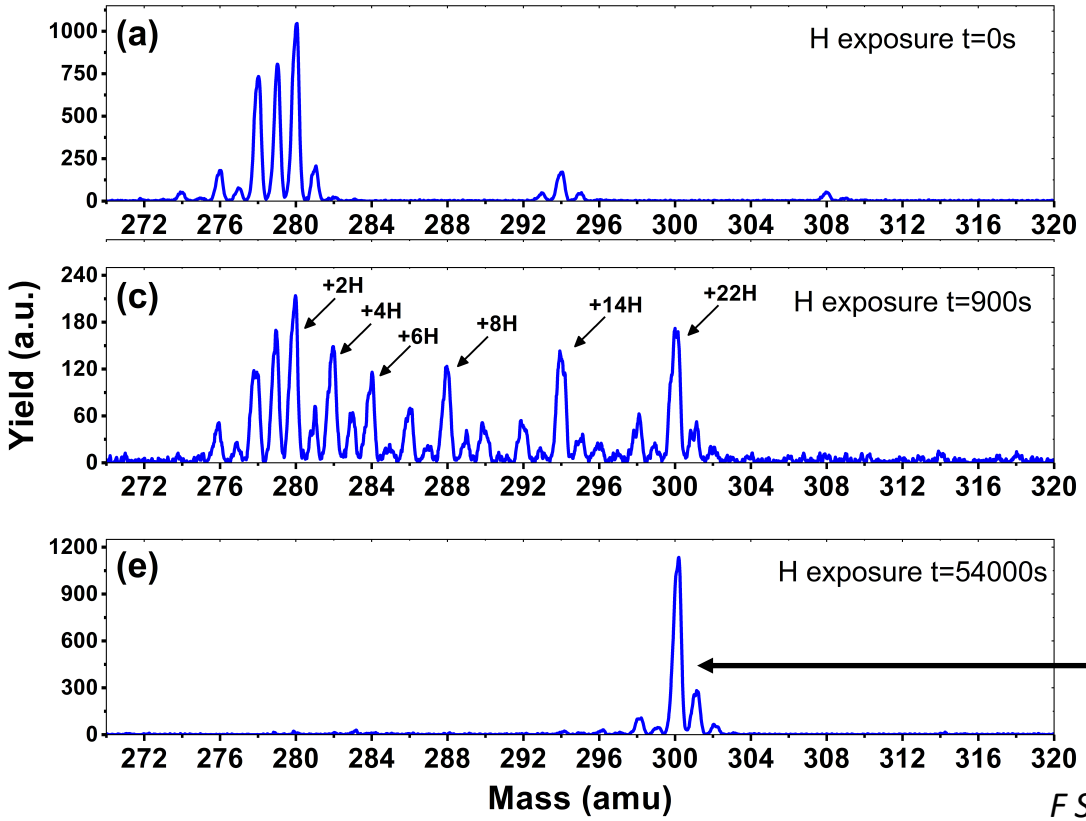
Jensen et al. 2019

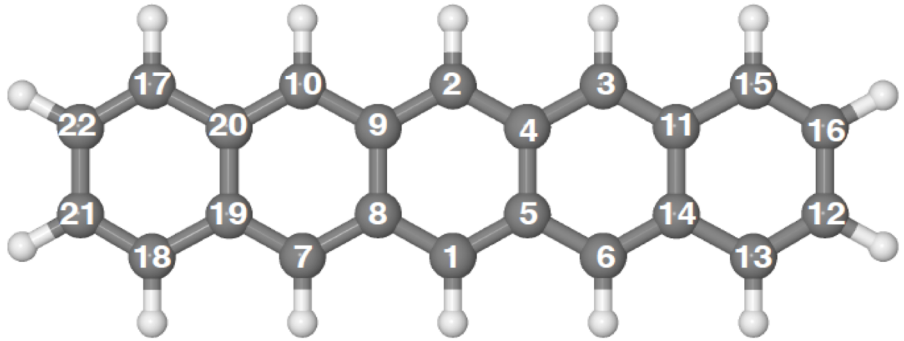
Interaction of Coronene Cation with H



Cazaux et al. 2016

Interaction of Pentacene with H

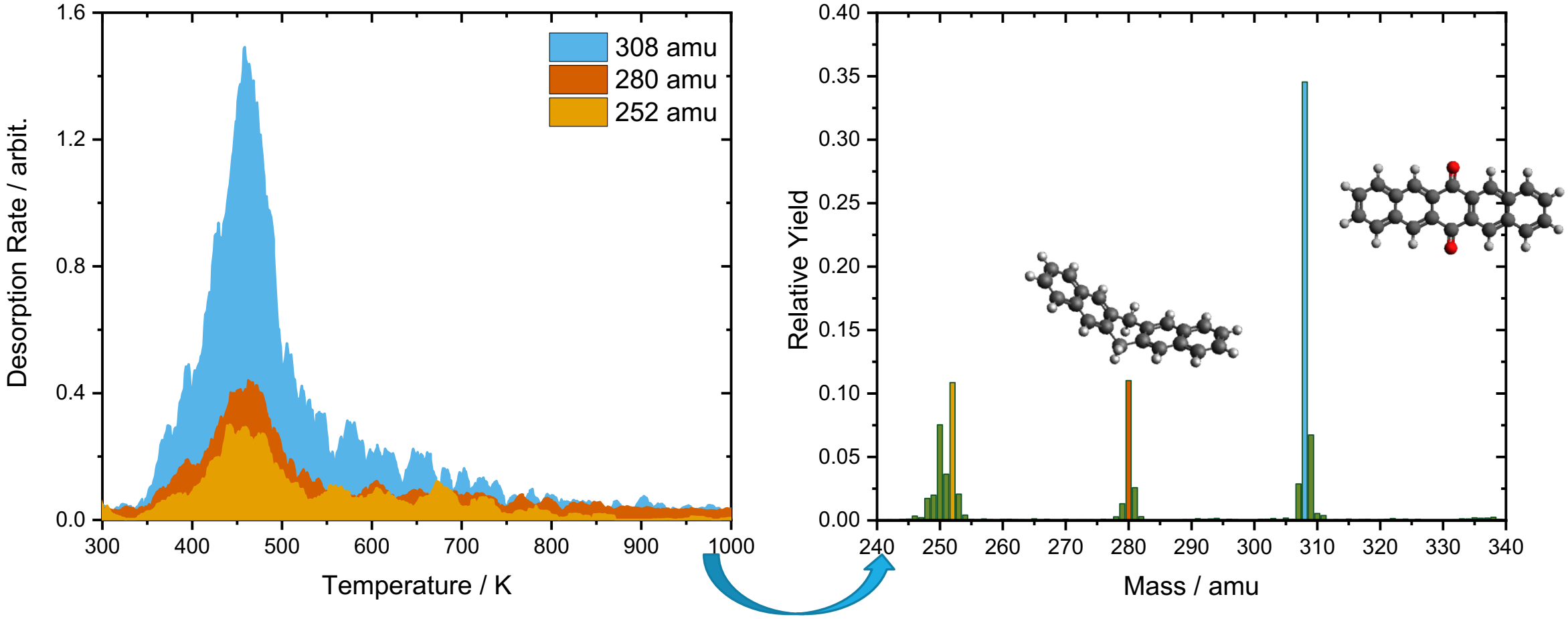




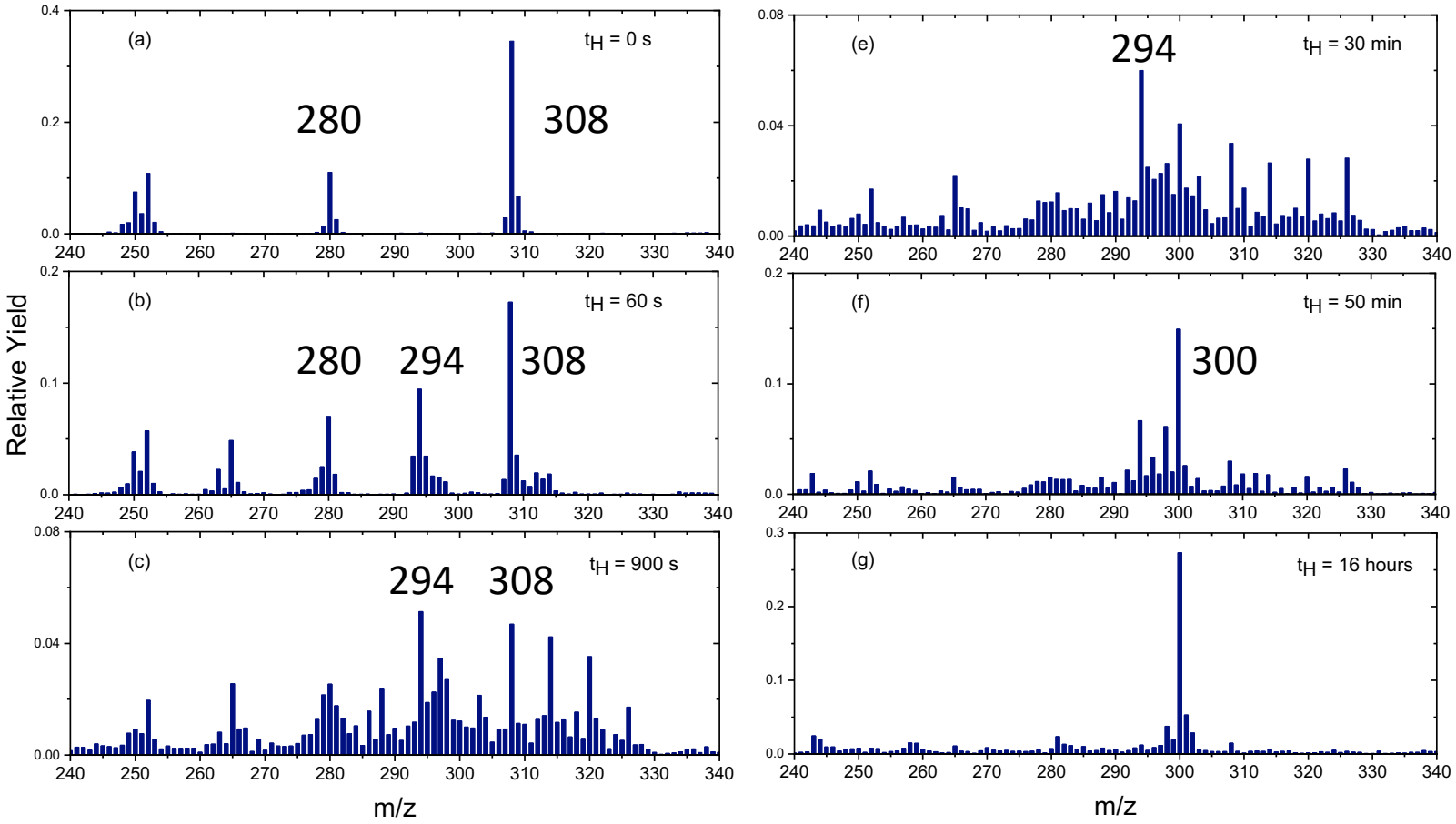
Fully superhydrogenated pentacene

F Simonsen, M Bulak, S Banhatti, G Wenzel, J D Thrower, J Palotas, R Delan, L M Fabiani D Campisi

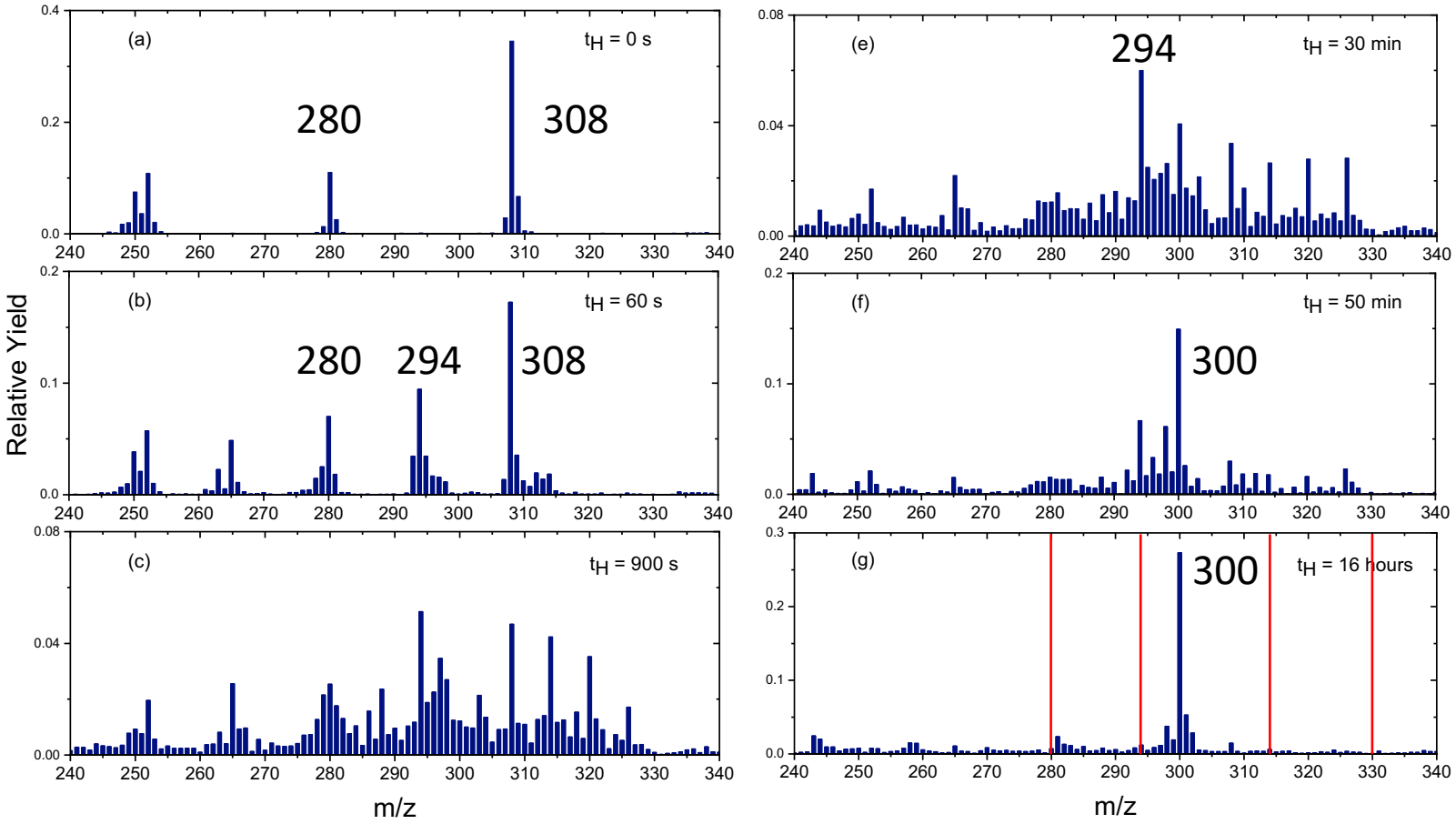
Pentacenequinone (PQ) Monolayer

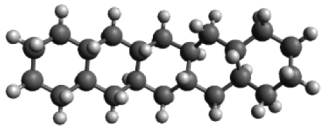


Interaction of PQ with H

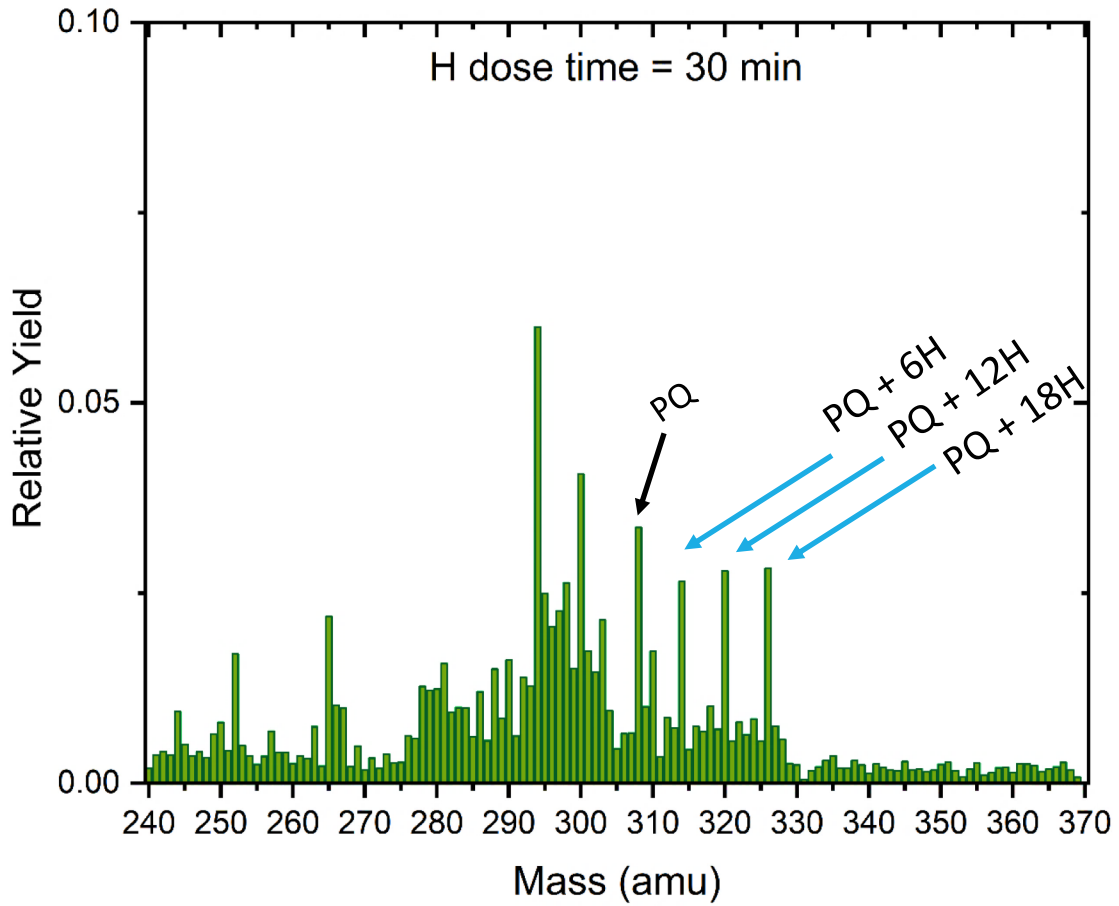


Interaction of PQ with H

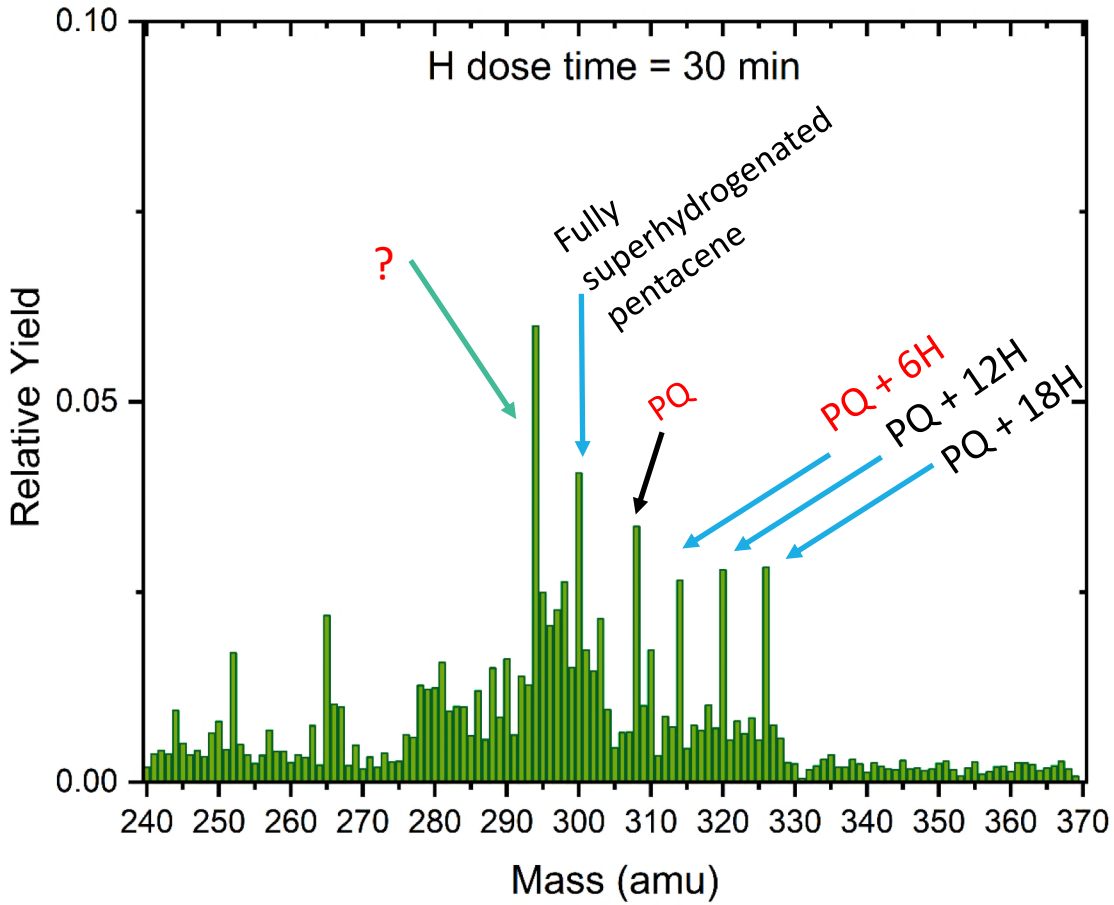




Important Masses

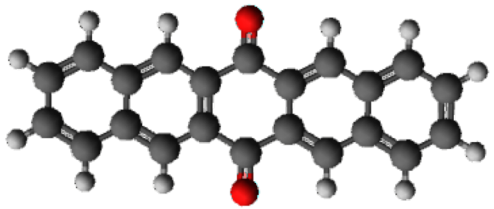


Important Masses



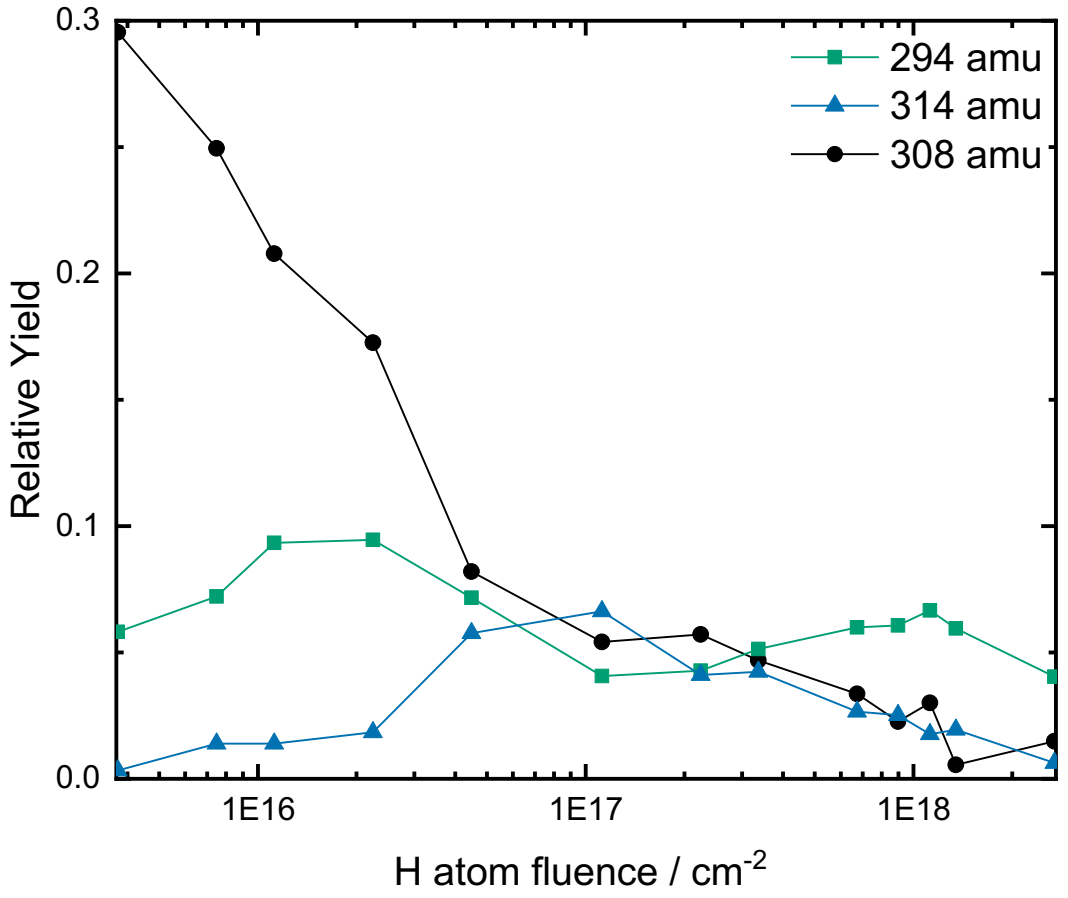
Products of PQ Hydrogenation

Abstraction

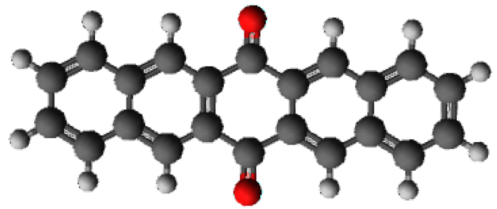


+ H

Pentacen-6-one/
Pentacen-6-ol



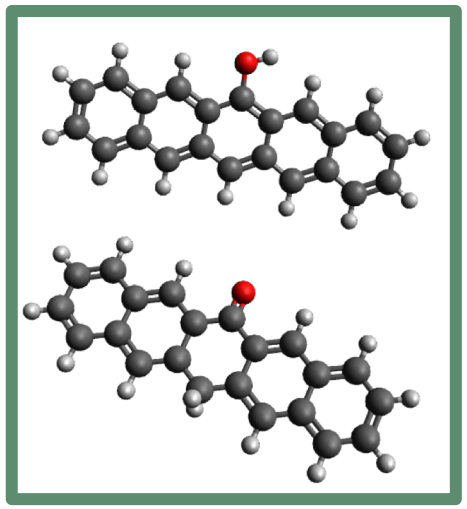
Addition

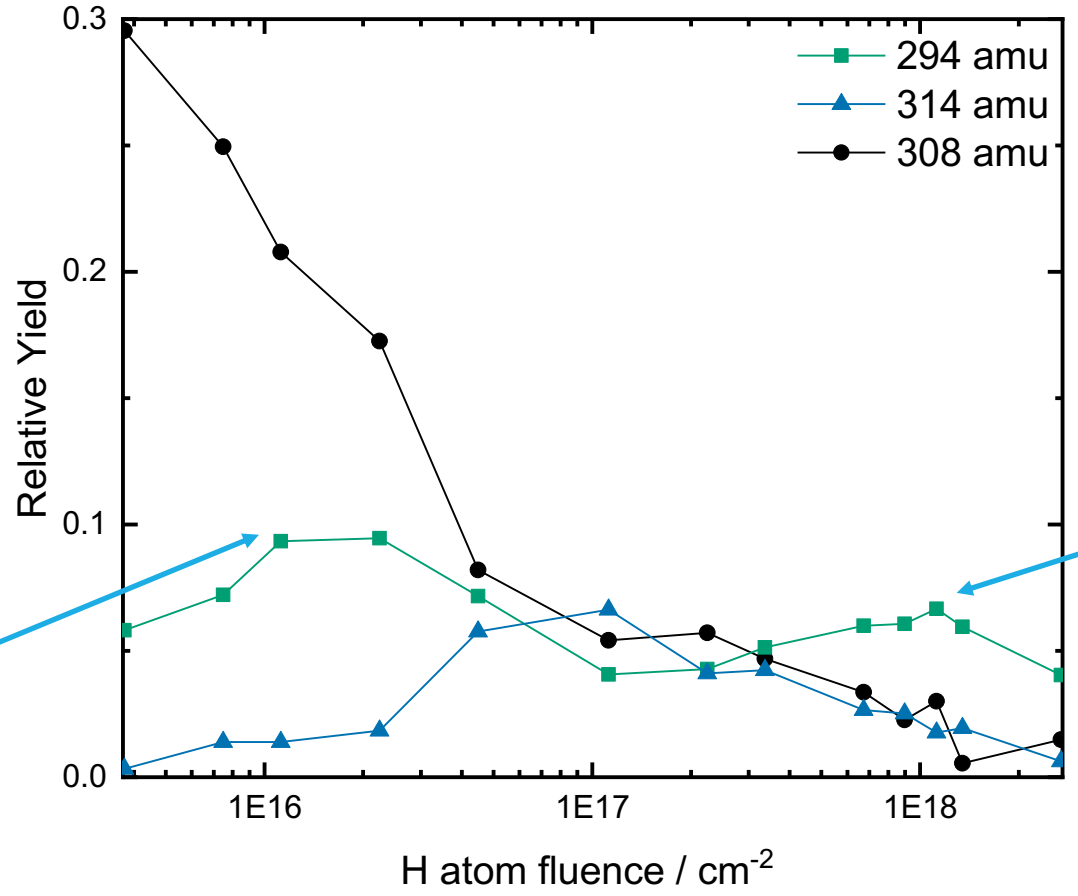


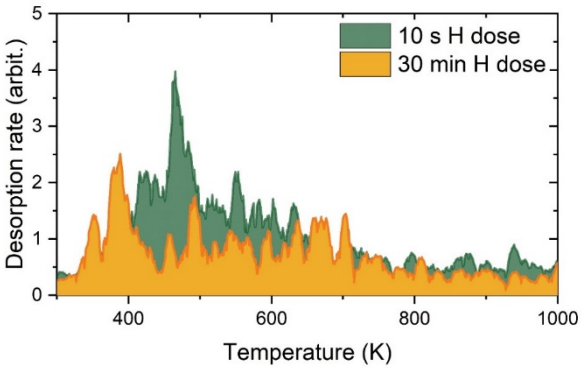
+ H

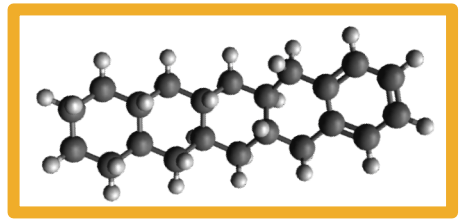
Superhydrogenated PQ

Products of Hydrogenation



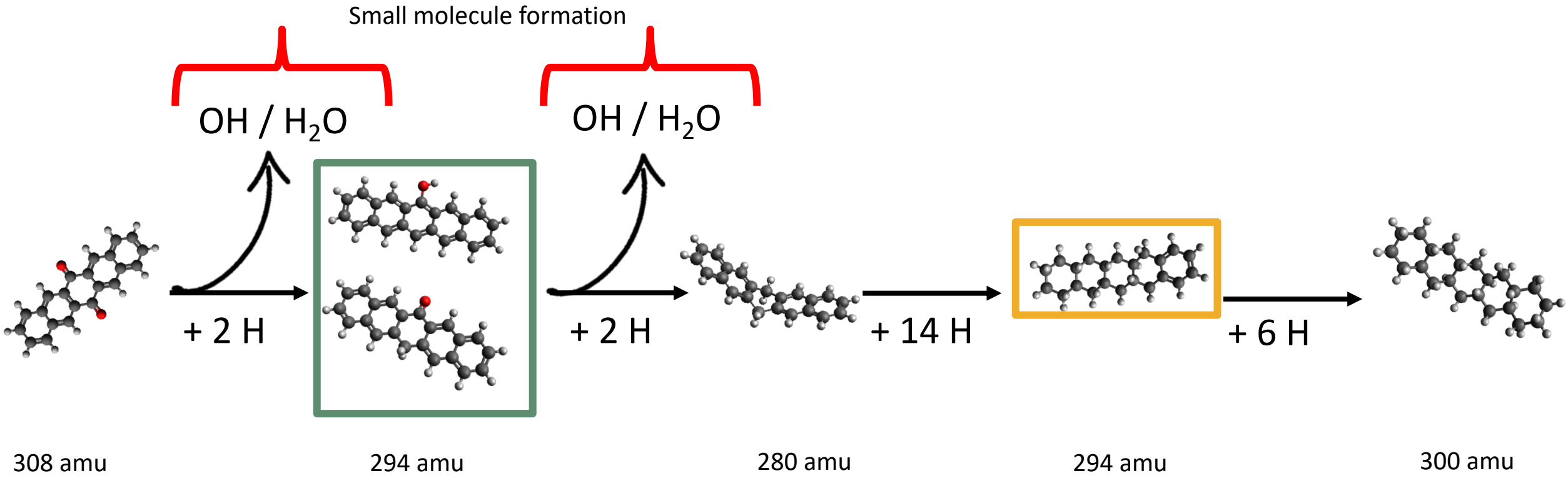




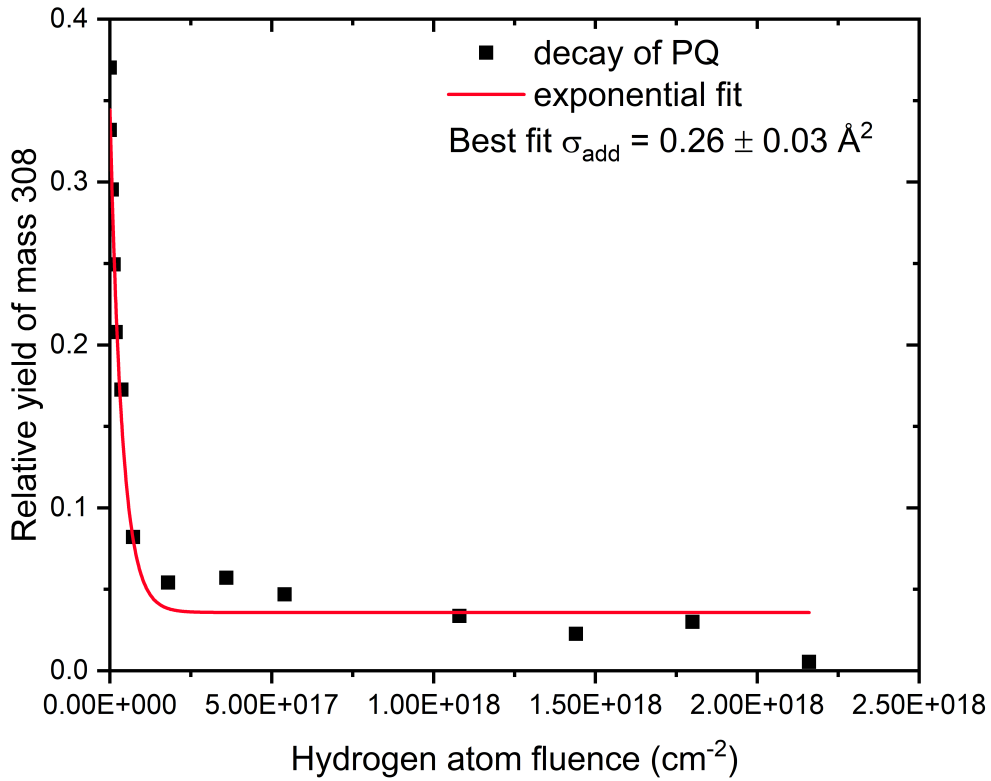


Pentacene + 14 H

Loss of O vs addition of H



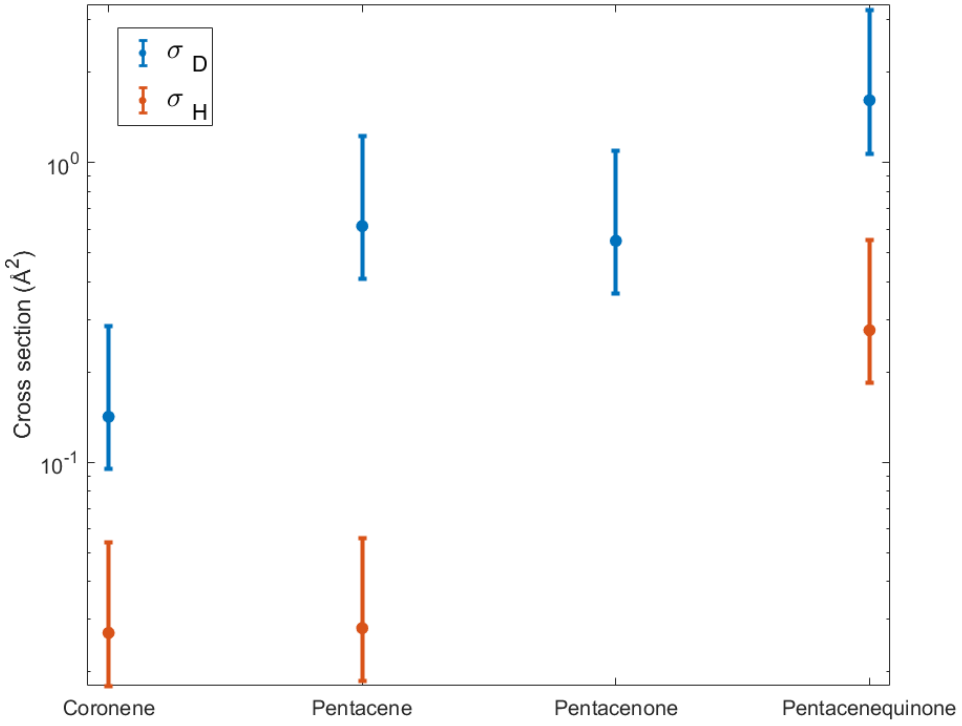
Reaction Cross Section

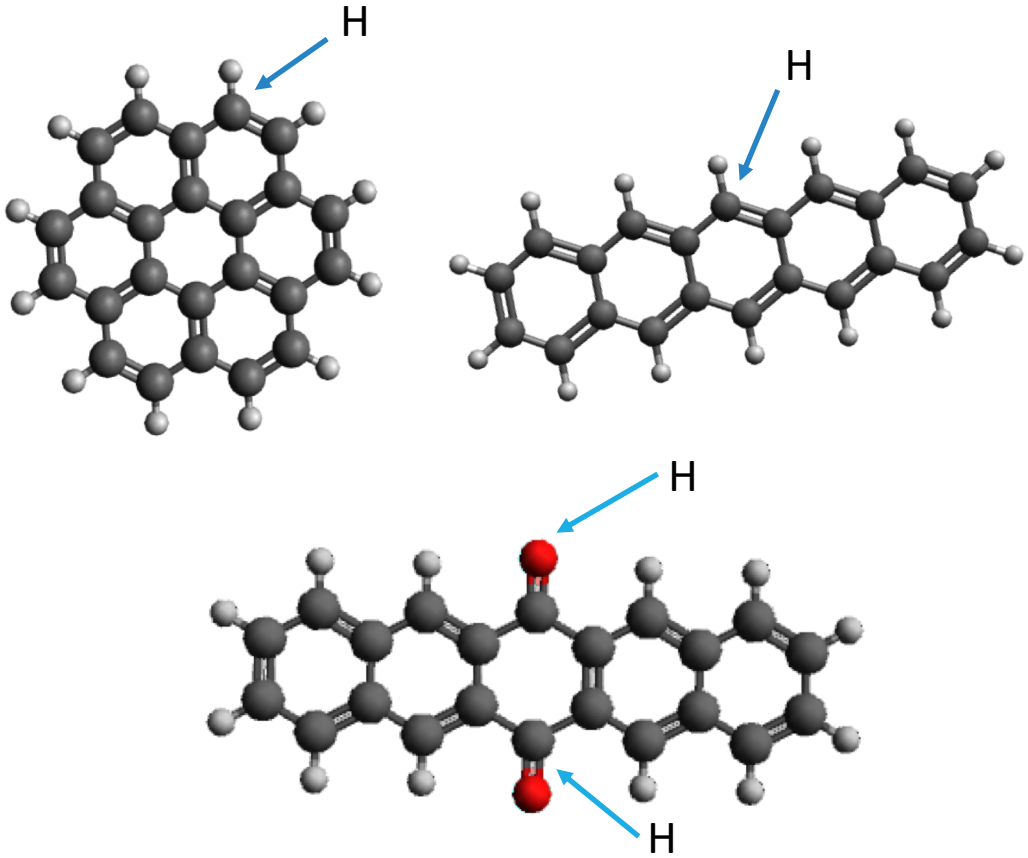


First order reaction kinetics:

$$I = I_0 \, e^{-\sigma\Phi} + I_\infty$$

Reaction Cross Section

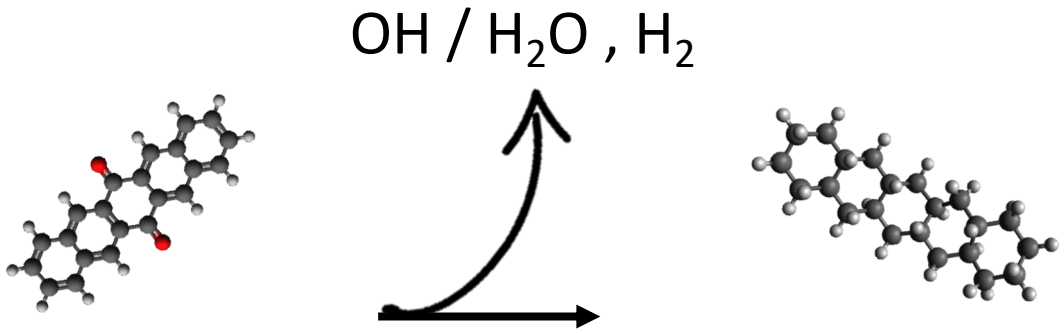




Simonsen et al., (in prep.)

Summary

- Reaction cross section is higher for oxygen functionalised pentacene
- Interaction of oxygen functionalised pentacene with H atoms leads to loss of oxygen atoms presumably in the form of OH / H_2O
- Upon H irradiation, oxygen functionalised pentacene is driven towards fully superhydrogenated pentacene



Acknowledgements

SDL group at Aarhus University



AARHUS UNIVERSITET

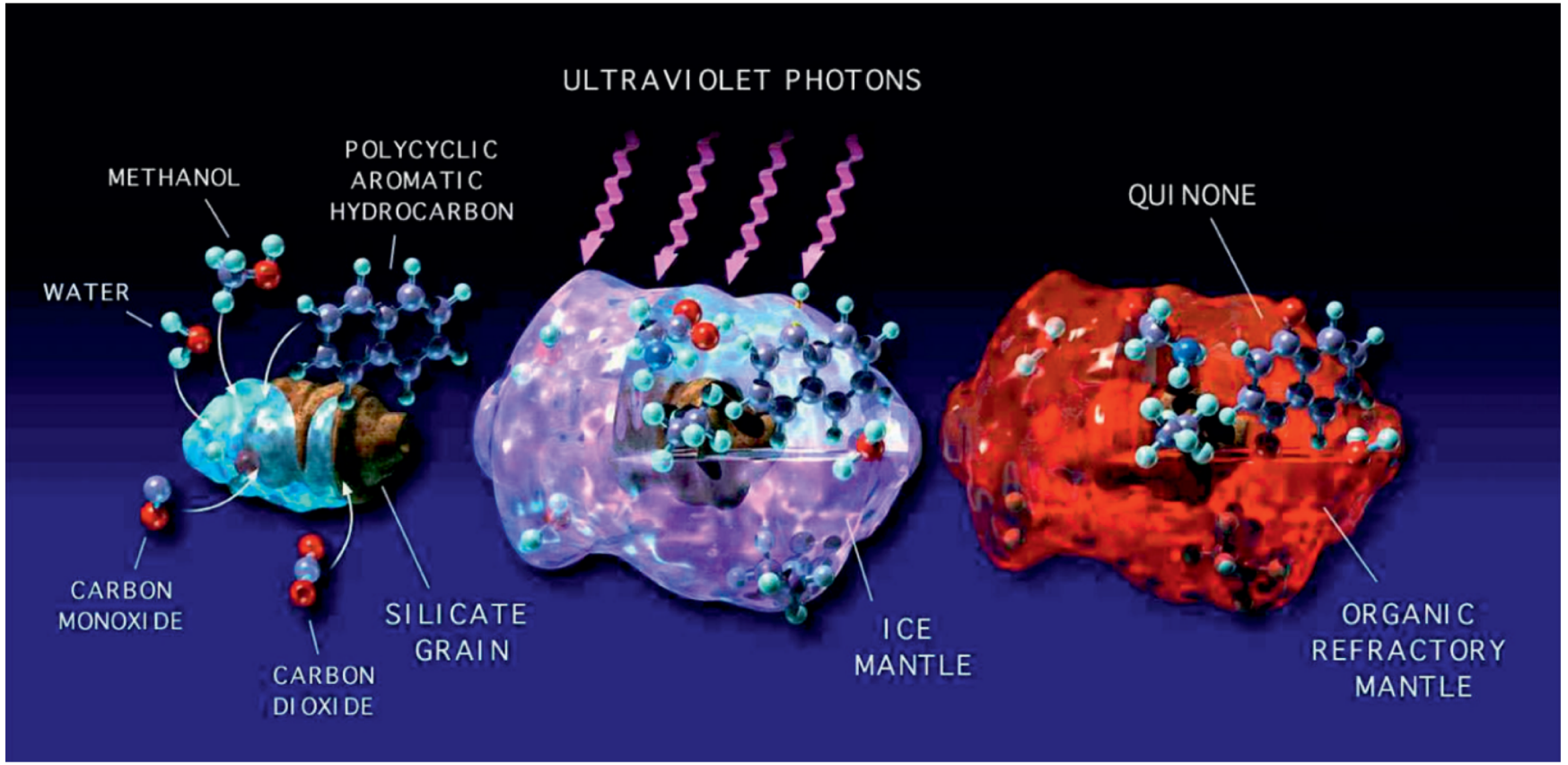
Collaborations within EUROPAH



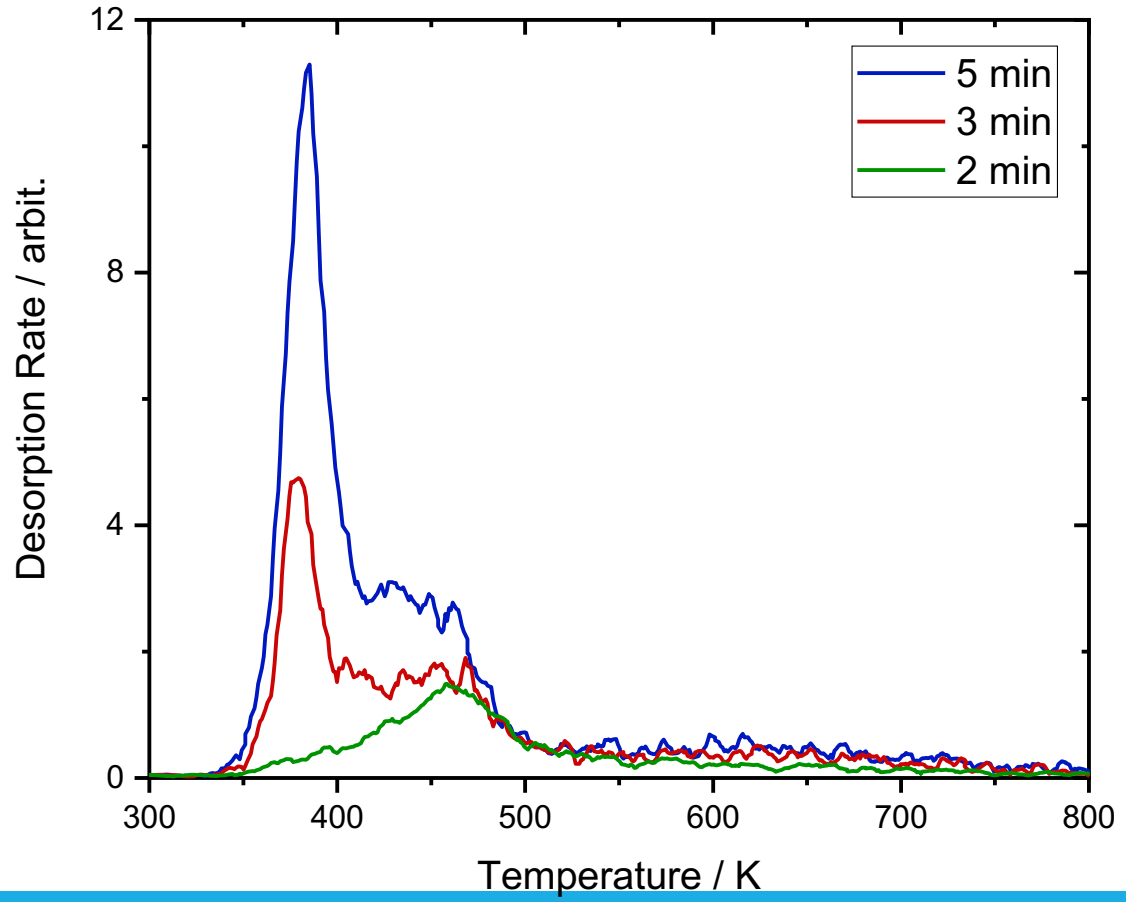


Horizon2020, Grant number 722346

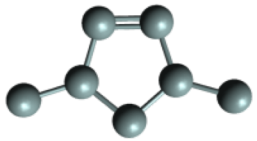
Why PQ ?


ULTRAVIOLET PHOTONS
METHANOL
POLYCYCLIC AROMATIC HYDROCARBON
WATER
QUINONE
CARBON MONOXIDE
CARBON DIOXIDE
SILICATE GRAIN
ICE MANTLE
ORGANIC REFRACTORY MANTLE

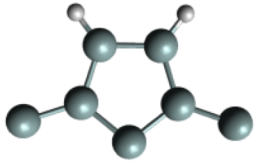
How to make a monolayer ?



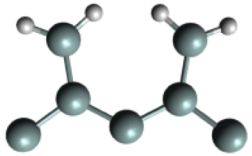
H Atom Flux calibration



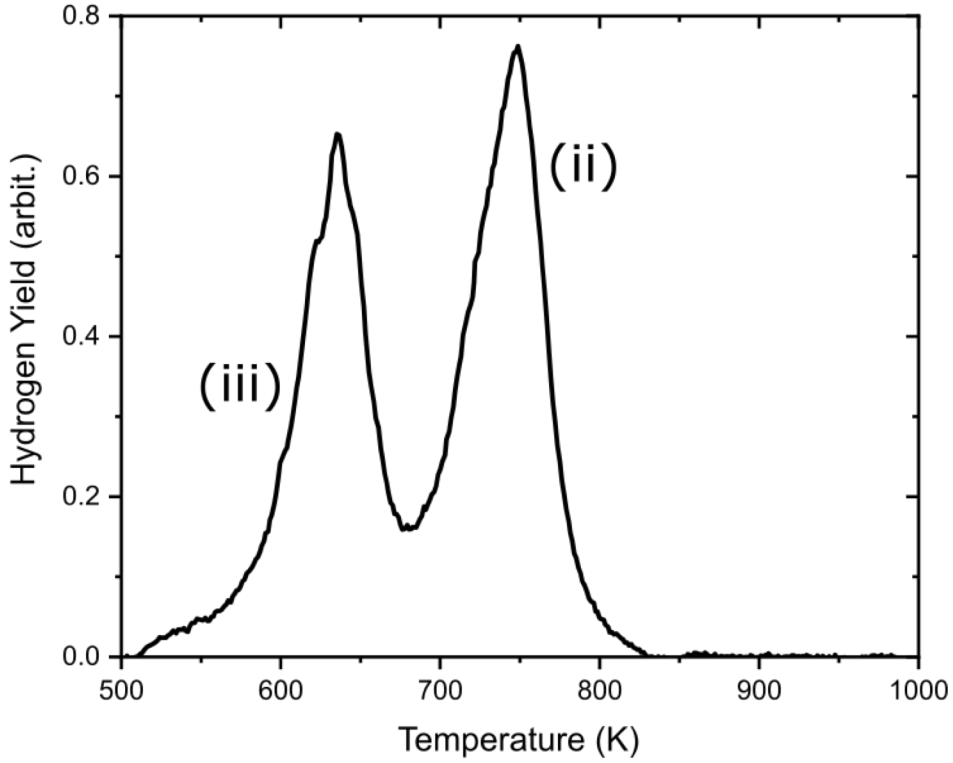
(i) Si (100) 2x1



(ii) Monohydride species



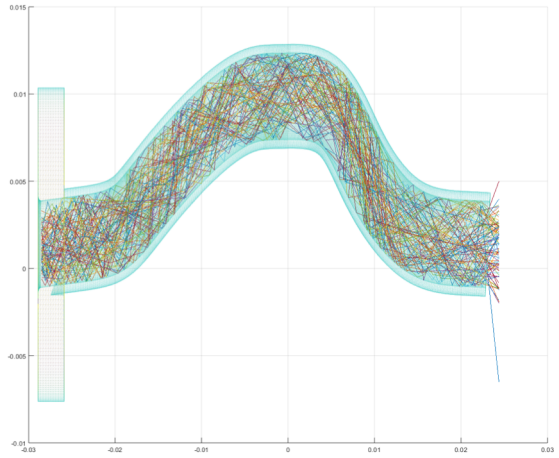
(iii) Dihydride species

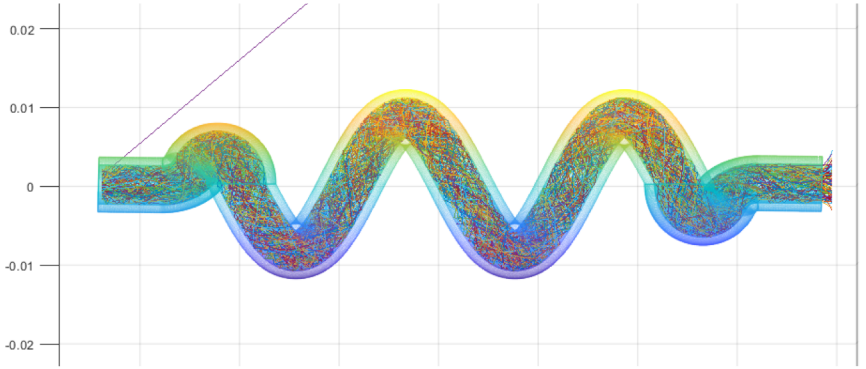


Nozzle Simulations



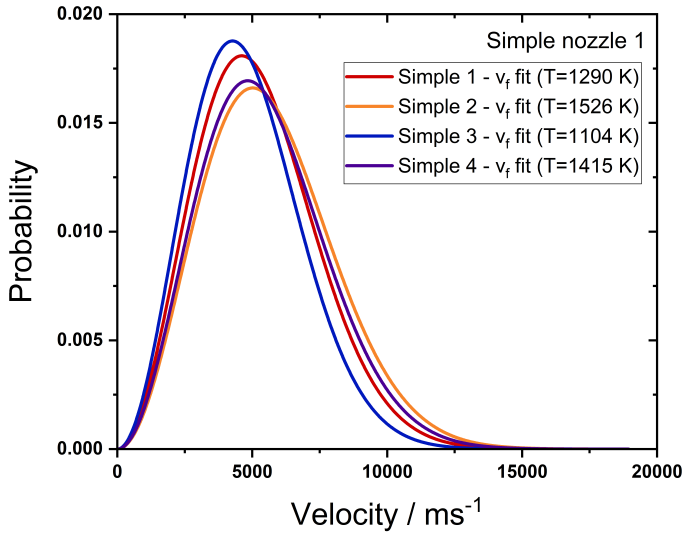






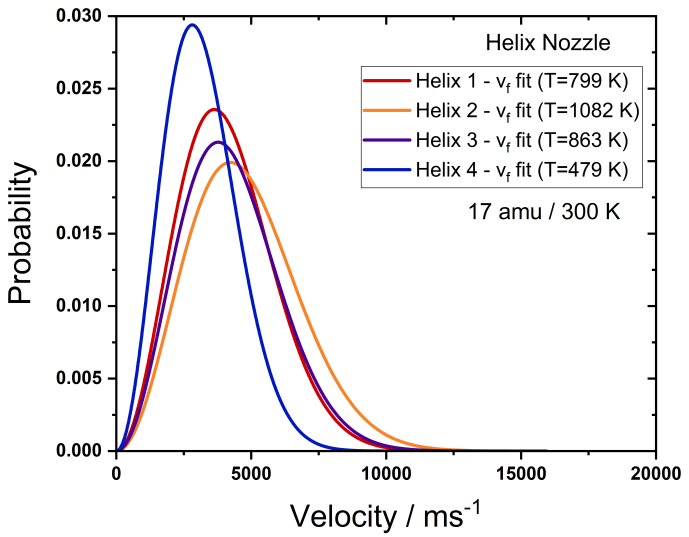
Temperature of H atoms





1300 K





1000 K