

UNRAVELLING SPECTRAL SIGNATURES AND PHOTOCHEMICAL PROCESSES OF PAHs

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The Physics and Chemistry of the Interstellar Medium

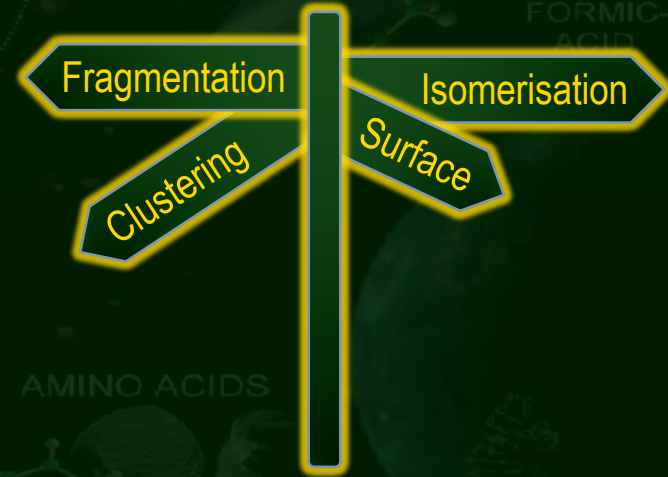
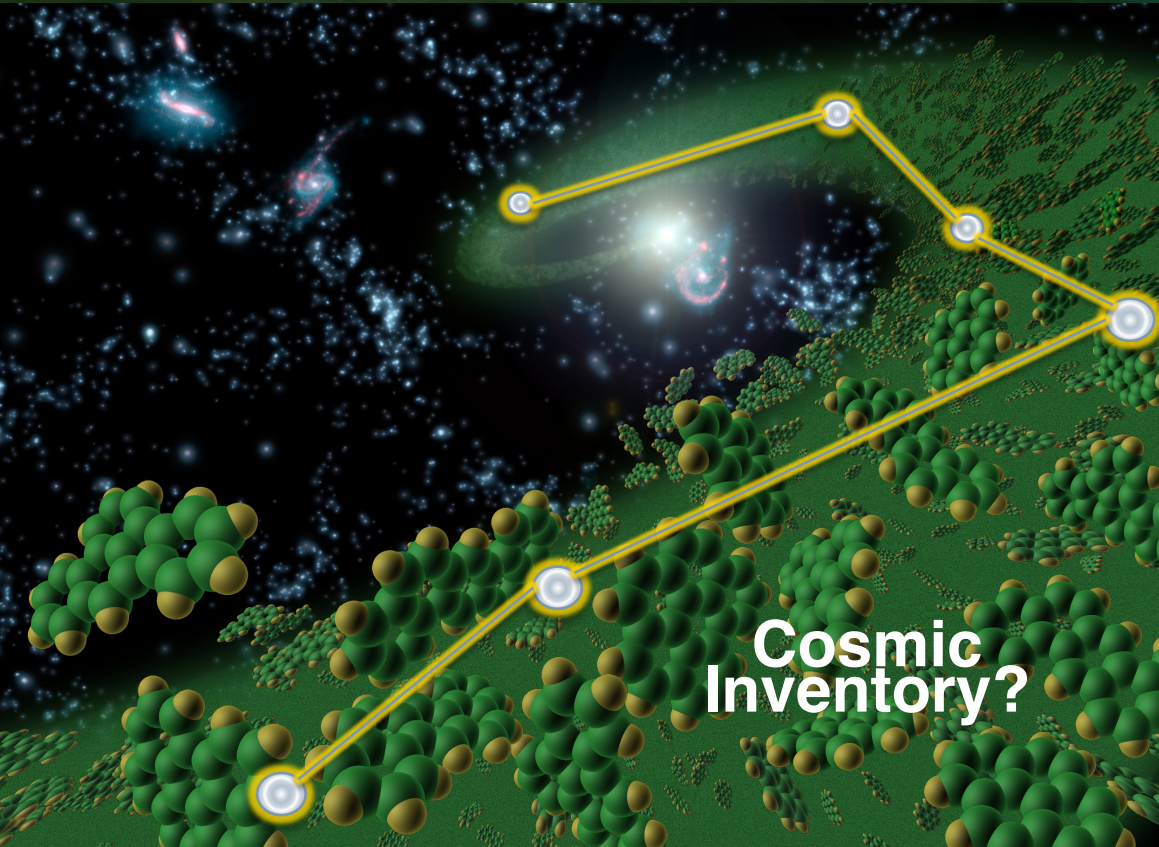
Celebrating the first 40 years of Xander Tielens' contribution to Science

Palais des Papes, Avignon, 3 Sep. 2019

OUTLINE

- The physics and chemistry of the ISM **IS PAHs**
- Electronic signatures of IS PAHs
- Photochemistry of PAHs as driver for D storage

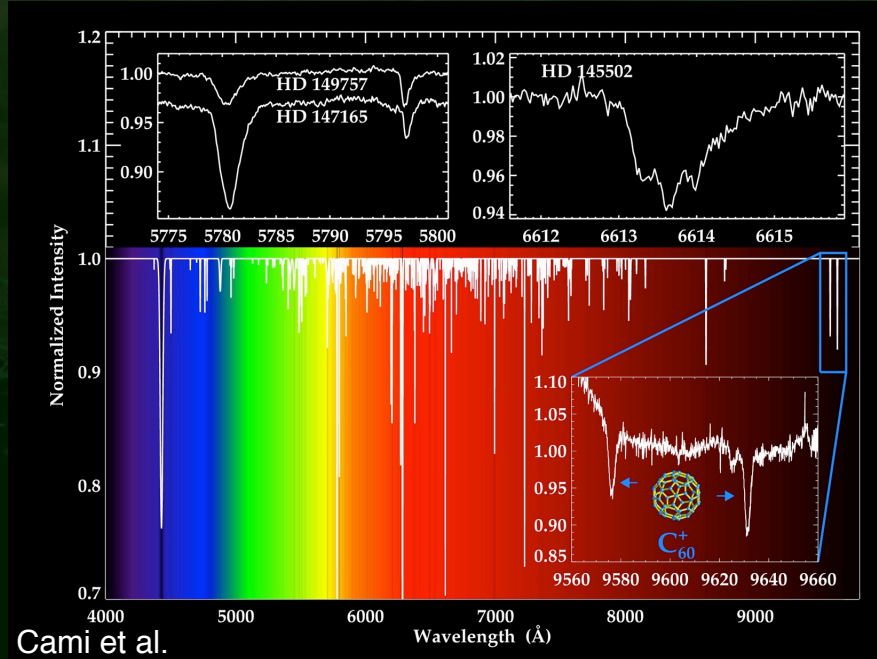
THE PHYSICS AND CHEMISTRY OF IS PAHs



Cosmic Chemistry?

THE PHYSICS OF IS PAHs

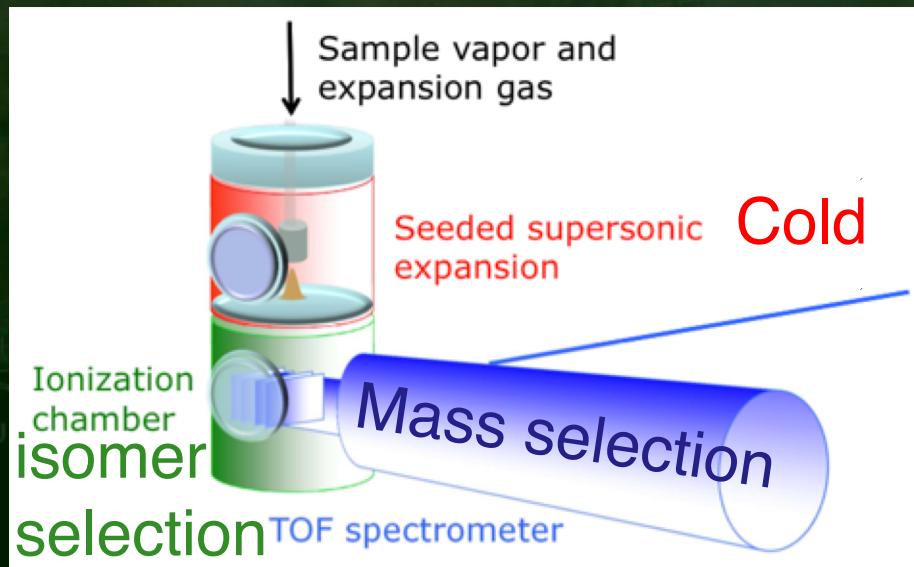
HOW TO IDENTIFY IS PAHs?



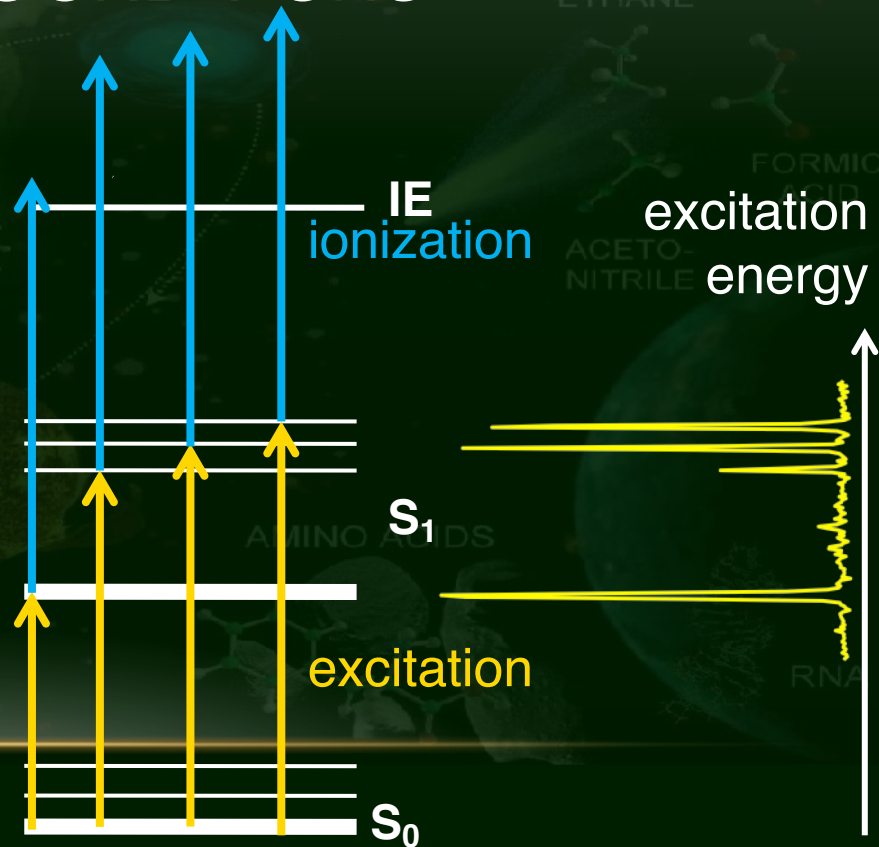
- Limited correlation
- Fortitude of possible isomers
- Individual abundances too low?
- No match found (yet)
- But... lack of accurate validated predictions and accurate experiments under IS conditions

Diffuse Interstellar Bands
PAHs as carriers?

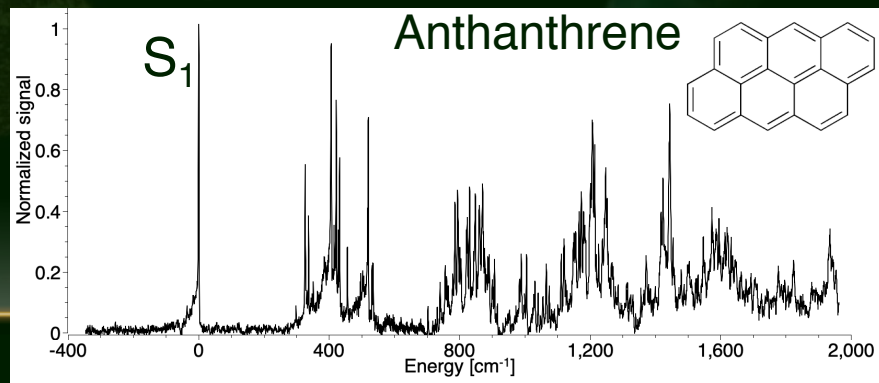
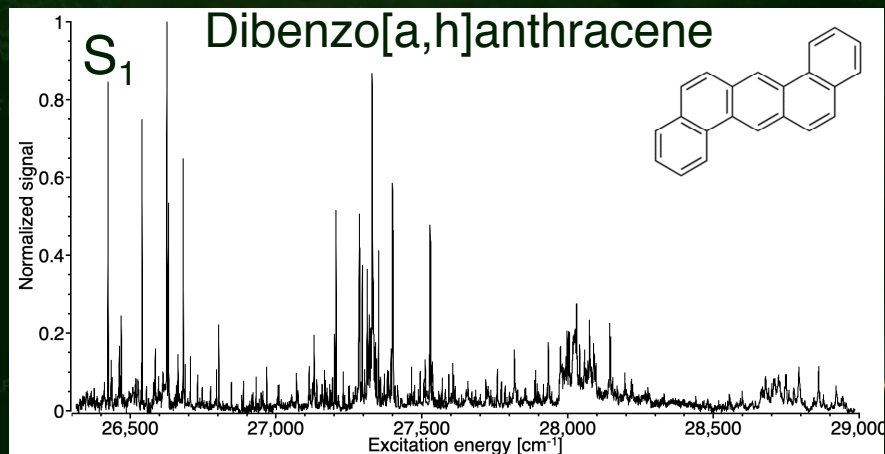
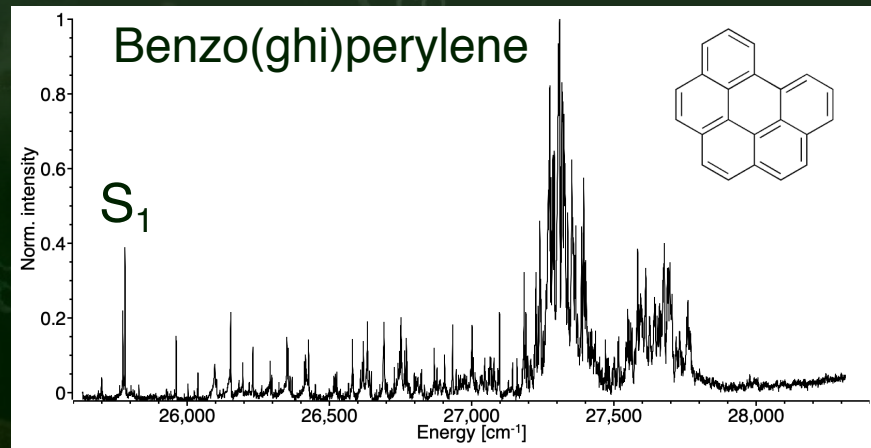
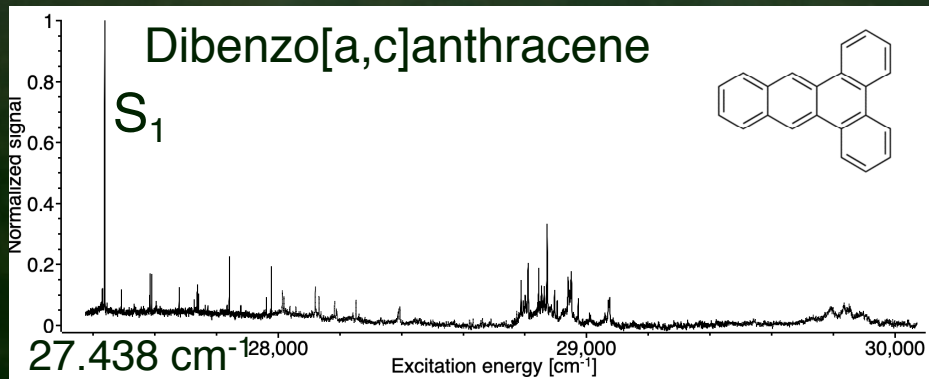
HIGH-RESOLUTION ACTION SPECTROSCOPY UNDER INTERSTELLAR CONDITIONS



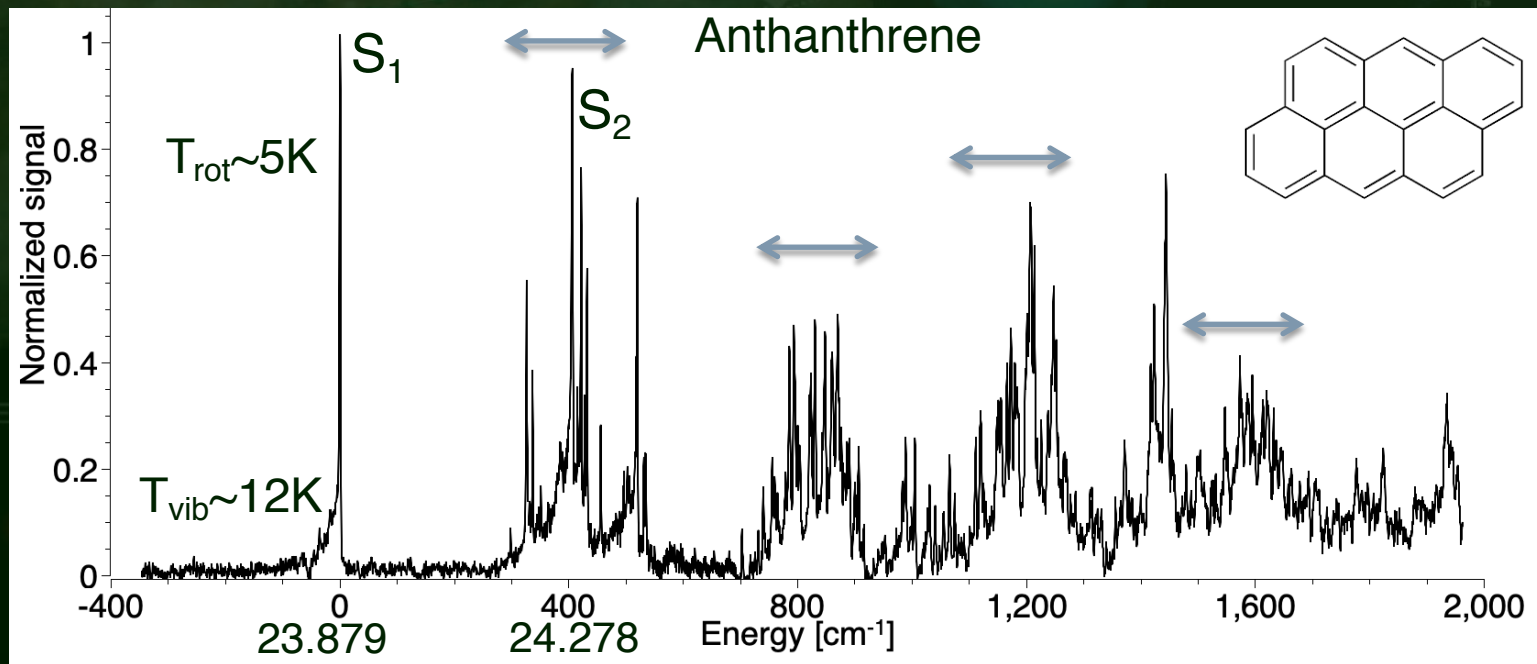
Resonant Enhanced MultiPhoton
Ionisation (REMPI)



GAS-PHASE ELECTRONIC SPECTRA

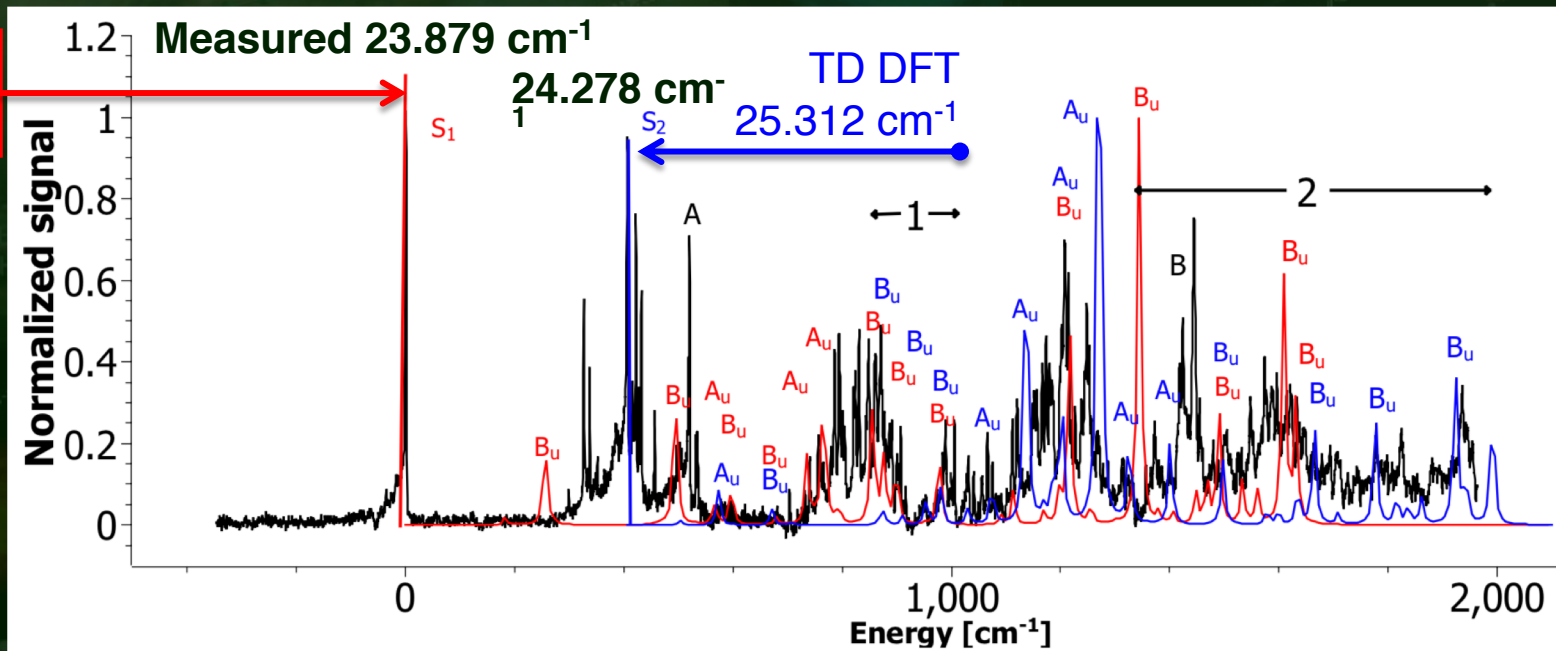


GAS-PHASE ELECTRONIC SPECTRA



GAS-PHASE ELECTRONIC SPECTRA

TD DFT
21.320 cm^{-1}



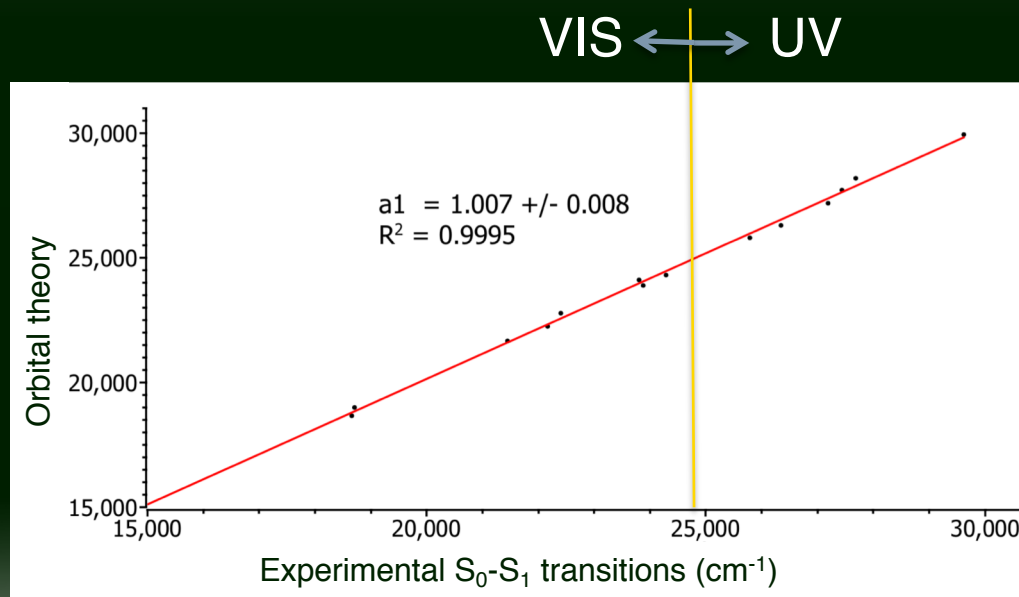
~11% deviation of $S_0 \rightarrow S_1$ transitions

VALIDATE AND IMPROVE PREDICTIONS

- Cold high-resolution laboratory data of isolated PAHs
- TD DFT <15%

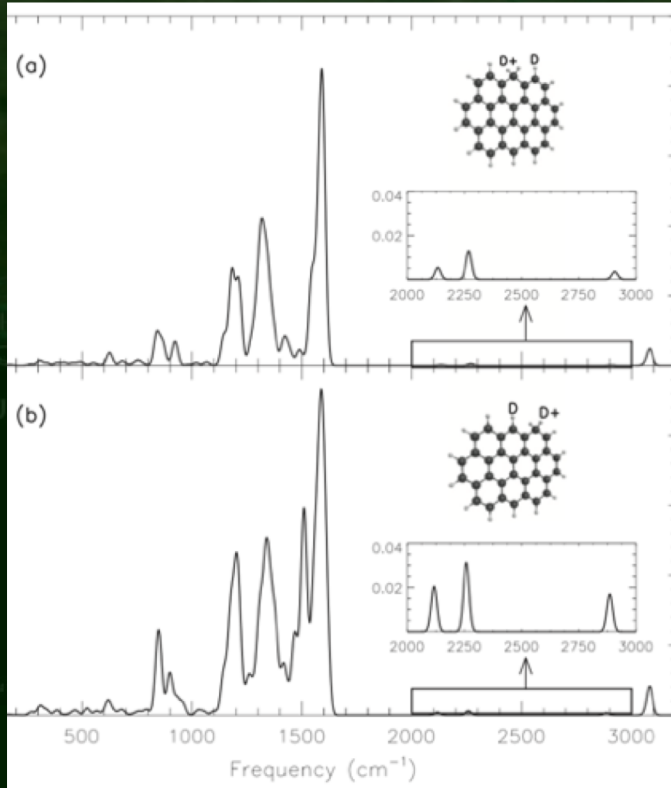
VALIDATE AND IMPROVE PREDICTIONS

- Cold high-resolution laboratory data of isolated PAHs
- TD DFT <15%
- Predictions ~1%!



THE PHOTOCHEMISTRY OF IS PAHs

PAHs AS SINK FOR DEUTERIUM

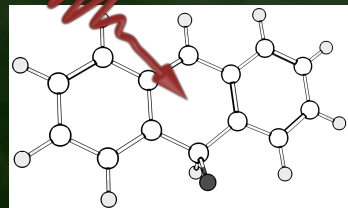


Buragohain et al. 2016

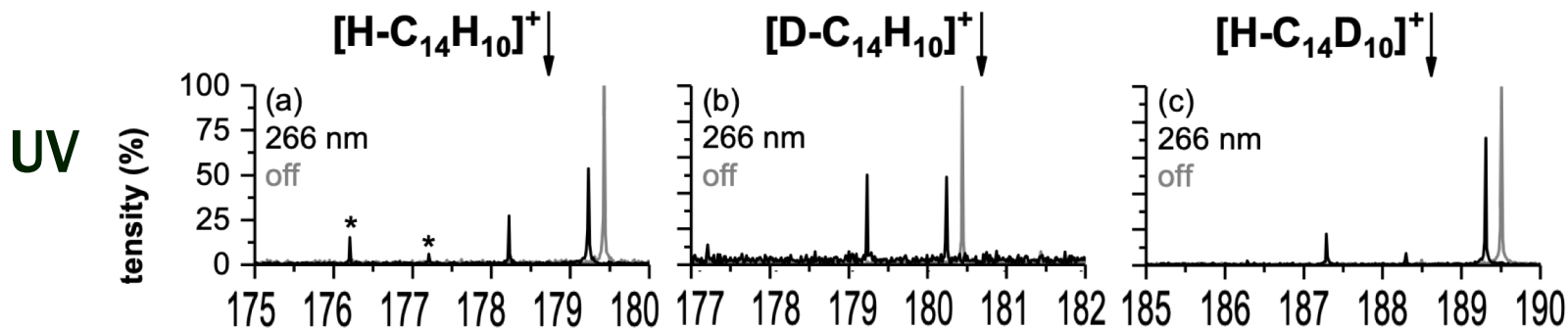
- D/H ratio Primordial ~26 ppm
ISM ~7 to 22 ppm
- Predictions & observations
- Experimental data lacking
- Mechanism?

Could PAHs form a sink
Does photochemistry play a role

PHOTOLYSIS OF D⁺-ANTHRACENE IONS

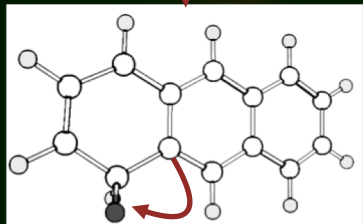
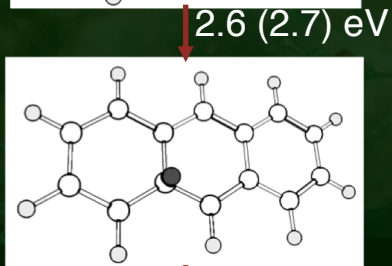
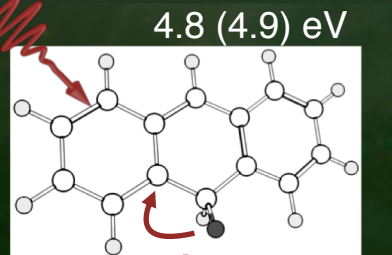


- D-PAH⁺ yields H loss only
- H-PAD⁺ yields D loss mostly



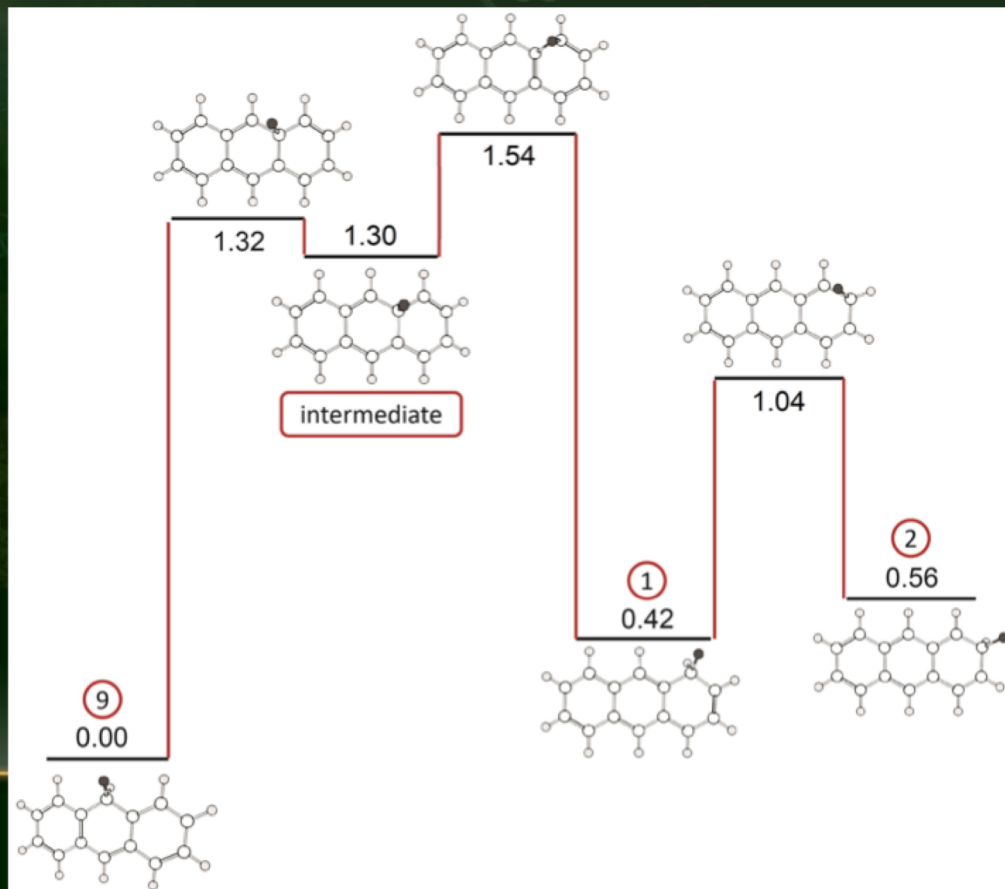
Wiersma et al. *in preparation*

PHOTO-INDUCED SCRAMBLING



Wiersma et al. *in preparation*

Castellanos et al. 2018



CONCLUSIONS

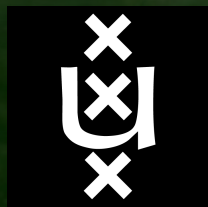
Photochemistry of IS PAHs

- Photolysis induces scrambling in D-PAH⁺
- Driver for D storage
- Structure and size dependency?
- Re-interpretation of C-D band observations?

Electronic Signatures of IS PAHs

- Laboratory data under interstellar conditions
- Validated predictions within 1% accuracy
- **Measuring DIB candidates in the lab!**

ACKNOWLEDGEMENTS



Sandra Wiersma
Wim Roeterdink
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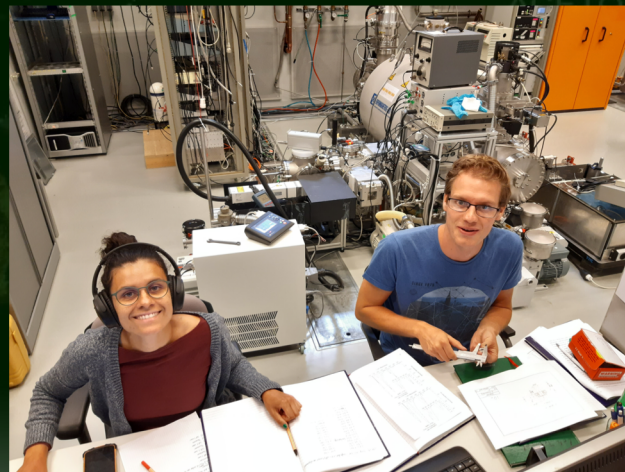


Alessandra Candian

Joost Bakker
Giel Berden
Jonathan Martens
Jos Oomens



Thank you Xander



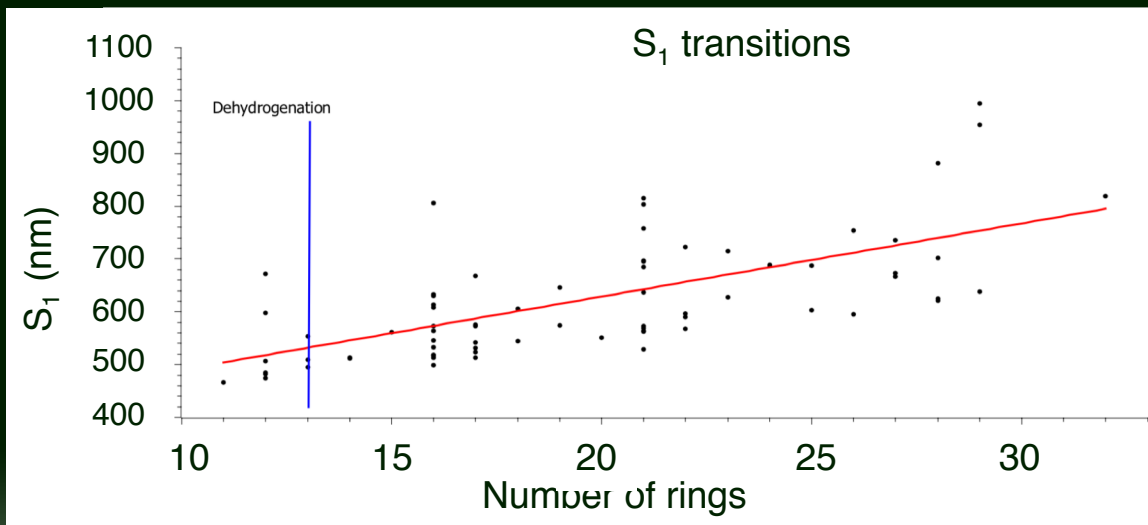
NWO VIDI Grant
VENI Grant



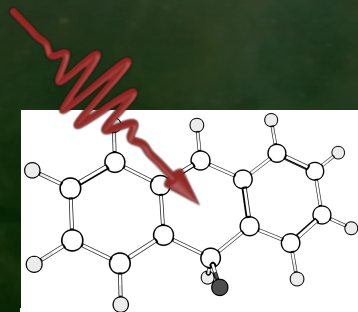


VALIDATE AND IMPROVE PREDICTIONS

- Cold high-resolution laboratory data of isolated PAHs
- TD DFT <15%
- Predictions <1%!
- Structure!



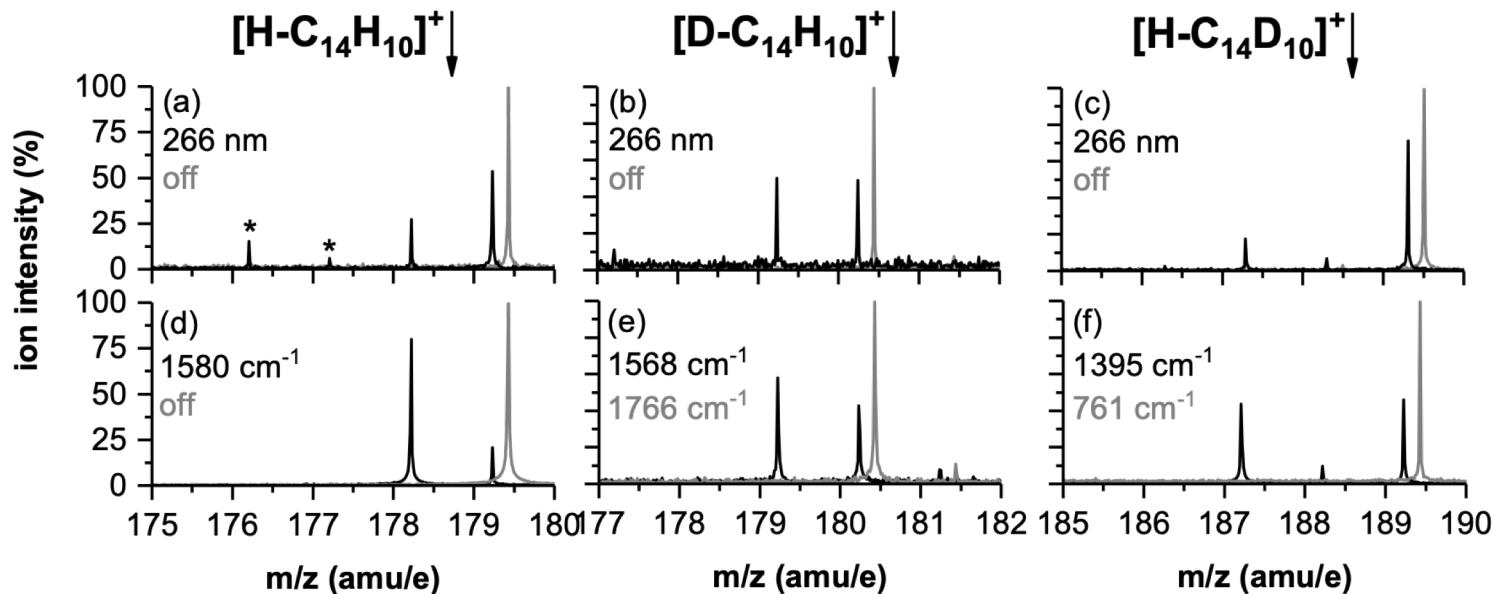
PHOTOLYSIS OF D⁺-ANTHRACENE IONS



Wiersma et al. *in preparation*

- D-PAH⁺ yields H loss only
- H-PAD⁺ yields D loss mostly
- IRMPD follows UV fragmentation

UV
IR MPD



PHOTOLYSIS OF ANTHRACENE

