Unmasking the Cosmic Fingerprint: Detecting Polycyclic Aromatic Hydrocarbons in Planetary Atmospheres

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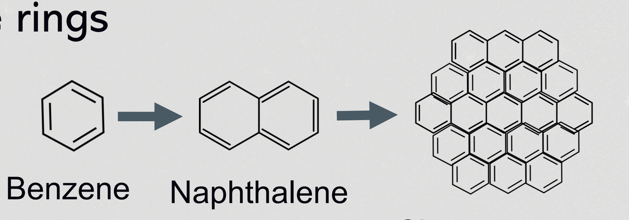
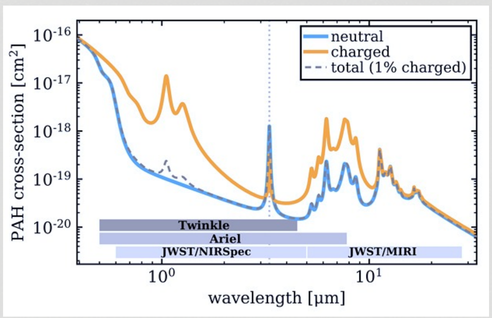
Poster round 3 – 20/06/2024
08:30 - 17:50 hrs.

Introduction

- Polycyclic Aromatic Hydrocarbons (PAHs) are a large group of organic compounds, made up of two or more benzene rings





- An optical slope is present around 0.6 μm
- Emission at longer wavelengths contaminated by silicate emission
- At 3.3 μm: Most prominent spectral feature in NIR.

- Important role in the thermo-chemo-dynamical evolution of gas atmospheres[1,2]
- High photoelectric yield
  - Extremely efficient at converting incoming far-ultraviolet radiation (FUV) into heating
  - Having a strong influence on atmospheric loss rates[2,3]
  - Emit fluorescent radiation in infrared
- Pre-biotic chemical reactions, leading to more complex molecules[4] (amino acids and nucleotides)

01. Methodology: Forward Model + Retrieval

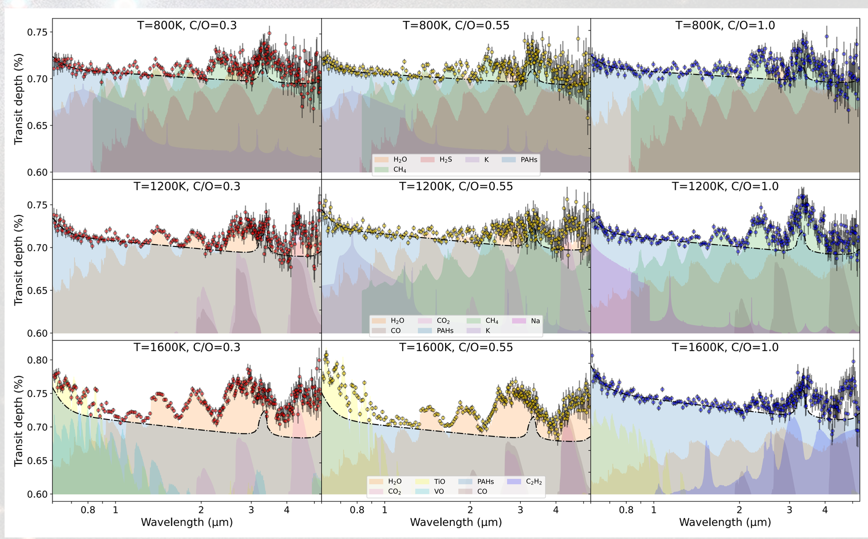
(i) petitCODE[3] for generating nine self-consistent models to calculate atmospheric abundances and temperature structure.

(ii) petitRADTRANS[4](pRT) to model the transmission spectra based on these forward models.

(iii) PandExo[5] to simulate observations with JWST and estimating uncertainties in these transmission spectra.

Input parameters from the synthetic spectra

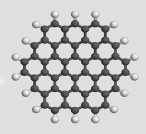
Parameter	Value	Parameter	Value
Temp	800, 1200, 1600K	f_{sed}	2.0
R_P	$0.83R_{Jup}$	σ_g	1.05
C/O	0.3, 0.55, 1.0	$\log(g)\ (cms^{-2})$	3.02
$[Fe/H]$	0	$\log(P/bar)$	-2
$\log(X_{PAH})$	-5, -6, -7		



(iv) pRT to retrieve the atmospheric abundances from these simulated observations and evaluate the potential detectability of PAHs. We run three retrieval models with PAH (**PAH-included models**) and three retrieval models without PAH (baseline models). Total number of retrievals: **27 × (3 + 3) = 162**

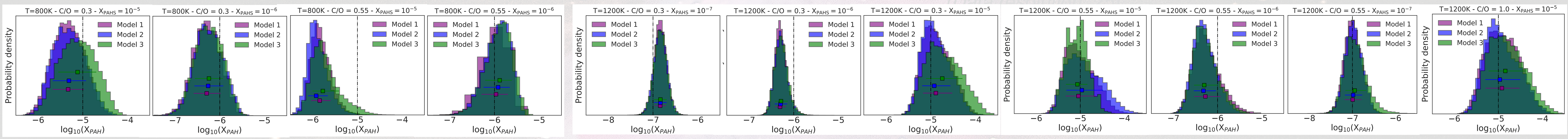
(iv) To assess the detectability of PAHs in each of the 27 forward models, we run retrievals and compare the results of the **three baseline models** with their corresponding PAH-included models. This involves calculating **Bayes factors** to perform model selection and determine if PAHs are favored for each forward mode.

Model	Baseline	Extra parameters
1	Cloud-free	-
2	Power-law Cloud	κ_0, γ_{scat}
3	Power-law and Grey cloud	κ_0, γ_{scat}, Pcloud

+ PAHs  Circumcoronene

02. Results:

PAH Detection – Posterior Distributions



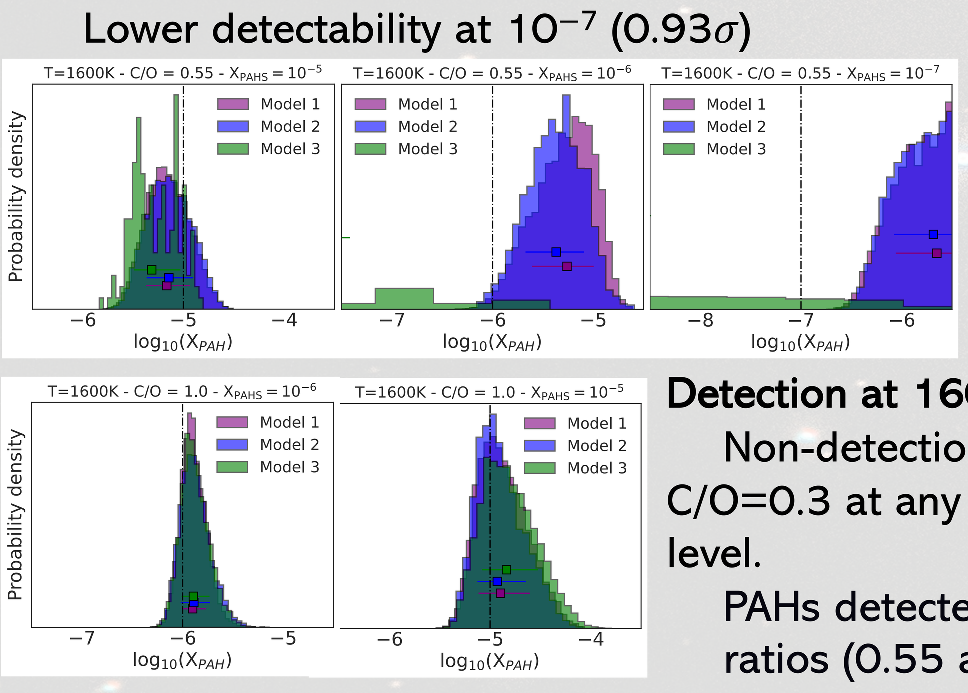
Detection at 800K:

PAHs detected at 1-σ confidence for abundances of 10^{-5} and 10^{-6}, with detection probabilities of 8.89σ and 4.59σ, respectively.

Lower detectability at 10^{-7} (0.93σ)

Detection at 1200K:

PAHs detectable at C/O ratios of 0.3 and 0.55 down to 10^{-7} and for C/O=1.0, at 10^{-5} PAH abundance at high confidence (>5σ)



Detection at 1600K:

Non-detection of PAHs at C/O=0.3 at any abundance level.

PAHs detected at higher C/O ratios (0.55 and 1.0) with strong probabilities.

- C/O=0.3:
  - Strong detections (> 3.6σ) of PAHs down to 10^{-6} for T=800K and 10^{-5} for 1200K
  - Non-detections for T=1600K
- C/O=0.55:
  - Strong detections (> 3.6σ) of PAHs down to 10^{-6} for T=800 and 1600K, and 10^{-7} for 1200K
  - Strong detections (> 3.6σ) of hazes down to 10^{-7} for 1600K
- C/O=1.0:
  - Strong detections (> 3.6σ) of PAHs down to 10^{-5} for T=800 and 1200K, and to 10^{-6} for 1600K

		T=800K			T=1200K			T=1600K		
C/O \ $\log X_{PAH}$		-5	-6	-7	-5	-6	-7	-5	-6	-7
0.3	Model 1	8.89σ	4.59σ	0.93σ	15.95σ	10.14σ	6.14σ	1.58σ	0.90σ	0.90σ
	Model 2	8.96σ	4.70σ	N/A	15.94σ	10.21σ	6.24σ	N/A	N/A	N/A
	Model 3	7.64σ	4.59σ	N/A	15.34σ	9.79σ	6.16σ	N/A	N/A	N/A
0.55	Model 1	8.92σ	4.65σ	0.93σ	10.30σ	6.85σ	5.12σ	12.61σ	8.01σ	6.47σ
	Model 2	9.39σ	4.70σ	N/A	10.34σ	6.72σ	5.06σ	15.27σ	7.98σ	6.66σ
	Model 3	8.83σ	4.49σ	N/A	10.36σ	6.93σ	5.02σ	6.61σ	1.67σ	0.96σ
1.0	Model 1	9.56σ	0.98σ	1.22σ	11.22σ	1.96σ	1.16σ	9.52σ	7.59σ	1.02σ
	Model 2	9.54σ	N/A	N/A	11.25σ	N/A	N/A	11.60σ	6.44σ	N/A
	Model 3	8.24σ	N/A	N/A	7.07	N/A	N/A	11.60σ	5.87σ	N/A

04. Conclusion

- We have investigated the detectability of Polycyclic Aromatic Hydrocarbons (PAHs) across a diverse range of exoplanet atmospheres, considering variations in atmospheric composition.
- We have explored the influence of three crucial parameters: atmospheric temperature, C/O ratio (carbon-to-oxygen ratio), and the presence of clouds, on the detectability of PAHs.
- First, we have created observation simulations of exoplanet atmospheres, employing JWST's NIRSpec instrument and the PandExo package. Finally, we have employed the retrieval package pRT to analyse and retrieve atmospheric properties, comparing the retrieved parameters with the model input and the bayes factor to assess its detectability.
- PAH detectability with optimal conditions found around 1200 K. Also, specific C/O ratios of 0.3 and 0.55 enhance the detectability of PAHs, with consistent detections observed under these conditions.
- Overall, our findings suggest that PAHs are most likely to be detected in exoplanetary atmospheres with temperatures around 1200 K and C/O ratios of 0.3 and 0.55, highlighting these conditions as prime candidates for future observational campaigns with JWST.

References:

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