Polycyclic aromatic hydrocarbons in exoplanet atmospheres (exploring equilibrium chemistry)

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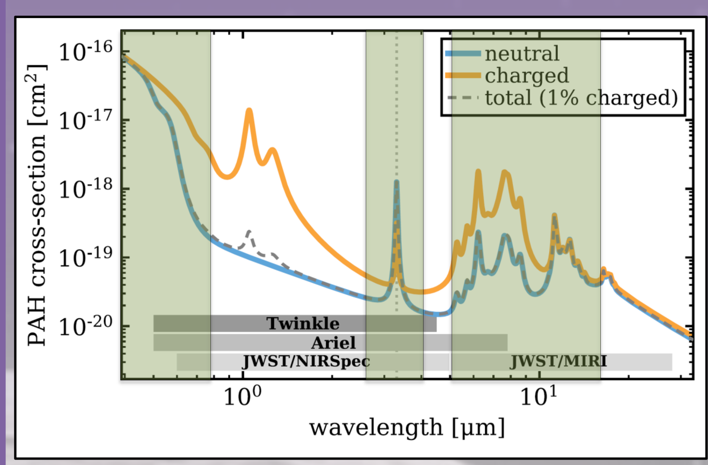
Motivation

- Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous in space, carrying 10–20% carbon budget of the interstellar medium (ISM) (*Joblin & Tielens 2011*).
- From the astrophysical and astrobiological standpoints, PAHs are considered one of the interesting complex organic structures for the following reasons:
  - They are crucial in studying the chemical and hydrodynamical evolution of protoplanetary disks and newborn planet atmospheres (*Gorti et al. 2009*; *Ercolano et al. 2022*) as well as in understanding the ionization balance of gaseous atmospheres (*Thi et al. 2019*).
  - They are anticipated to have a significant influence on prebiotic chemistry and abiogenesis, leading an important step toward life formation (*Ehrenfreund & Charnley 2000*; *Ehrenfreund et al. 2006, 2007*; *Rapacioli et al. 2006*; *Kim et al. 2012*; *Puzzarini et al. 2017*; *Closs et al. 2020*).
- They are present in the ISM with a relative number density of 3×10^{-7} respective to hydrogen nuclei (*Tielens 2008*). They could mimic the cloud/haze properties during observation. However, their presence and abundance on exoplanets are largely unknown.

Introduction

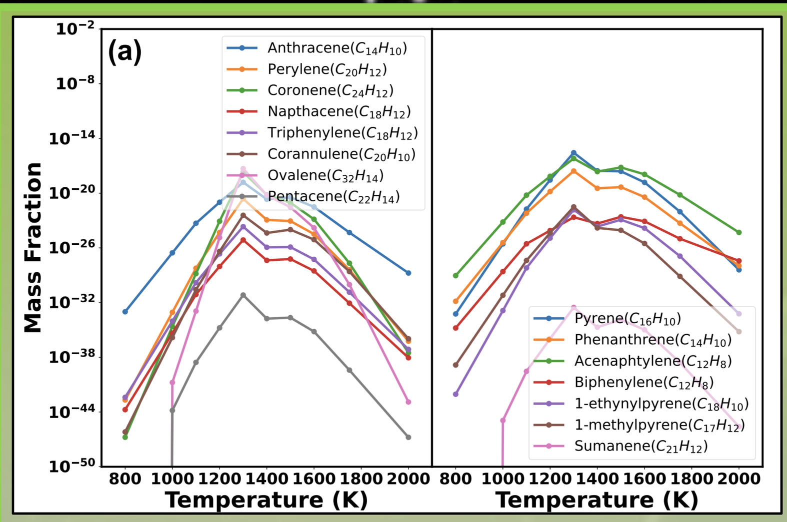
Ercolano et al. 2022



- PAH cross-sections are calculated following *Li & Draine (2001)* and including updates from *Draine & Li (2007)* for Circumcoronene PAHs consisting of 54 carbon and 16 hydrogen atoms.
- These cross-sections represent optical-properties of "astroPAHs" and are consistent with astronomical observations in the ISM.

Spectroscopic Features:
- Optical slope around 0.6 μm for neutral PAH
- 3.3 μm feature is independent of charge
- A collection of features at longer wavelength (6-12 μm)

Effective Planet Temperature (T_{eff})



0-D model for a wide temperature grid and at a pressure level consistent with the planetary photosphere (10^{-2} bar)

T_{eff} = [800K, 1000K, 1100K, 1200K, 1400K, 1500K, 1600K, 1750K, 2000K]

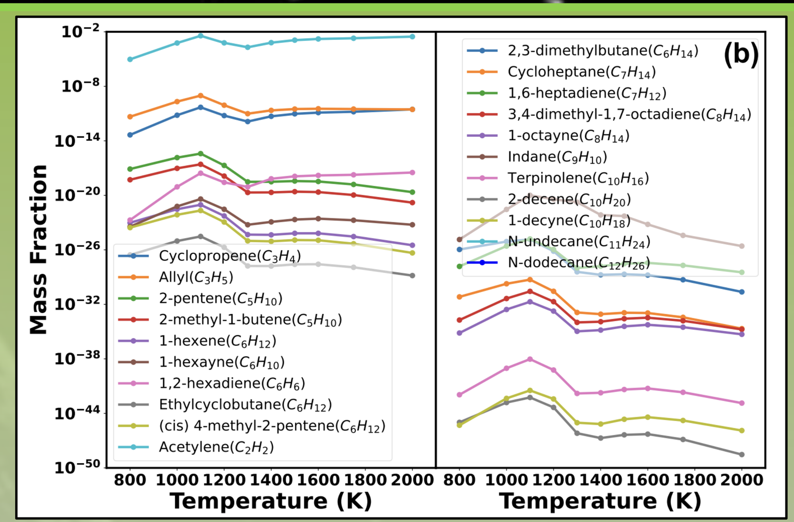
$$\beta = \frac{n_C}{n_H}$$

Class I: $\beta > 1$ — Species with more unsaturation

Class II: $\beta < 1$ — Species with low unsaturation or saturated species

n_C = Number of Carbon atom present in the molecule

n_H = Number of Hydrogen atom present in the molecule



- Peak at an optimum temperature ~1300K for PAHs.
- Lower temperatures are not sufficient to form PAHs while higher temperatures lead to thermal destruction of PAHs.
- Anthracene, Perylene, Coronene, Ovalene, Pyrene, Phenanthrene are the most abundant PAH species among all.

- An opposite trend to that of PAHs. This class of molecules undergoes a dip at the optimum temperature ~1300K.
- While getting formed in the lower temperature regions, these molecules contribute towards formation of heavy organic structures: highly unsaturated aliphatic hydrocarbons and PAHs.

180 organic species are introduced into the chemical network of petitCODE

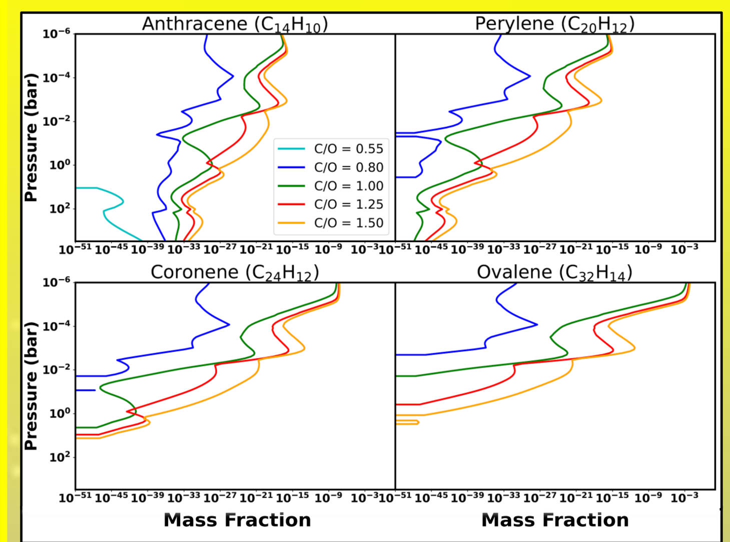
Saturated (alkanes) and unsaturated hydrocarbons (alkene, alkyne, and aromatics) in the cloud free atmosphere

1D Radiative Convective Equilibrium Model → Parameter Space Study

Irradiated hot Jupiters ($R_P = 1R_{Jup}$, $M_P = 1M_{Jup}$, log(g) = 3.0) around G5 stars ($T_* = 5660$ K, V = 9, K = 7.5, $R_* = 1R_\odot$)

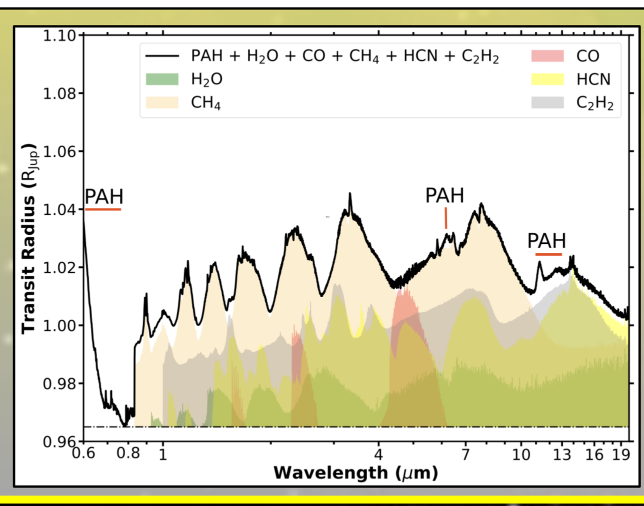
C/O ratio

T_{eff} = 1300K, [Fe/H] = 1.0

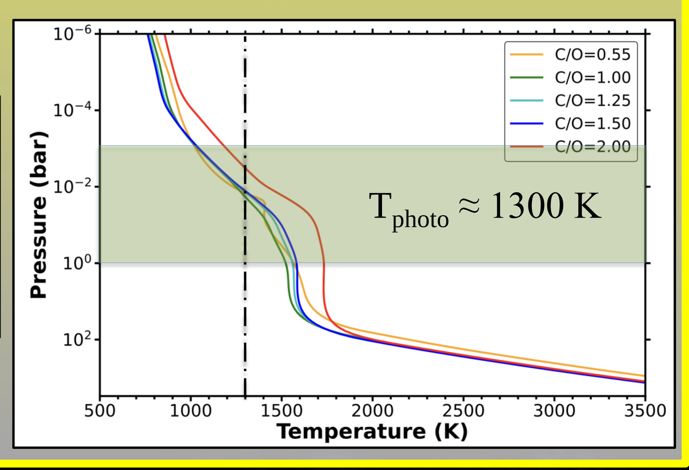


Parameter space: C/O = [0.55, 0.80, 1.0 , 1.25, 1.50]

- No *in-situ* PAH feature at solar C/O ratio
- Enhanced C/O ratio favors PAH formation.
- An average photospheric temperature ~1300K is evident from the pressure-temperature profiles – support to 0-D models.



The contribution from different molecules to the net transmission spectrum of the planet for C/O = 1



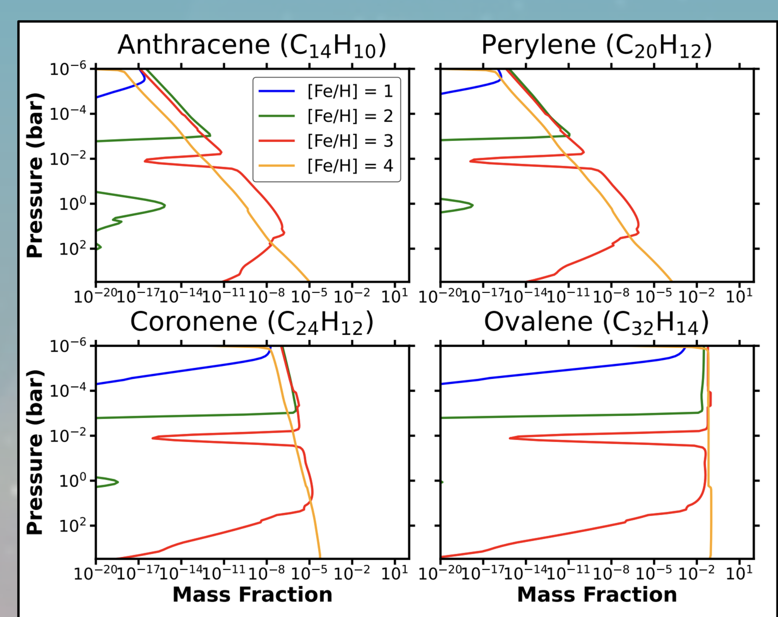
Metallicity [Fe/H]

- Metallicity also impacts the formation of PAHs in a similar way as the C/O ratio does: enhanced metallicity favors PAH formation.

Parameter space: [Fe/H] = [0, 1, 2, 3, 4] (in log scale)

- However, for Solar C/O ratio, the PAH abundance does not change significantly with the increase of the metallicity.
- C/O ratio is the dominant parameter over metallicity for the PAH formation.

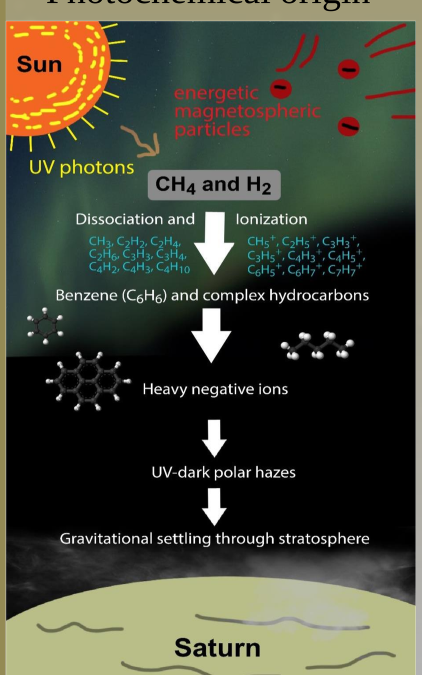
T_{eff} = 1300K, C/O= 1.0



Extraplanetary Origin of PAHs

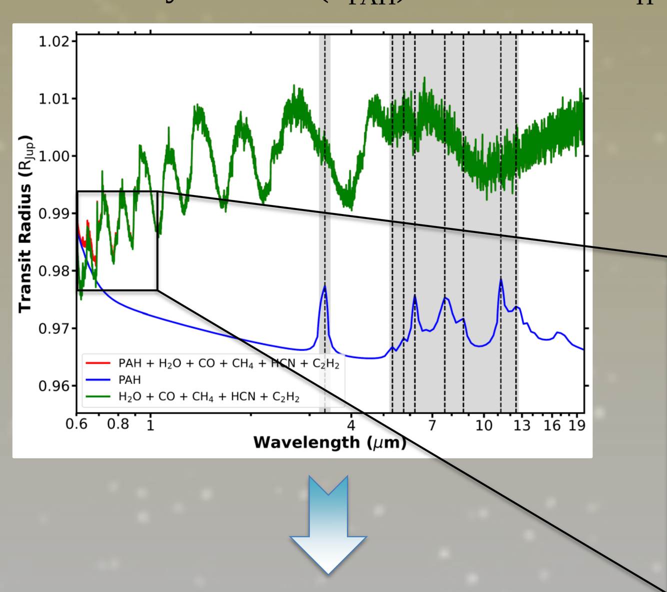
- Ex-situ PAH accumulation through primordial gas accretion or through asteroid/comet impact.

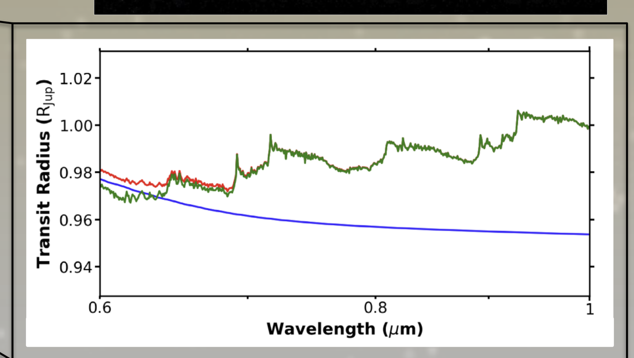
Photochemical origin



Solar case: C/O = 0.55

Number density of PAH (n_{PAH}) ≈ 3 × 10-7 × n_H

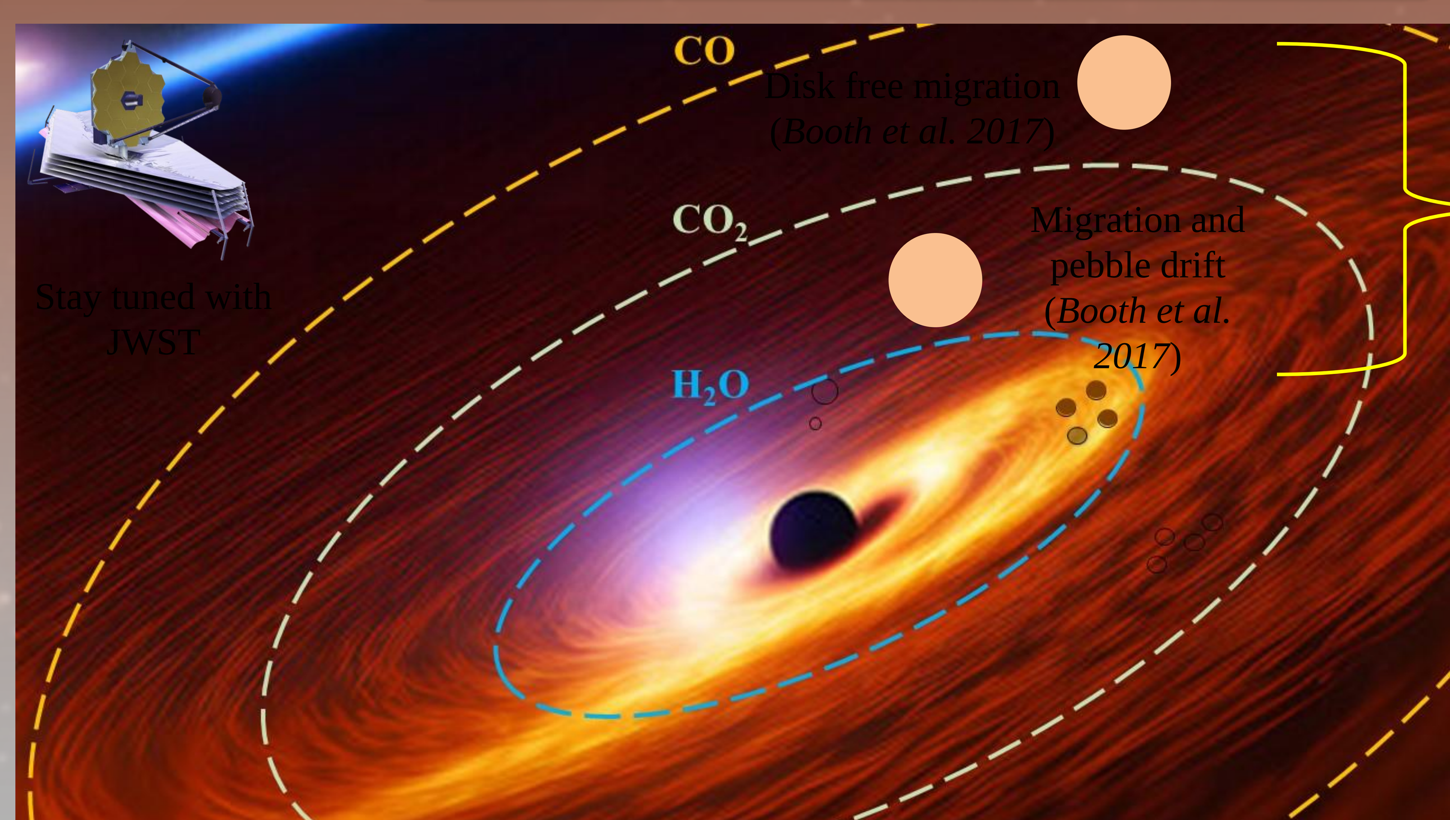




Demands significant retrieval...

Asteroid impact

Constraining Planet Formation Pathways



Rainout of O-rich refractories (*Burrows et al. 1999*)

C/O-rich hot Jupiter atmosphere

Summary and Future Prospects

- **An optimum effective temperature is required for PAH formation in thermalized atmosphere (T_{eff} ~1300 K).**
- **Enhanced metallicity and C/O expedites PAH formation.**
- **Overall impact on PAH formation: C/O ratio > Effective planet temperature >> Metallicity**
- **From Solar system perspective, PAHs are not expected to form thermally on transiting planets.**
- **Hence, studying chemical kinetics and photochemistry became important to understand the formation and destruction processes of PAH on exoplanets: a lead towards disequilibrium chemistry.**

1. Ercolano B., Rab C., Molaverdikhani K., Edwards B., Preibisch T., Testi L., Kamp I., Thi W.F., 2022, Monthly Notices of the Royal Astronomical Society, 512, 430
2. Dubey, Dwaipayan, et al. "Polycyclic aromatic hydrocarbons in exoplanet atmospheres - I. Thermochemical equilibrium models." *Astronomy & Astrophysics* 678 (2023): A53

We need you…

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