NASA Ames *PAH IR Spectroscopic Database*

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&

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JWST ERS PDRs4All JWebbinar

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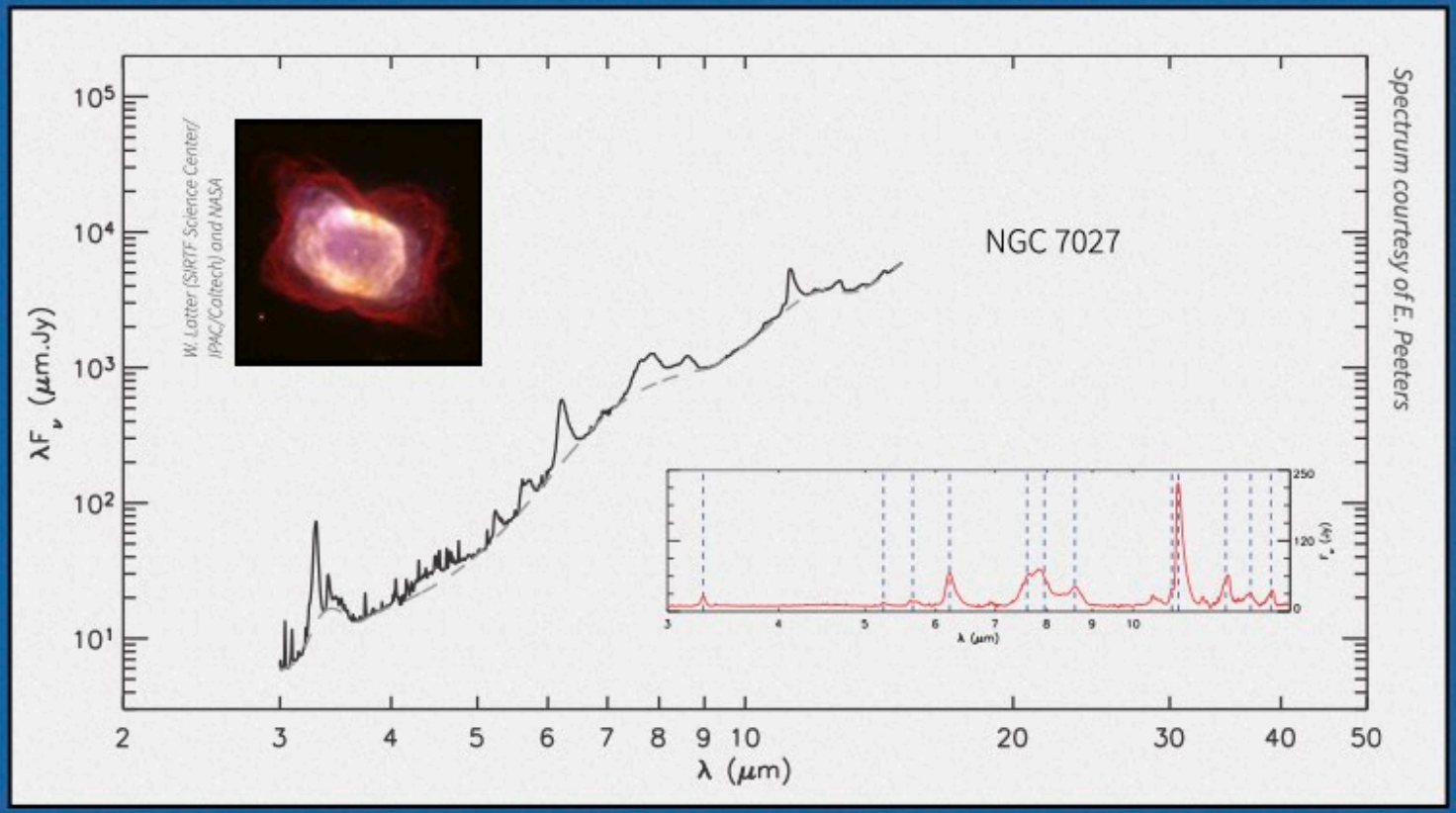
Outline

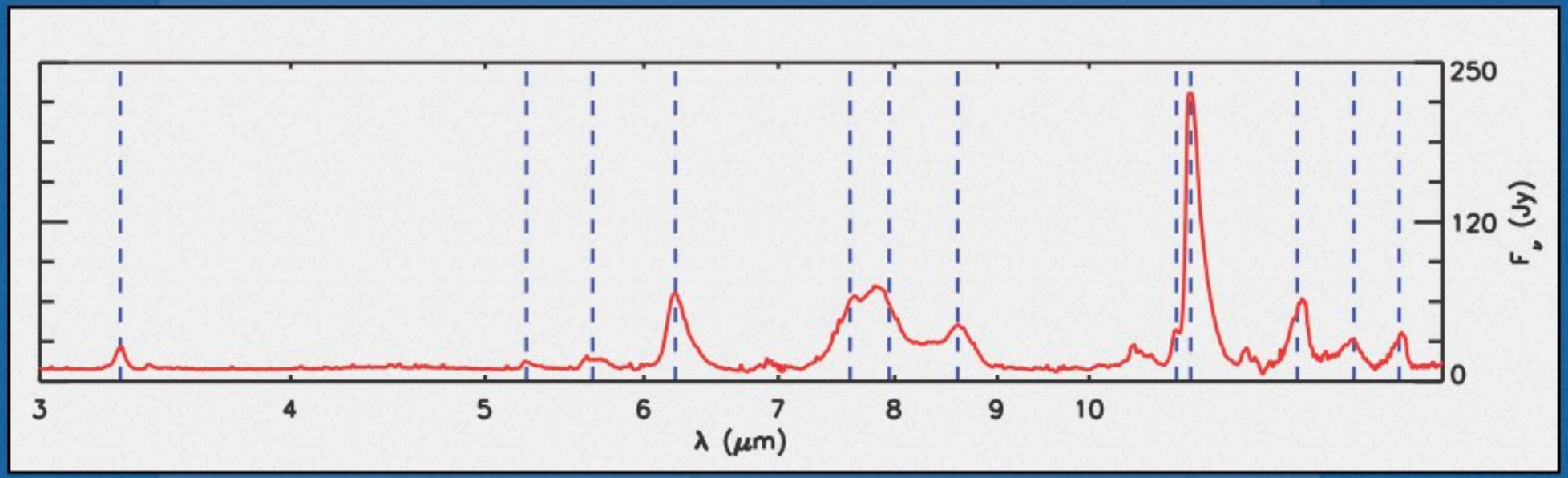
- PAH Spectral Databases
- PyPAHdb

PAH SPECTRAL DATABASES

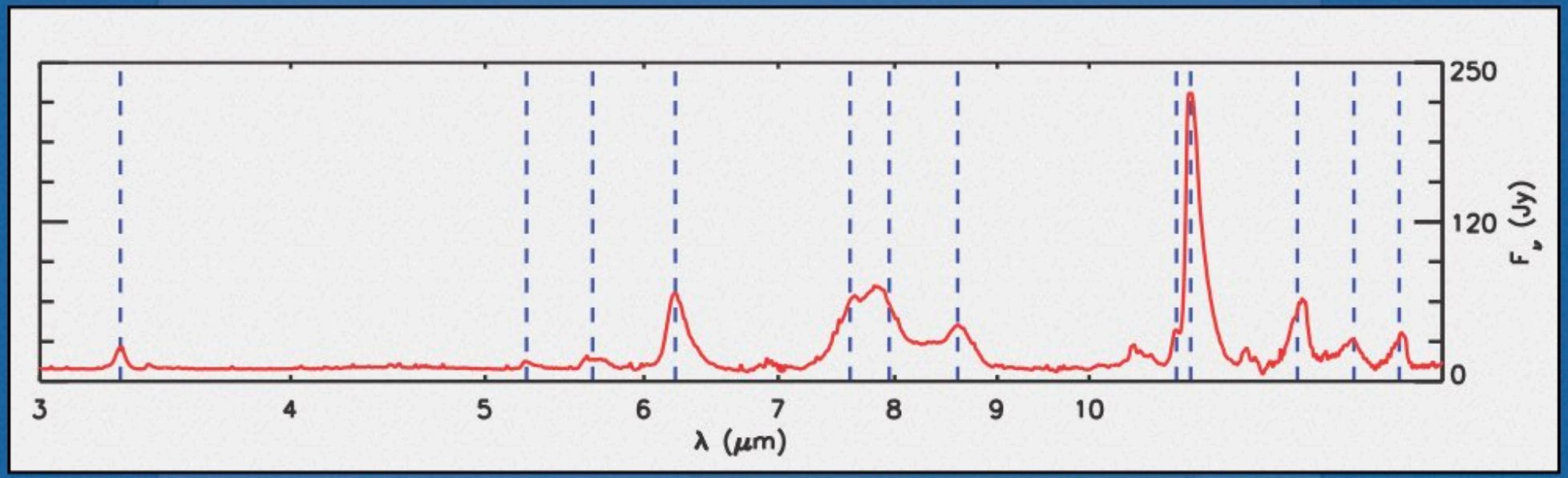
Richness: Mid-IR vibrational spectroscopy



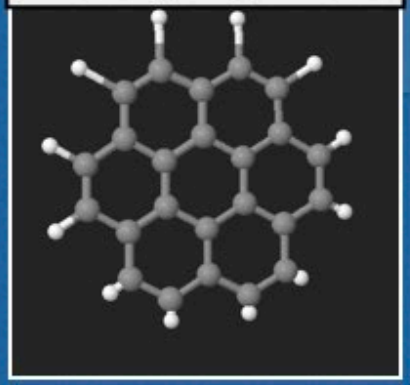
Richness: Mid-IR vibrational spectroscopy



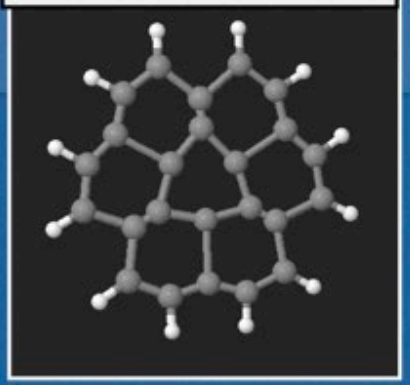
Richness: Mid-IR vibrational spectroscopy



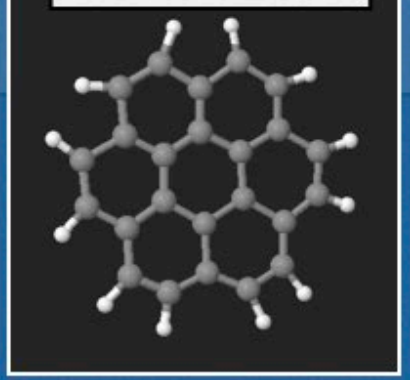
3.3 μm: $CH_{stretch}$



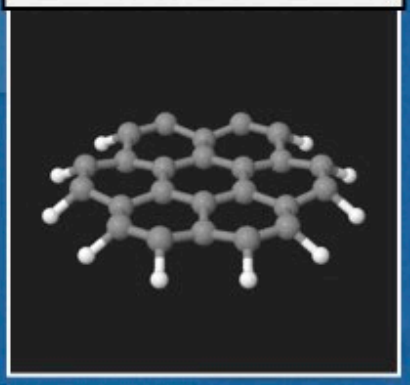
6.2 μm: $CC_{stretch}$



8.6 μm: CH_{ip}



10-15 μm: CH_{oop}



Richness: Mid-IR vibrational spectroscopy

Goal: Explain the richness of the astronomical IR PAH spectrum and, through this, gain an understanding of the astrophysical environment.

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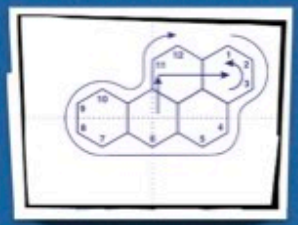
NASA Ames PAH IR Spectroscopic Database

PAH IR Spectral Database
Ames Research Center

www.astrochem.org/pahdb/

Bauschlicher+ 2010, ApJS; Boersma+ 2014, ApJS; Mattioda+ 2021, ApJS; Bauschlicher+ 2018, ApJS

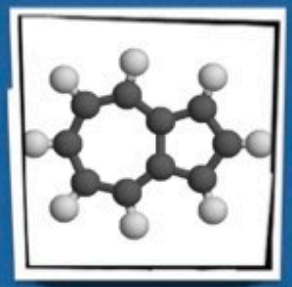
NIST



pah.nist.gov

Sander & Stephen 1997; NIST Special Publication 922

Italian/French



astrochemistry.oa-cagliari.inaf.it/database/

PAHdb

Malloci+ 2007, Chem. Phys.

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Trinity

PAH Spectral Libraries

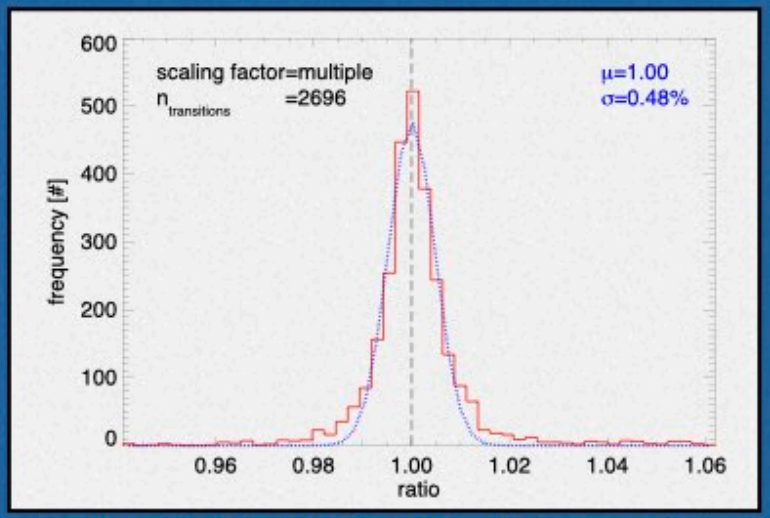
Software Tools
github.com/pahdb/

Website
www.astrochem.org/pahdb/

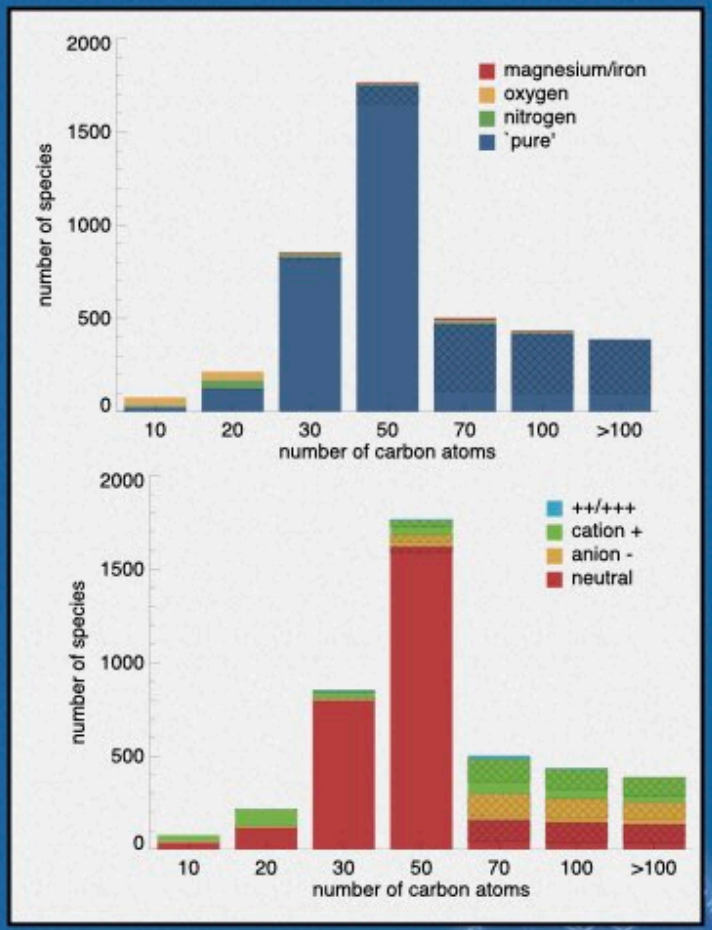
Bauschlicher+ 2010, ApJS; Boersma+ 2014, ApJS; Bauschlicher+ 2018, ApJS; Mattioda+ 2021, ApJS

Spectral Libraries

- Computed library contains ***4,233*** theoretical spectra
- Laboratory library contains ***84*** measured spectra
- Computed library of PAH-*clusters* contains ***103*** spectra



comparison of the calculated PAH band positions with those determined from experiment, showing an accuracy of 0.5%



cross-hatched areas show additions, hatched areas removals between versions 3.00 and 3.20 of the database

Bauschlicher+ 2010, ApJS; Boersma+ 2014, ApJS; Bauschlicher+ 2018, ApJS; Mattioda+ 2021, ApJS

PYPAHDB

Purpose

"The purpose of pyPAHdb is to derive astronomical PAH parameters directly from JWST observations. pyPAHdb uses a ***database-fitting*** *approach with a* ***pre-computed*** *matrix of theoretically calculated PAH emission spectra from a the library of computed spectra. This matrix has been constructed from a collection of* ***'astronomical' PAHs****."*

Why Database Fitting?

"Spectroscopic assignments are based on computed spectra of aromatic molecules in specific charge states, structures, sizes and so on. This allows the analysis of the spectra without the need of an ad-hoc interpretation of the state of the PAH population since the average synthesized spectra can be traced back to the fully characterized individual PAH molecules."

Ingredients

Astronomical PAHs

The collection of "astronomical" PAHs meet the following criteria and have the fullerenes C_{60} and C_{70} added:

‘magnesium=0 oxygen=0 iron=0 silicium=0 chx=0 ch2=0 c>20 hydrogen>0’

Emission Model

- A calculated vibrational temperature upon the absorption of a **7 eV** photon
- A calculated integrated band intensity after following the **entire emission cascade**
- A **red shift of 15 cm^{-1}** to mimic some anharmonic effect
- A **Gaussian** emission profile with a **FWHM of 15 cm^{-1}**

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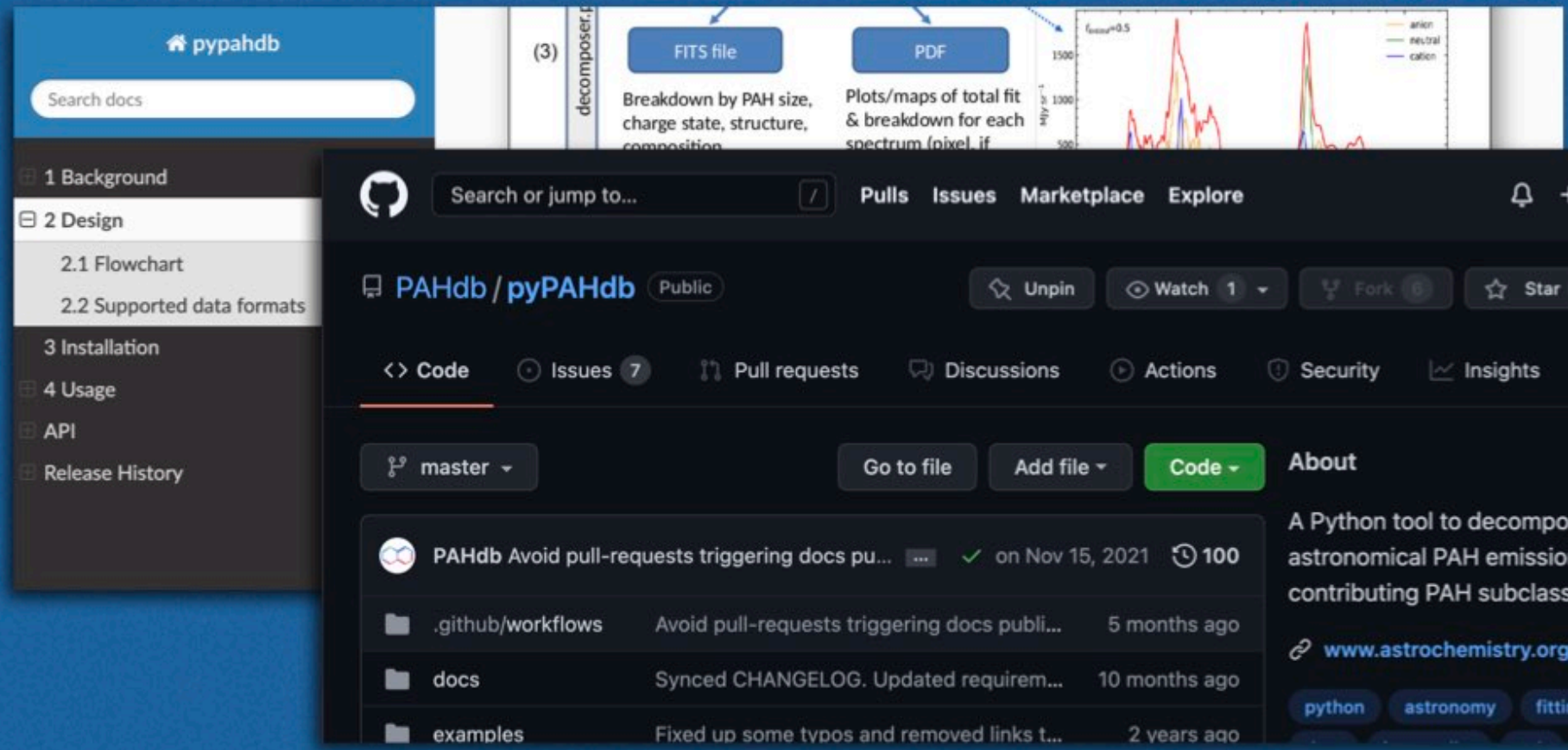

Workflows • CI • Unit Tests • Sphinx Docs • codecov • Examples • Flake

github.com/pahdb/pypahdb


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Organic Molecules in Space: Insights from the NASA Ames Molecular Database in the era of the James Webb Space Telescope

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More…

https://doi.org/10.25080/majora-4af1f417-00f

Thank You!

PAHdb