

NASA Ames PAH IR Spectroscopic Database



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JWST ERS PDRs4All JWebbinar

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Outline

- PAH Spectral Databases
- PyPAHdb



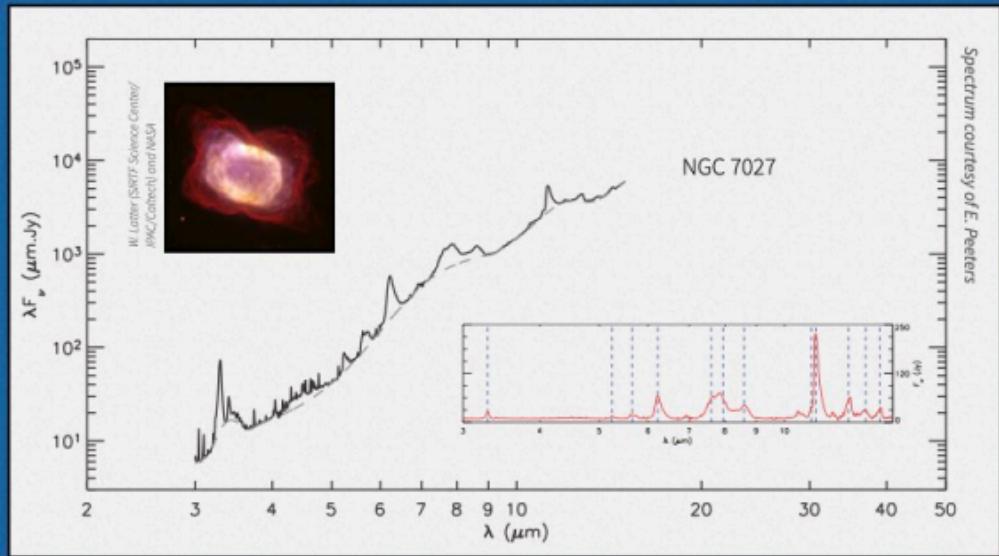


PAH SPECTRAL DATABASES



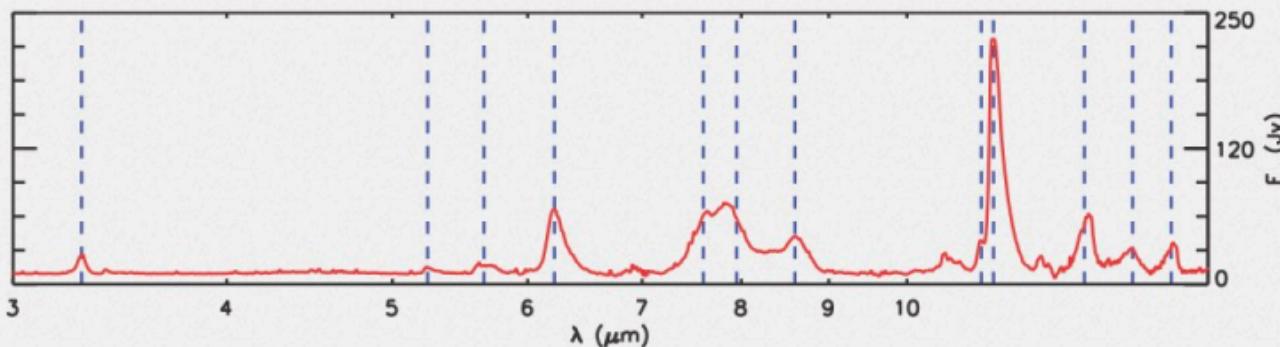


Richness: Mid-IR vibrational spectroscopy



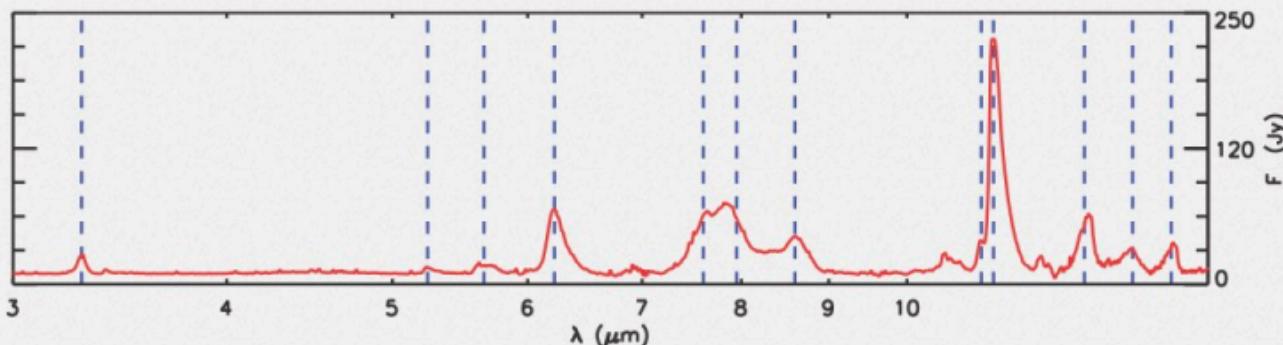


Richness: Mid-IR vibrational spectroscopy

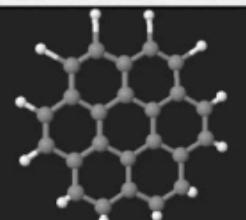




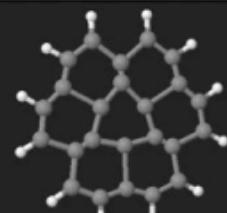
Richness: Mid-IR vibrational spectroscopy



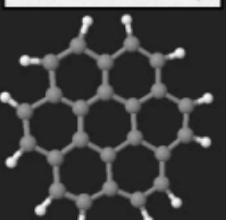
3.3 μm : CH_{stretch}



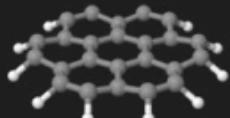
6.2 μm : CC_{stretch}



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.



NASA Ames PAH IR Spectroscopic Database

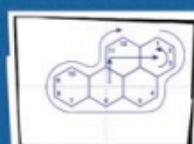


NASA Ames PAH IR Spectroscopic Database



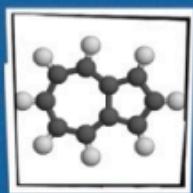
www.astrochem.org/pahdb/

NIST



pah.nist.gov

Italian/French



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



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

Sander & Stephen 1997; NIST Special Publication 922

Malacci+ 2007, Chem. Phys.

NASA Ames PAH IR Spectroscopic Database



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2021, ApJS; Bauschlicher+ 2018, ApJS



Trinity

PAH Spectral Libraries



Software Tools

github.com/pahdb/

Website

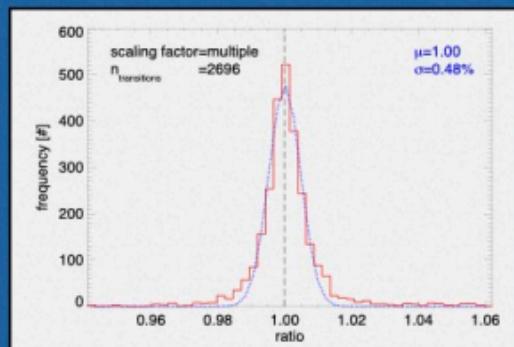
www.astrochem.org/pahdb/



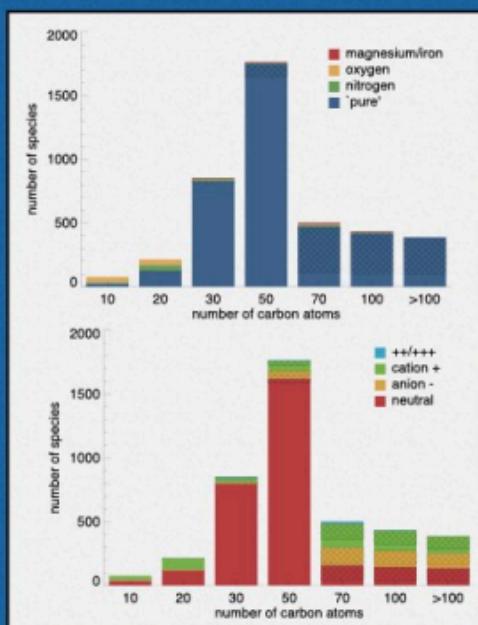


Spectral Libraries

- 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 bond 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

PAHDB



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 C₆₀ and C₇₀ 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**



NASA Ames PAH IR Spectroscopic Database



github.com/pahdb/pypahdb

(3) decomponests

FITS file PDF

Breakdown by PAH size, charge state, structure, composition
Plots/maps of total fit & breakdown for each spectrum (pixel), if

Search docs

1 Background

2 Design

2.1 Flowchart

2.2 Supported data formats

3 Installation

4 Usage

API

Release History

Search or jump to... Pulls Issues Marketplace Explore

PAHdb / pyPAHdb Public Unpin Watch 1 Fork 6 Star 4

Code Issues 7 Pull requests Discussions Actions Security Insights ...

master Go to file Add file Code About

PAHdb Avoid pull-requests triggering docs pu... on Nov 15, 2021 100

.github/workflows Avoid pull-requests triggering docs publi... 5 months ago

docs Synced CHANGELOG. Updated requirem... 10 months ago

examples Fixed up some typos and removed links t... 2 years ago

A Python tool to decompose astronomical PAH emission into contributing PAH subclasses.

www.astrochemistry.org/pahdb/

python astronomy fitting

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 ...

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Thank You!

