

Cosmic PAHs

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IRAP, Toulouse

Réunion OV-GSO, IRAP, Toulouse

10/03/2022



Osservatorio
Astronomico
di Cagliari



Cosmic PAHs: context & outline

- AROMA DB: *cosmic (star) dust analogues, meteorites, sample returns (e.g. Hayabusa 2), PEPR Origins*
 - AROMA DB web application, mMass_IRAP desktop application
- LAIBrary project: *aromatic infrared bands, polycyclic aromatic hydrocarbons, fullerenes, synthetic spectra for JWST (ERS PDRs4All)*
 - Hot PAHs IR web application, CosmicPAHmfit desktop application
 - QChITool: set of web applications for the theoretical PAH database (query, visualize, feed)
- Cosmic PAH portal: *dissiminate news and information about tools, projects, and services*
 - Web portal: dokewiki

AROMA DB

- Show Samples
- Search Data
- FAQ
- Contact

Murchison

AROMA DB: Mass spectrometry

<http://aroma.irap.omp.eu/>



Reference: H. Sabbah, A. Bonnamy, D. Papanastassiou, J. Cernicharo, J.-A. Martin-Gago, C. Joblin, Identification of PAH Isomeric Structure in Cosmic Dust Analogs: The AROMA Setup. *Astrophys. J.* 843 (2017), doi:10.3847/1538-4357aa73dd

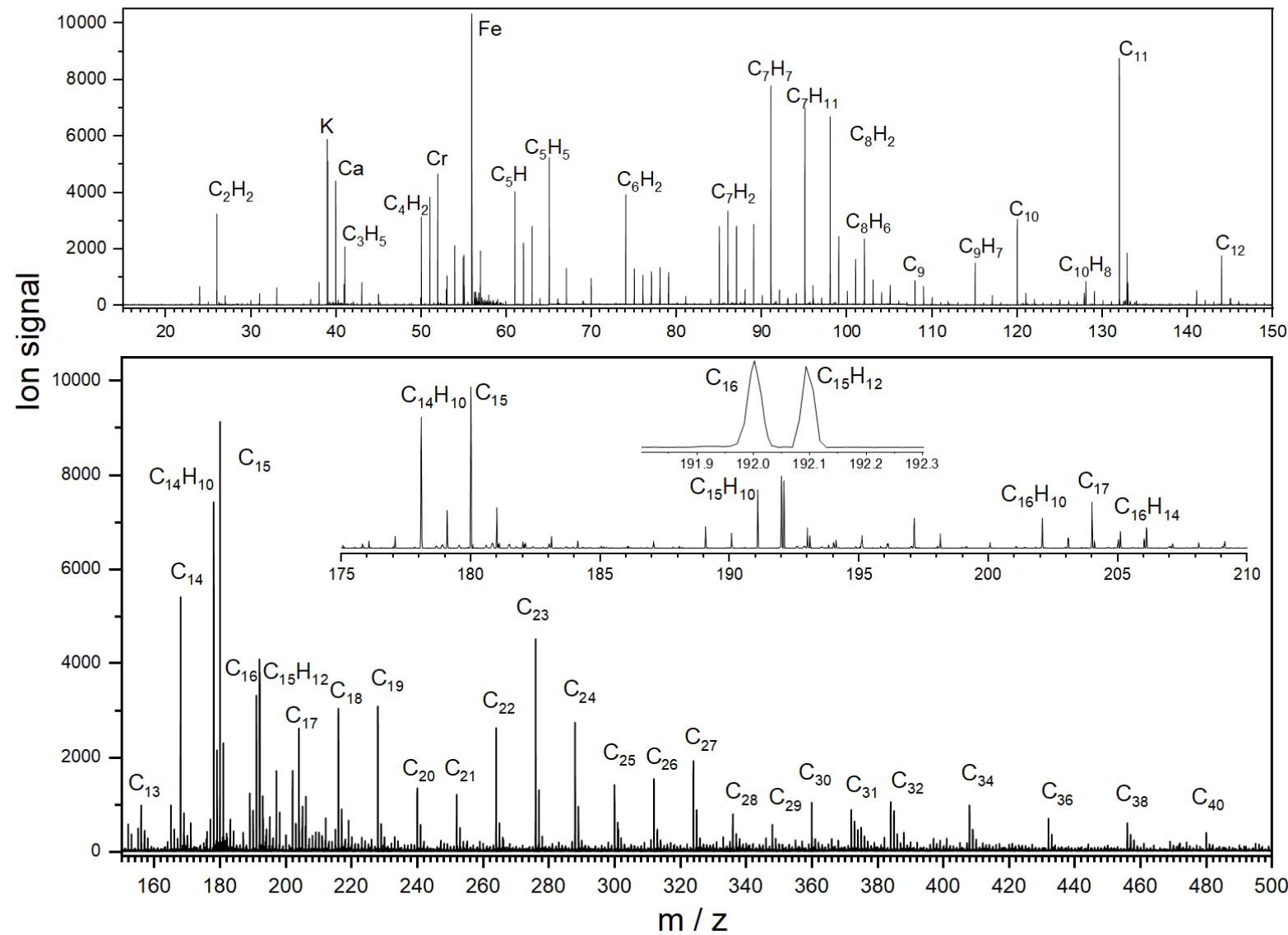
Spectrum (highlighted with a red oval)

Description	
Identity	
Name:	Murchison
Date:	2016-06-21
Version:	1
Operator:	Hassan Sabbah
Contact:	hassan.sabbah@irap.omp.eu
Institution:	IRAP
Category:	meteorite
Phase:	powder
Precursors:	
Instrument:	AROMA
Preparation:	few mg of meteorite rock powdered and fixed with conductive double tape
Comments:	

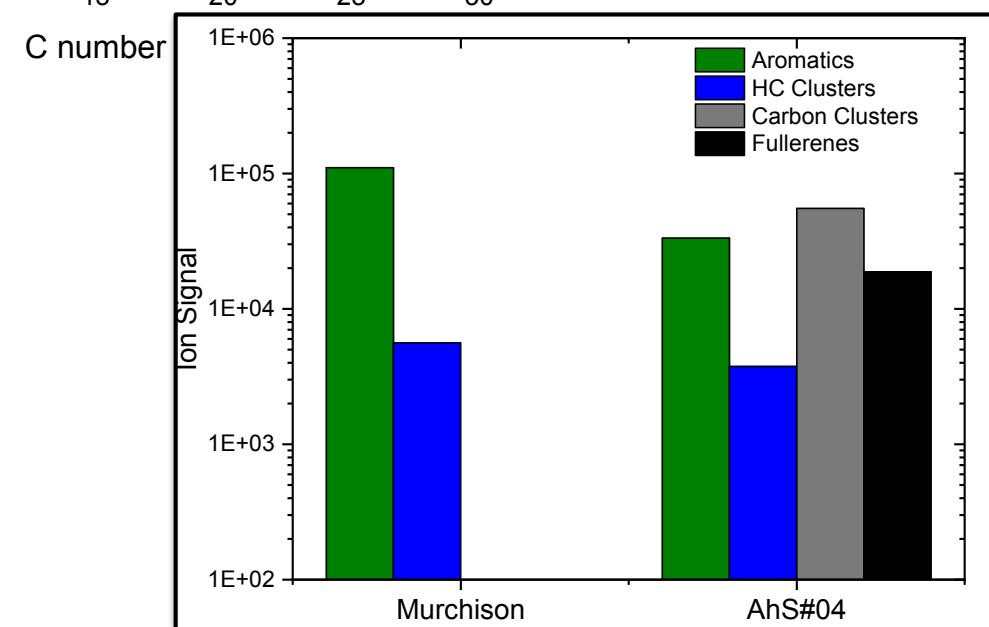
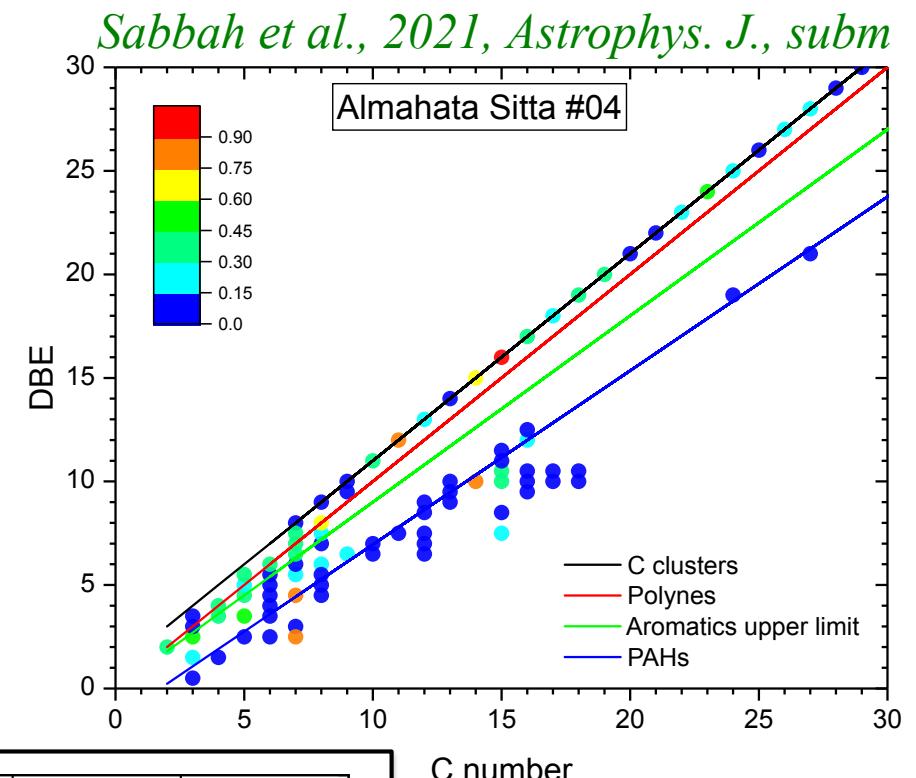
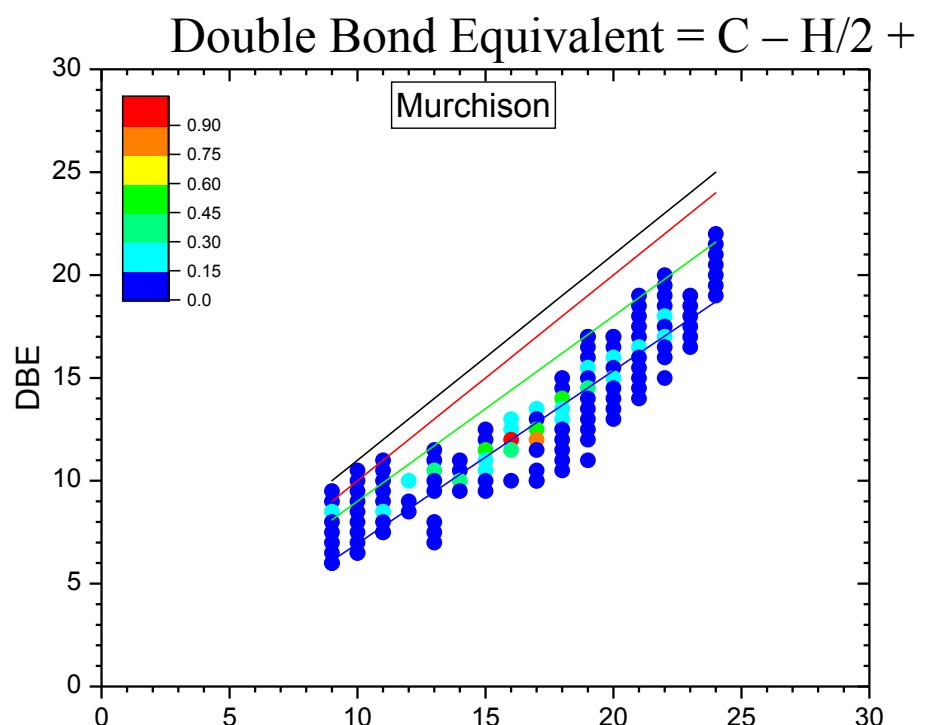
mMass: mass peak assignmemnt

Sabbah et al., 2021, Astrophys. J., subm

Almahata Sitta #04



Classification of carbonaceous molecular families



→ Different chemistries involved?

AROMA DB: family analysis

Analysis tools

AROMA DB Login

Show Samples

Search Data

FAQ

Contact

Stardust_3

Reference: Santoro, G., Martínez, L., Lauwaet, K., et al. 2020, The Astrophysical Journal, 895:97, doi.org/10.3847/1538-4357/ab9086

Infos Spectrum Data Family Analysis Dbe Media Export

Family composition by number of peaks (Tot: 47)

Elements	Count	Percentage
Hydrocarbons (CxHy)	33	70.21%
Carbon Species (Cx)	11	23.4%
Oxygen Species (CxHyOk)	3	6.38%
Nitrogen Species (CxHyNz)	0	0%
CxHyOkNz Species	0	0%

Carbon families by number of peaks (Tot: 44)

Carbon Families	Count	Percentage
Carbon Clusters	11	25%
Fullerenes	0	0%
HC Clusters	14	31.82%
Aromatics	19	43.18%

Family composition by absolute intensity peaks

Elements	Intensity	Percentage
Hydrocarbons (CxHy)	2.10e+4	58.76%
Carbon Species (Cx)	8.97e+3	25.13%
Oxygen Species (CxHyOk)	5.75e+3	16.11%
Nitrogen Species (CxHyNz)	0.00e+0	0%
CxHyOkNz Species	0.00e+0	0%

Carbon families by absolute intensity peaks

Carbon Families	Intensity	Percentage
Carbon Clusters	8.97e+3	29.95%
Fullerenes	0.00e+0	0%
HC Clusters	1.69e+4	56.59%
Aromatics	4.03e+3	13.46%

AROMA DB: Status

- Database publicly available on 10/2020
- Tools connected to the DB + mmass software (updated version mmass_IRAP)
- 05/2020 - 08/2020: mmass software development, upgrade for mac OS 64-bits. (Student project in OVGSO: E. Mauger)
- 11/2020 – 07/2021 : mmass software development by adding several functionalities including chemical family analysis (“alternance” E. Charbonnel)
- 06/2022-08/2022: internship (E. Planteur, M1) – similarity index between mass spectra
- Need: internship 2023 (6 months) evolution of mmass and AROMA DB tools to include metal family.

JWST Early Release Science program PDRs4All

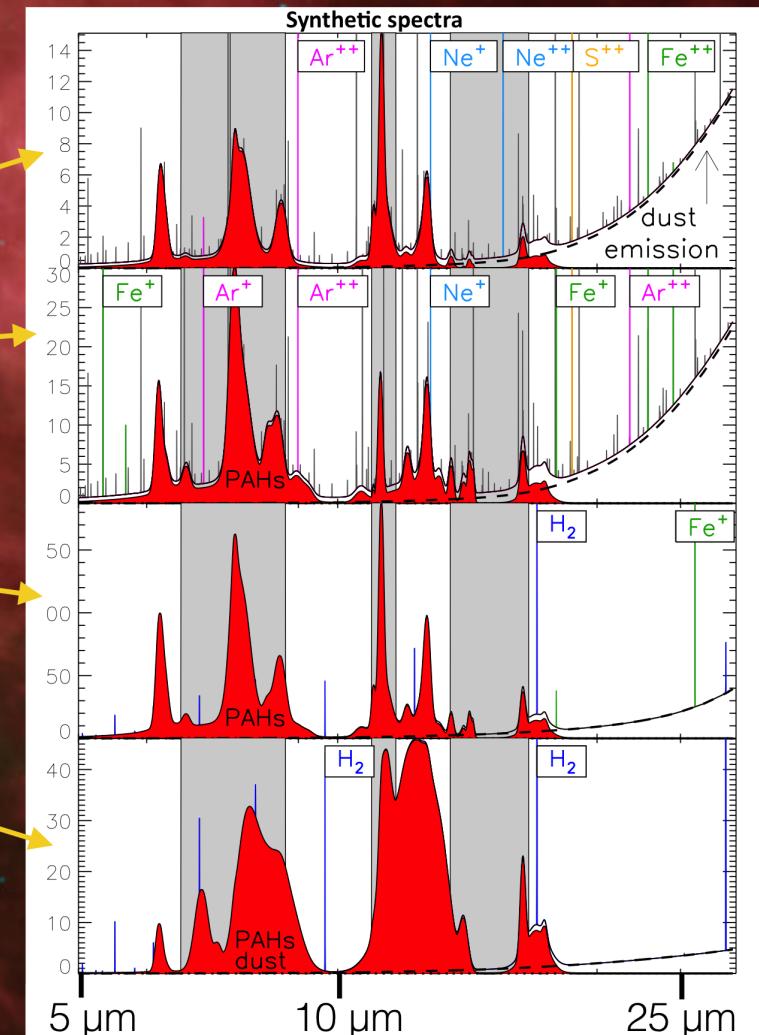
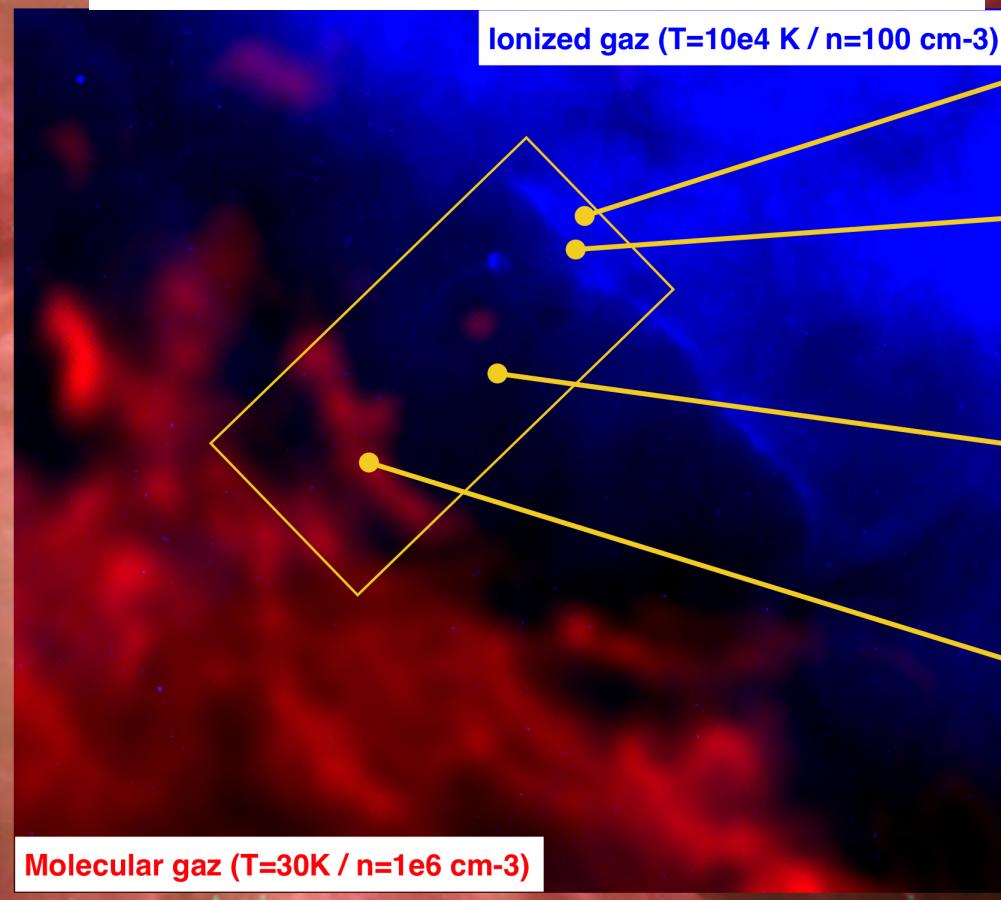
*Radiative feedback from massive stars
as traced by multiband imaging and spectroscopic mosaics*

PI team: Olivier Berné (France), Emilie Habart (France), Els Peeters (Canada)

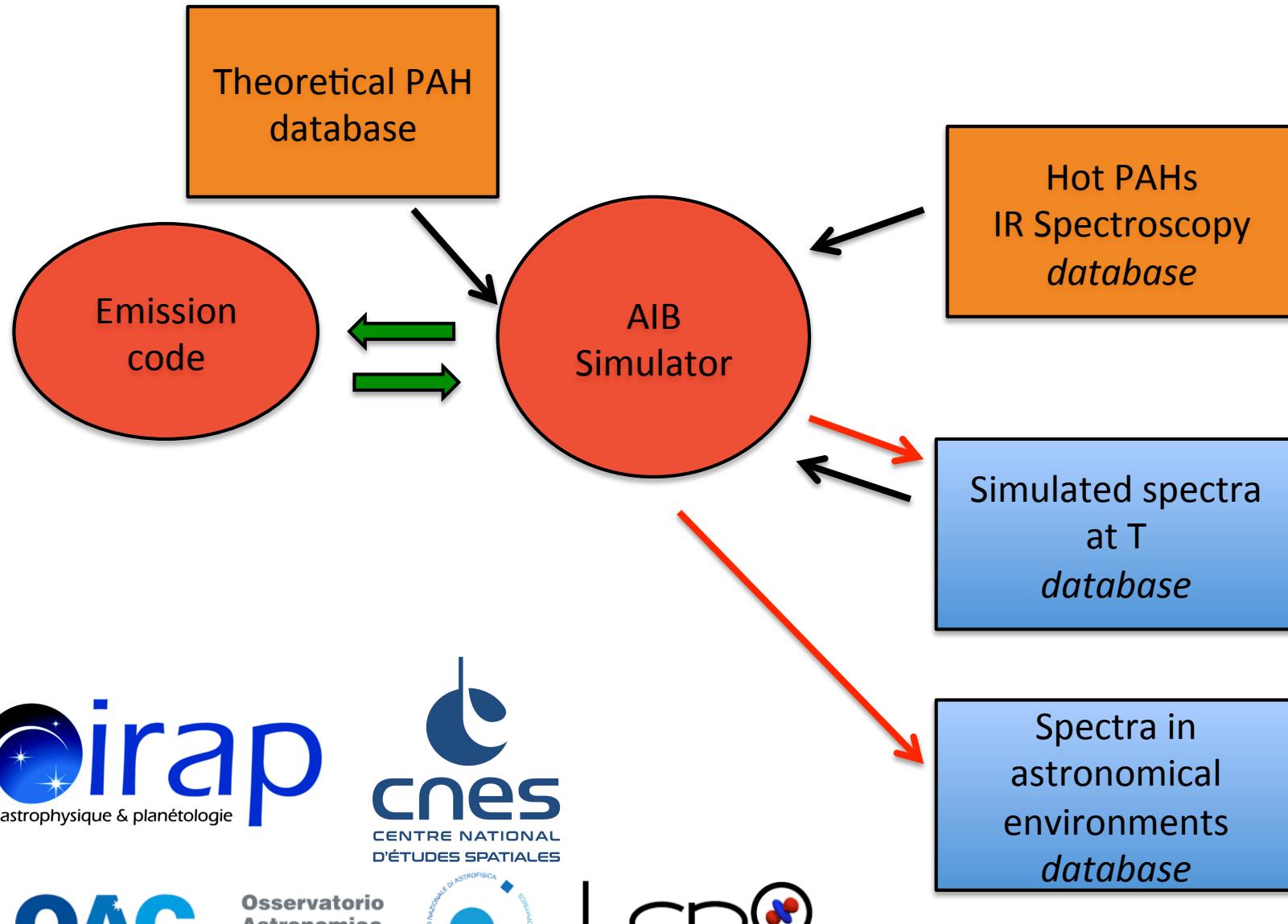
Core team of 19 members (Europe, Canada, US, Japan)

119 Science collaborators from 18 countries

Berné, Habart, Peeters et al., 2022, subm
A&A, eprint arXiv:2201.05112



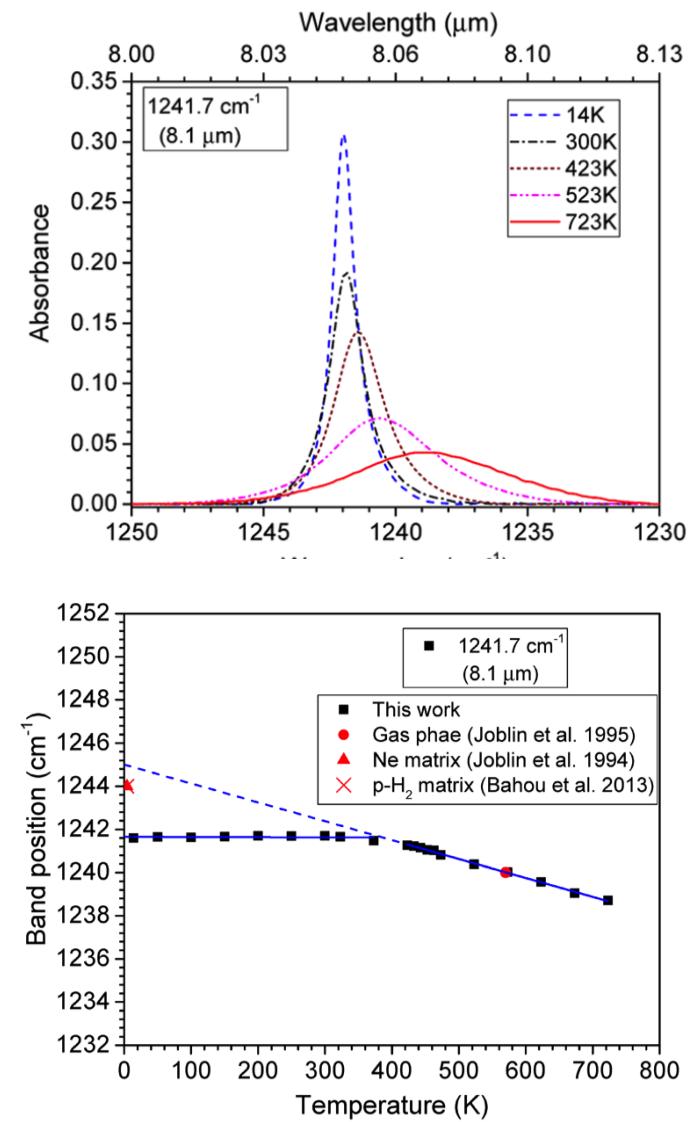
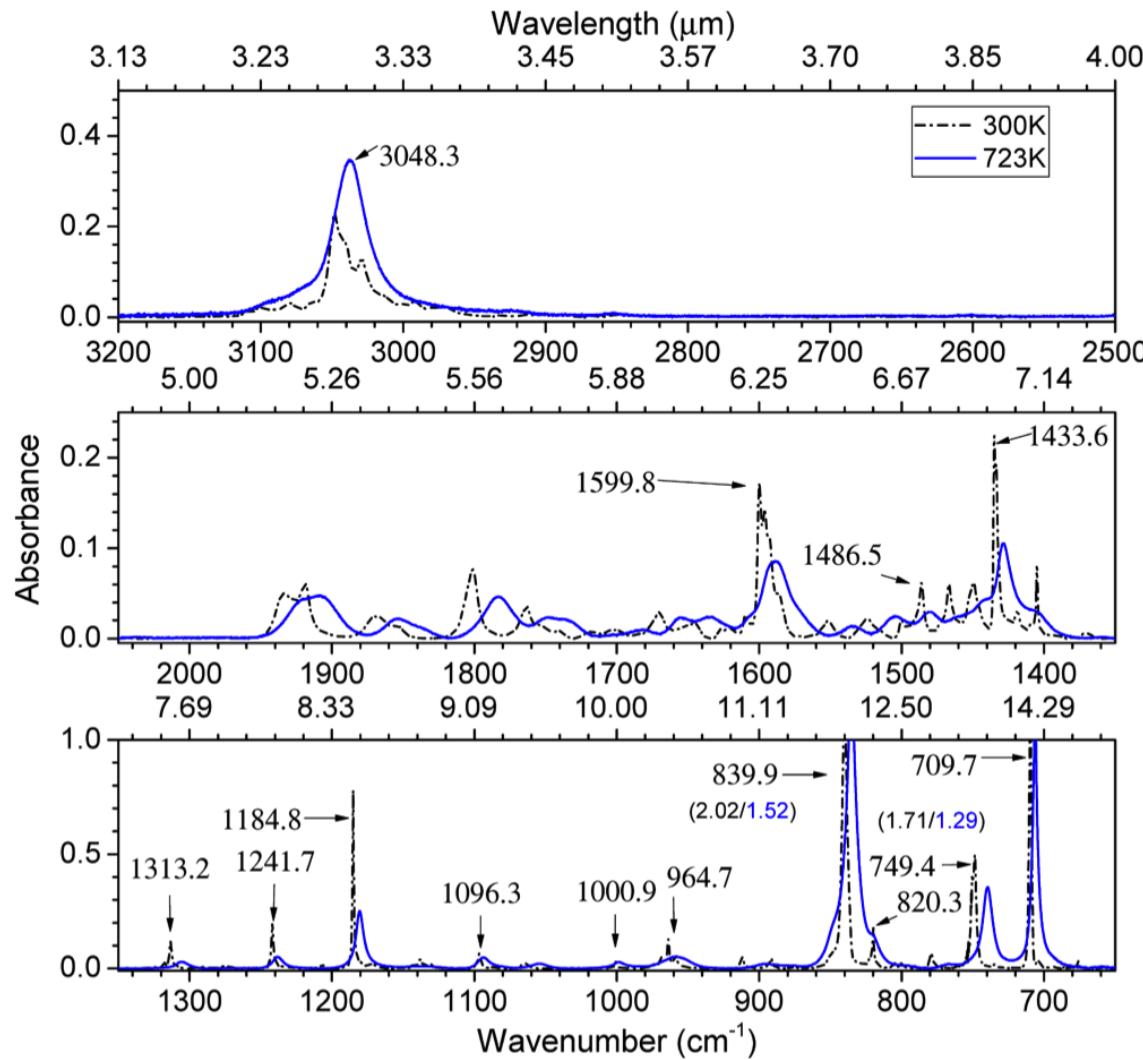
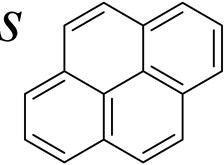
LAIBrary: Library of simulated AIB spectra





IR spectroscopy of hot neutral PAHs

Chakraborty et al., 2019, JPCA 123, 4139

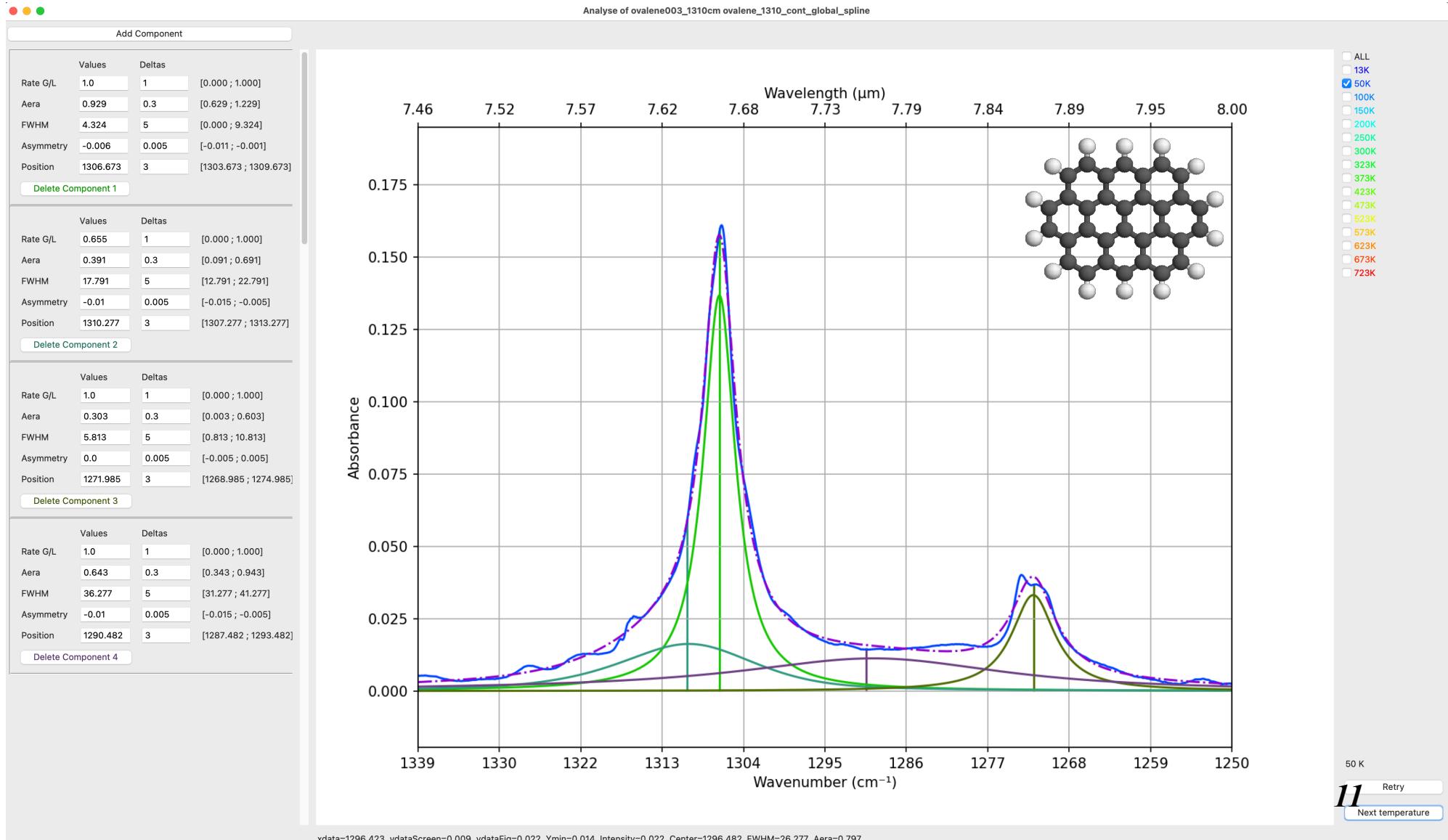


CosmicPAHfit: multicomponent fitting tool

Python3 code

Asymmetric Gaussian + Lorenztian functions

Interactive definition of the components



Hot PAHs IR spectroscopy database

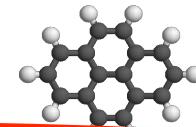
Hot PAHs IR

Show Samples

Profile

Log in

Pyrene : C₁₆H₁₀ - Solid - Experimental



Infos

Full spectrum

Analysed bands & multi-fit

Anharmonicity parameters

Export

Information

Identity

Name	Pyrene
Date	None
Version	1
Operator	UserA, UserB
Contact	emails, tel, etc
Institution	IRAP - Toulouse

Species

Formula	C ₁₆ H ₁₀
Structure	None
Phase	Solid
Origin	Institution Y - Country A
Purity	95.0

Experiment

Category	Experiment
Instrument	ESPOIRS

Instrument: ESPOIRS

Cell	KBr
Sample preparation	Méthode A
Temperature range (K)	14 - 723
Spectral range (cm ⁻¹)	650 - 3200
Spectral resolution (cm ⁻¹)	0,06027
Number of scans	XX
Beam splitter	xxxx123
Source	abc789
Detector	456yyy

Reference

DOI	
-----	--

Hot PAHs IR DB: specific bands

Hot PAHs IR

Show Samples

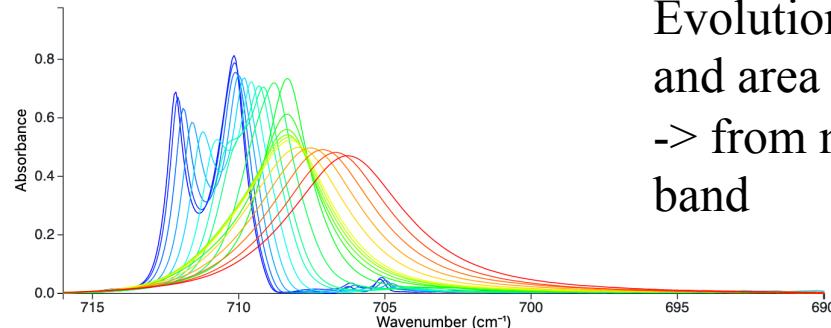
Profile

Log in

Study of mode 711 for Pyrene: C₁₆H₁₀

Download everything:

[Pyrene C₁₆H₁₀ 711.zip](#)



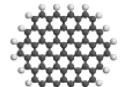
Evolution of peak position, FWHM
and area with temperature
-> from multi-component fit of the
band

Method	Graph	Fit Range (K)	Empirical anharmonicity factors ($\times 10^{-2} \text{ cm}^{-1} \text{ K}^{-1}$)
Area weighted position		[150 ; 723]	-0.8
		[14 ; 150]	-0.3
Area weighted FWHM		[523 ; 723]	0.0071
Area evolution		---	---

Theoretical spectral database of PAHs (Cagliari/ Toulouse)

<http://astrochemistry.oa-cagliari.inaf.it/database/>

Malloci, Joblin, Mulas, Chem. Phys. 332 (2007) 353



Polycyclic aromatic hydrocarbons

Mirrors

- Astronomical Observatory - Cagliari

Resources

- Linux cluster (OAC)
- INAF-CINECA
- CALMIP

Programs

- NWChem
- Octopus

Theoretical spectral database of polycyclic aromatic hydrocarbons

(A red oval highlights Coronene (C₂₄H₁₂))

- Azulene (C₁₀H₈)
- Naphthalene (C₁₀H₈)
- Acenaphthylene (C₁₂H₆)
- Biphenylene (C₁₂H₈)
- Acenaphthene (C₁₂H₁₀)
- Fluorene (C₁₃H₁₀)
- Anthracene (C₁₄H₁₀)
- Phenanthrene (C₁₄H₁₀)
- Pyrene (C₁₆H₁₀)
- Tetracene (C₁₈H₁₂)
- Chrysene (C₁₈H₁₂)
- Triphenylene (C₁₈H₁₂)
- Benzo[a]anthracene (C₁₈H₁₂)
- Corannulene (C₂₀H₁₀)
- Perylene (C₂₀H₁₂)
- Benzo[a]pyrene (C₂₀H₁₂)
- Benzo[e]pyrene (C₂₀H₁₂)
- Anthanthrene (C₂₂H₁₂)
- Benzo[g,h,i]perylene (C₂₂H₁₂)
- Pentacene (C₂₂H₁₄)
- Coronene (C₂₄H₁₂)
- Dibenzop[cd,im]chrysene (C₂₄H₁₄)
- Dibenzo[cd,lm]perylene (C₂₆H₁₄)
- Hexacene (C₂₆H₁₆)
- Bisanthene (C₂₈H₁₄)
- Benzo[a]coronene (C₂₈H₁₄)
- Dibenzo[bc,kl]coronene (C₃₀H₁₄)
- Dibenzo[bc,ef]coronene (C₃₀H₁₄)
- Terrylene (C₃₀H₁₆)
- Ovalene (C₃₂H₁₄)
- Tetrabenzocoronene (C₃₆H₁₆)
- Circumbiphenyl (C₃₈H₁₆)
- Circumanthracene (C₄₀H₁₆)
- Quaterrylene (C₄₀H₂₀)
- Circumpyrene (C₄₂H₁₆)
- Hexabenzocoronene (C₄₂H₁₈)
- Dicoronylene (C₄₈H₂₀)
- Pentarylene (C₅₀H₂₄)
- Circumcoronene (C₅₄H₁₈)
- Circumovalene (C₆₆H₂₀)

Maintained by G. Malloci

Last modified: Fri Mar 2 13:56:19 CET 2007

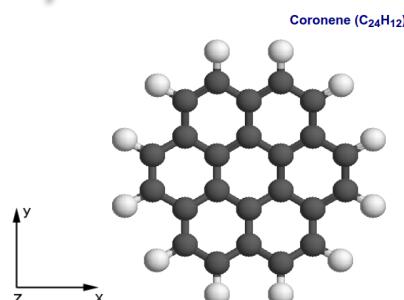


Carbon clusters

- Contribute
- Citation
- Acknowledgements

Links

- OAC - Cagliari
- Physics Dept - Cagliari
- IRAP - Toulouse
- The Astrochymist
- PAHs in Wikipedia
- Diffuse interstellar bands



- NIST WebBook page
- General properties
- Ground-state optimized geometries
- Harmonic vibrational frequencies
- Anharmonic vibrational spectrum
- Photo-absorption cross-sections
- Bibliographic references

The fully relational database

- 2018: partly connected to the VAMDC portal
https://portal.vamdc.eu/vamdc_portal/home.seam



Home VAMDC databases Guided query Advanced query Saved queries | Discr

Choose a request type ([reset page](#))

By species
 For radiative process
 For collisional process

Please, enter the number of species you wish to query

Number of atoms

Number of molecules

Number of particles

[Validate](#) [Add more](#)

Molecule

Chemical name Anthracene

Stoichiometric formula

Structural formula

Spin isomer

Standard InChIKey

Results by node						
Name	Response	Last database update	Download	Species	States	
KIDA: Kinetic Database for Astrochemistry - TAP service	OK	Not available	XSAMS file	6	0	
Photodissociation - MolD database	OK	Not available	XSAMS file	0	0	
Theoretical spectral database of polycyclic aromatic hydrocarbons	OK	Not available	XSAMS file	4	66	
VAMDC species-DB	OK	Not available	XSAMS file	4	0	

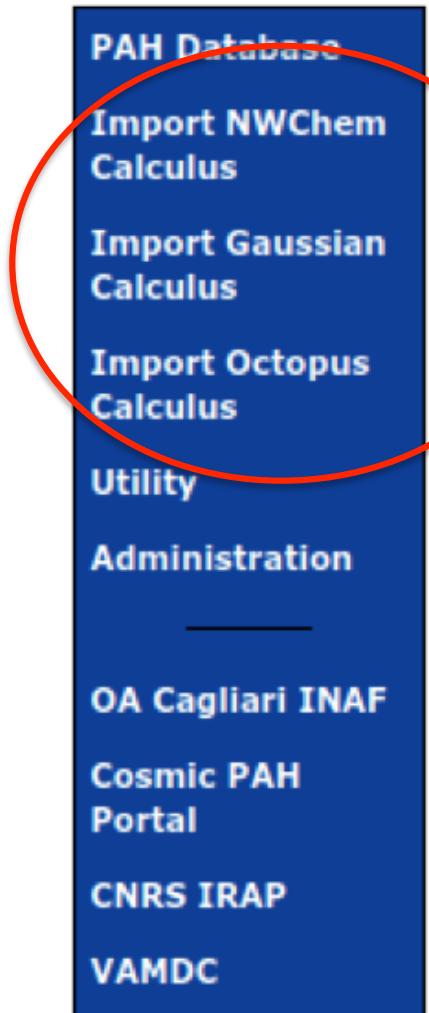
To be done:

- Develop tools for automatic (supervised) data ingestion (import from QChem codes)
<https://qchitool-pah-dev.oa-cagliari.inaf.it/>
- Implement the new database at
<astropah-qcalcs.oa-cagliari.inaf.it> and
<astropah-qcalcs.irap.omp.eu>

Theoretical spectral database of Polycyclic Aromatic Hydrocarbons

Improved QChiTool

<https://qchitool-pah-dev.oa-cagliari.inaf.it>



The screenshot shows the 'Import calculus' page. The title is 'Import calculus' and the subtitle is 'gaussian import'. A red arrow points from the 'Select what to import...' box in the previous screenshot to this page. The main content area displays a warning message: 'Calculation NOT Found in QChiTool DB' and 'Choose tasks to save :'. It lists two tasks:

- Task 0 - Warning : No Checkpoint File Found
 - Theory: DFT
 - Operation: OPTIMIZE
 - Molecule: Warning : Molecule NOT Found in DB
 - Formula: C60H₂
 - Inchi: 1S/C60H₂ /c1-2-5-6-3(1)-8-12-10-4(1)-9-11-7(2)-17-21-13(5)-23-24-14(6)-22-18(8)-28-20(12)-30-26-16(10)-15(9)/h1,5H/t1-,5+
 - InchiKey: TUYISFDQPLCFIA-CUODSJINSA-N
 - Aromatic Cycles: 0
 - Charge: 0
- Task 1
 - Theory: DFT
 - Operation: FREQUENCIES
 - Molecule: Warning : Molecule NOT Found in DB
 - Formula: C60H₂
 - Inchi: 1S/C60H₂ /c1-2-5-6-3(1)-8-12-10-4(1)-9-11-7(2)-17-21-13(5)-23-24-14(6)-22-18(8)-28-20(12)-30-26-16(10)-15(9)/h1,5H/t1-,5+
 - InchiKey: TUYISFDQPLCFIA-CUODSJINSA-N
 - Aromatic Cycles: 0
 - Charge: 0

At the bottom right of the page, there are 'Cancel' and 'Continue >' buttons. The 'Continue >' button is circled in red. The footer at the bottom of the page includes links: Home, About Us, PAH Database, Our Services, and Contact Us.

Theoretical spectral database of Polycyclic Aromatic Hydrocarbons

Improved QChITool <https://qchitool-pah-dev.oa-cagliari.inaf.it>

Molecules

Name	Formula	Weight (u.)
Benzene	C ₆ H ₆	78.047
Chrysene	C ₁₈ H ₁₂	228.094
Corannulene	C ₂₀ H ₁₀	250.078
Corannulene	C ₂₀ H ₁₀ +	250.078
Coronene	C ₂₄ H ₁₂	300.094
Ovalene	C ₃₂ H ₁₄	398.110
HexaBenzoCoronene	C ₄₂ H ₁₈	522.141
C ₆₀ H ₂ test2	C ₆₀ H ₂	722.016

PAH Database

- Import NWChem Calculus
- Import Gaussian Calculus
- Import Octopus Calculus
- Utility
- Administration

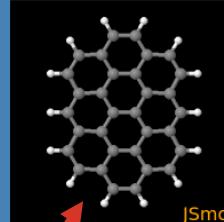
OA Cagliari INAF

- Cosmic PAH Portal
- CNRS IRAP
- VAMDC

O
Animated, interactive visualization

Ovalene (C₃₂H₁₄)

Molecular Formula: C₃₂H₁₄
 Mass: 398.109550 u.
 InChIKey: LSQODMMMSXVCN-UHFFFAOYSA-N
 InChI: 1S/C32H14/c1-2-16-6-10-20-14-22-12-8-18
 Related Molecules



JSmol: an open-source Java viewer for chemical structures in 3D. <http://www.jsmol.org/>

Electronic States :

Task: FREQUENCIES C₃₂H₁₄/0 DFT/B3LYP/4-31G

Energy (eV)	Description	Multiplicity	Symmetry
-1226.41400	S ₀	1	-
Is Minimum	Theory Level	Basis Sets	
no	DFT B3LYP	4-31G	<input type="button" value="Load geometry"/>

Rotational Constants (cm ⁻¹)	a	b	c
	0.00795	0.00491	0.00304

Dipole Moments (Debye)	mu_x	mu_y	mu_z
	0.00000	0.00000	0.00000

Vibration Analysis

Harmonic: link
Anharmonic: None

Vibration Analysis Harmonic :

#	Frequency (cm ⁻¹)	IR Intensity (km/mol)	Symmetry
1	63.37200	0.00000	-

- All service (DB, QChITool, VAMDC node) is containerized. Mirroring/failover policy needs to be defined (between OAC and IRAP).

Theoretical spectral database of PAHs -status

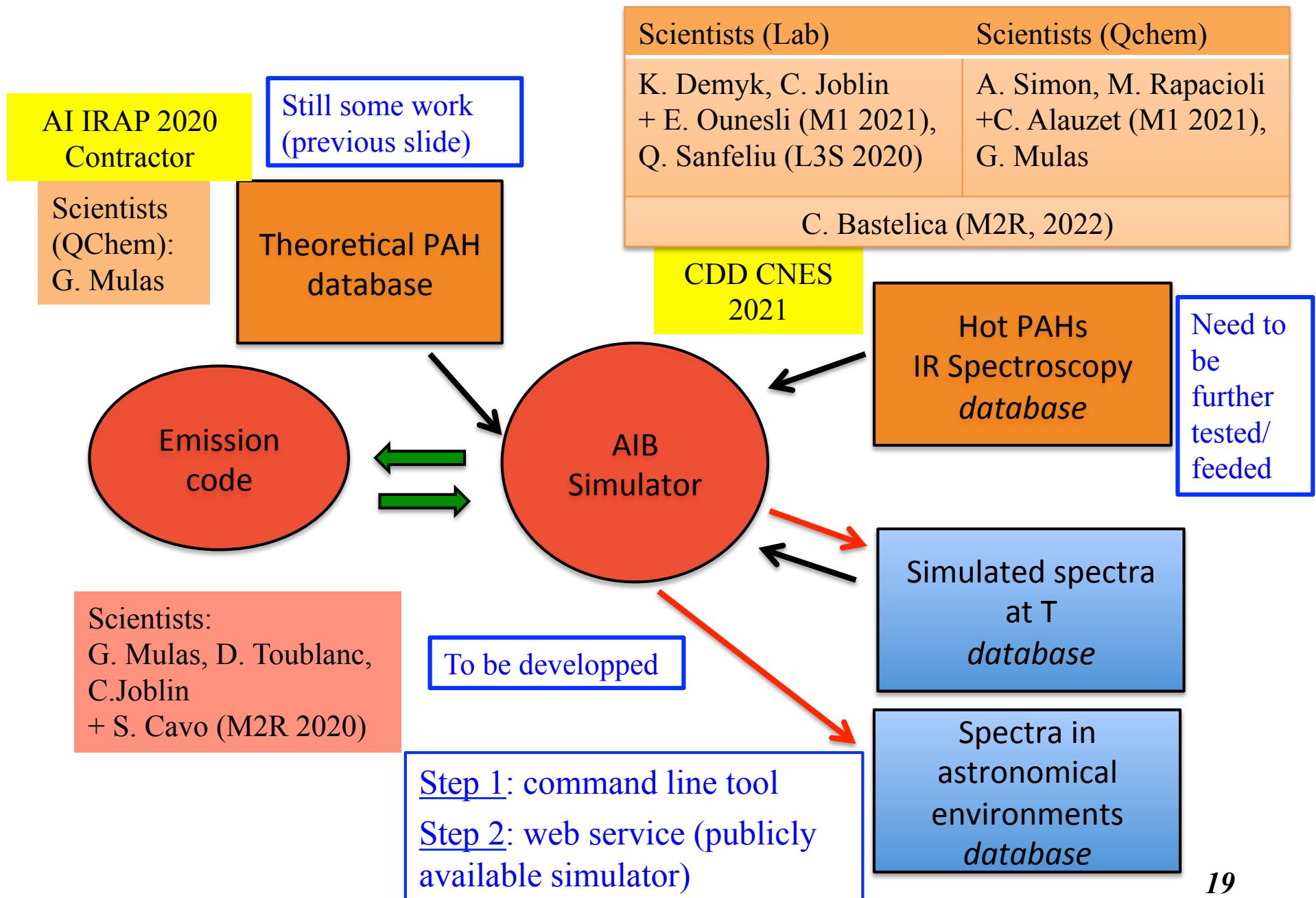
QChITool:

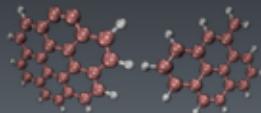
- import of Gaussian and NWChem calcs working and deployed;
- web visualisation of DB contents working but should be improved with testing & feedback
- import of octopus calcs in final development, almost ready
- service containerized, but mirroring/failover policy to be defined

VAMDC node:

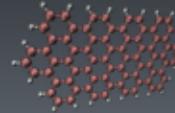
- service containerized, but mirroring/failover policy to be defined
- upgrade VAMDC node software to adapt to slight modifications of DB structure that come with the new QChITool; till then it works but we cannot import calcs supported only by new QChITool.
- port VAMDC node software to python 3, works fine but still runs on python 2 (will soon become unsupported)

LAIBrary - status





Cosmic PAH portal

 [Recent Changes](#) [Media Manager](#) [Sitemap](#)[News](#)[Activities](#)[Platforms](#)[Production](#)[Databases](#)[Tools](#)[Teams](#)

DATABASES

- ✓ **AROMA database** This is a mass spectrometry database providing information on the molecular content of meteorites, stardust analogues and soot samples. Targeted molecules include polycyclic aromatic hydrocarbons, carbon clusters, fullerenes and various hydrocarbons.

It is accessible via the AROMA DB web application:



 <http://aroma.irap.omp.eu/>

- ✓ **Theoretical spectral database of polycyclic aromatic hydrocarbons**



 <http://astrochemistry.oa-cagliari.inaf.it/database/>

 <https://qchitool-pah-dev.oa-cagliari.inaf.it/>

- ✓ **Hot PAHs IR spectroscopy** *in progress*

- ✓ **Simulated IR spectra at T** *in progress*

- ✓ **IR spectra in astronomical environments** *in progress*



TOOLS

* PAHTAT

Description

The PAHTAT tool aims to analyze astronomical mid-infrared spectra containing PAH emission. It uses spectral templates that were derived from observations.  <https://doi.org/10.1051/0004-6361/201015915>

Tool access  <http://userpages.irap.omp.eu/~cjoblin/PAHTAT/Site/PAHTAT.html>

* mMass_updated

→ AROMA DB

Description

mMass_updated is a modified version of  mMass with new functionalities such as double bond equivalent calculation and separation into families of compounds (compatible with 64-bit MacOS). [More](#)

Tool access *planned in 2022*

* Qchitool

→ Theoretical database of PAHs

Description

QChITool is a web application for easy extraction of information from the log files of some quantum chemistry calculations, and import in the theoretical PAH database. [More](#)

Tool access  <https://qchitool-pah.oa-cagliari.inaf.it> (restricted use of the tool to add data to the PAH database)

cosmicPAHmf

→ Hot PAHs IR spectroscopy

Description

cosmicPAHmf provides a multi-component spectral fit and a graphical interface to derive area-weighted peak position and width of selected infrared features. [More](#)

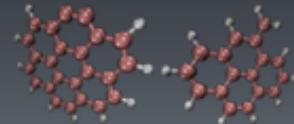
Tool access *planned in 2022*

* AIBsimulator

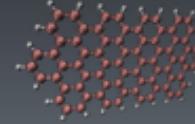
→ LAIBrary project

Description

The AIBsimulator is a simulator for a fast calculation of the emission of a given PAH in a given radiation field. The synthetic spectra are based on theoretical and experimental molecular data. [More](#)



Cosmic PAH portal



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<http://cosmic-pah.irap.omp.eu>

Table of Contents

COSMIC PAH portal

Description

Polycyclic aromatic hydrocarbons (PAHs) and related molecular species (e.g. fullerenes) are key species in astrophysical environments. The primary objective of the Cosmic PAH portal is to ease access to databases and tools in order to:

- **Identify** these species in astrophysical environments and in extraterrestrial samples.
- **Understand** their formation pathways and their link with related molecular species such as carbon clusters and fullerenes.
- **Model** their evolution in astrophysical environments and their impact on the physical and chemical conditions.

Link content

- **Molecular databases** developed by the team, both theoretical and experimental.
- **Simulated spectra databases** for PAH infrared emission in various astrophysical environments.
- **Spectral analysis tools** to analyze in a consistent way spectra from experiments, theoretical calculations, and astrophysical observations.
- **Tools to model spectra** in astrophysical environments using experimental and theoretical data.

- Portal publicly available on 08/2021
- Need to improve the design of the web portal
- Tools, DBs & services: Limited manpower. “Tâche de service” → “Labelisation”