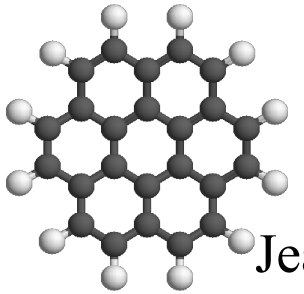


Cosmic PAHs

Christine Joblin, Hassan Sabbah, Karine Demyk

Jean-Michel Glorian, Axel Pérignon (05/22-12/22, CDD CNES),
Emma Charbonnel (11/20-7/21; M2 alternance)

Institut de Recherche en Astrophysique et Planétologie
Université de Toulouse [UPS] – CNRS

Giacomo Mulas, (Andrea Saba)
INAF, Osservatorio Astronomico di Cagliari
IRAP, Toulouse

Réunion OV-GSO, IRAP, Toulouse
10/03/2022

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)*

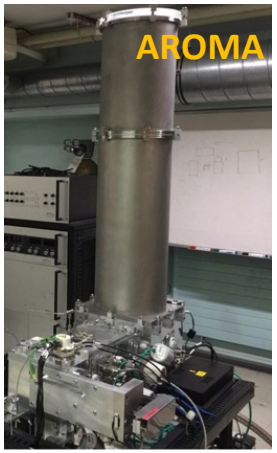
  → Hot PAHs IR web application, CosmicPAHmfit desktop application

  → 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: dokuwiki

AROMA DB: Mass spectrometry



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

AROMA DB

Show Samples

Search Data

FAQ

Contact

Murchison

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

Infos | Spectrum | Data | Family Analysis | Dbe | Media | Export

Identity

Name:	Murchison
Date:	2016-06-21
Version:	1
Operator:	Hassan Sabbah
Contact:	hassan.sabbah@irap.omp.eu
Institution:	IRAP

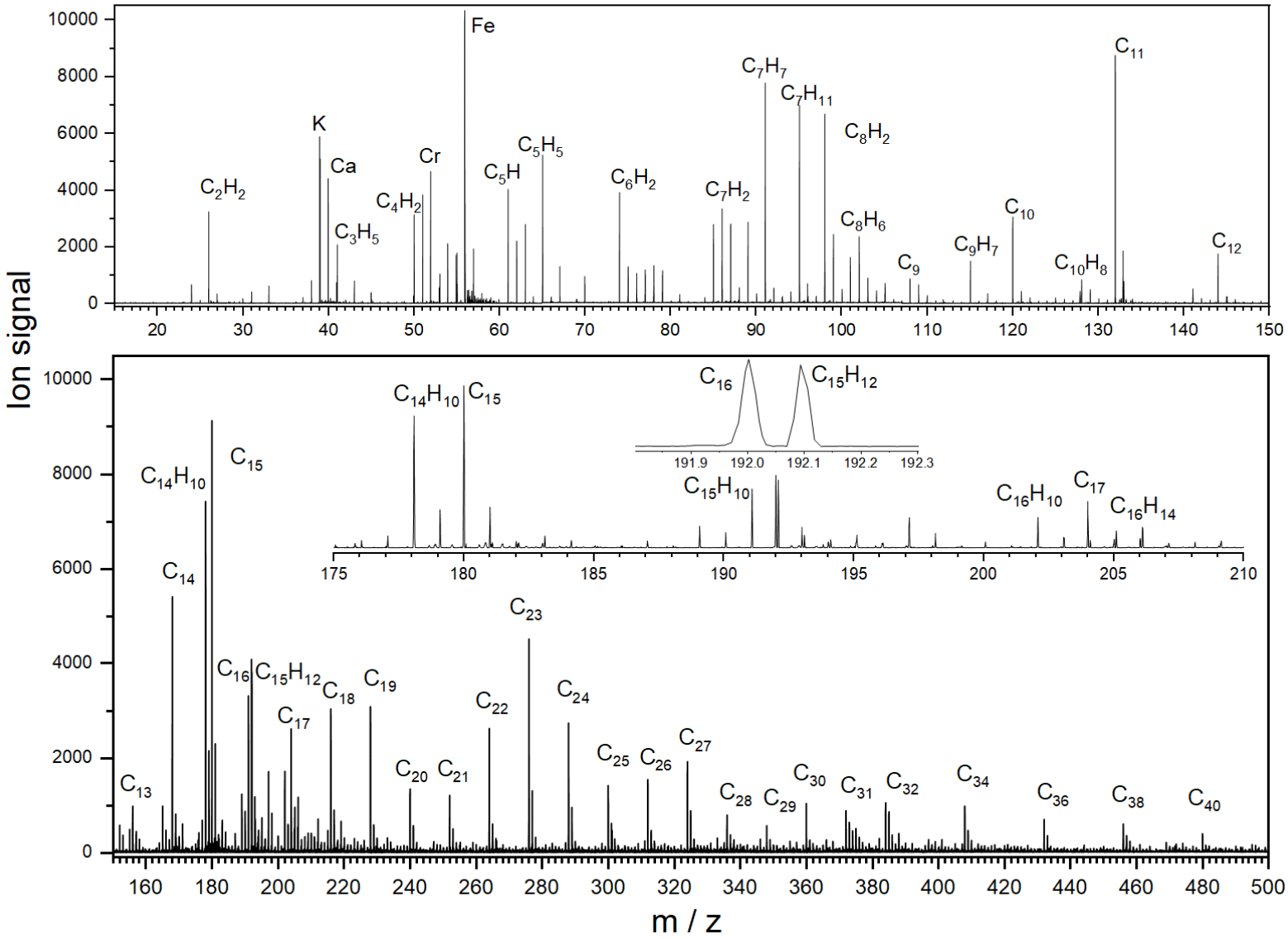
Description

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

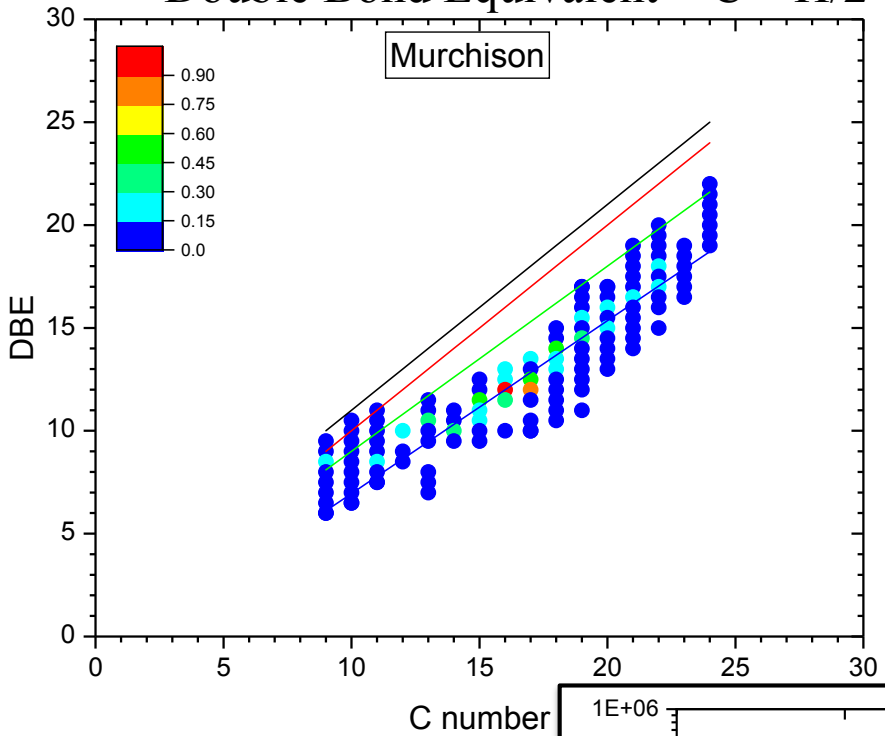
Sabbah et al., 2021, Astrophys. J., subm

Almahata Sitta #04

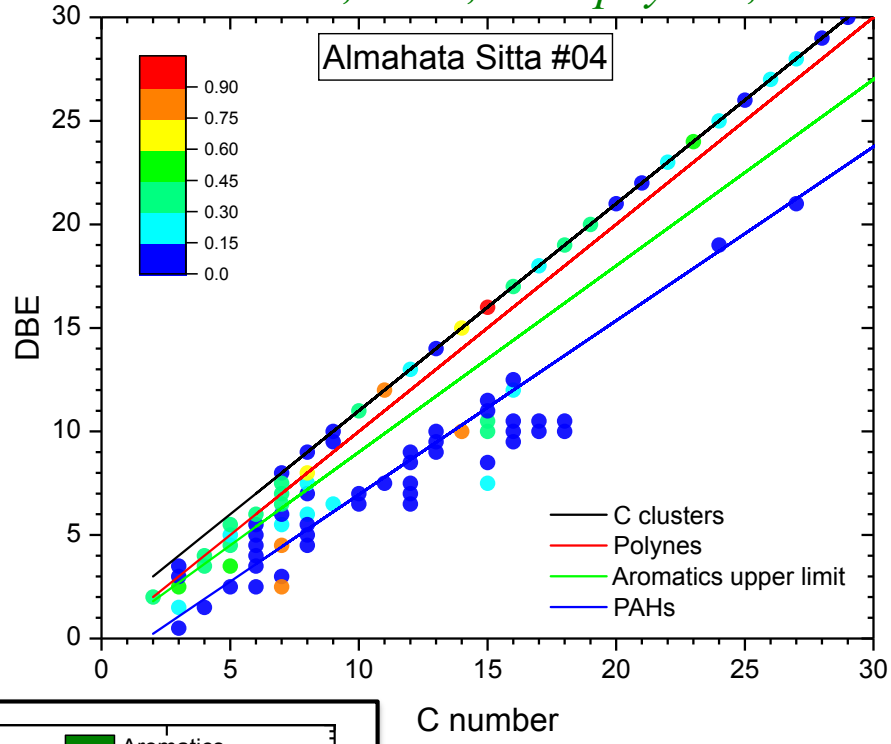


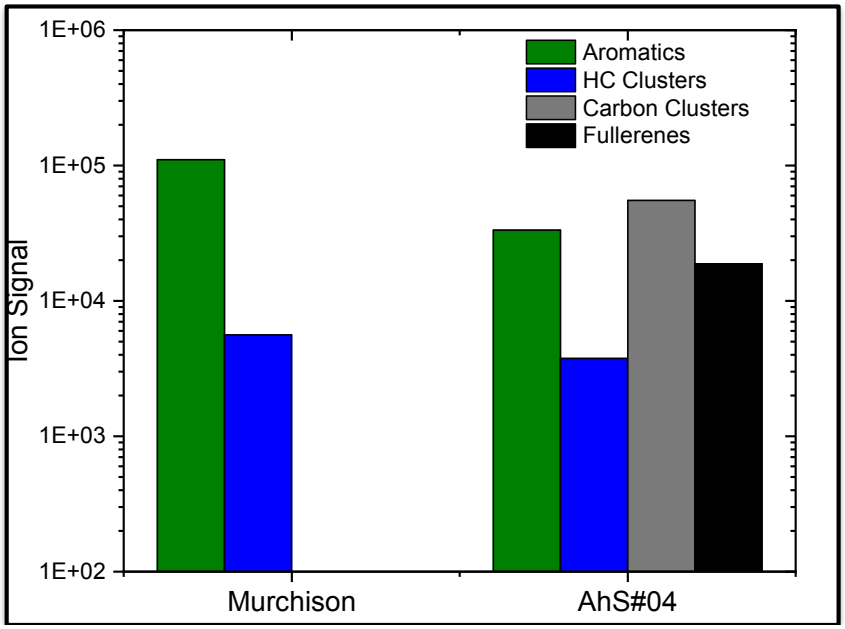
Classification of carbonaceous molecular families

Double Bond Equivalent = C – H/2 + 1



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

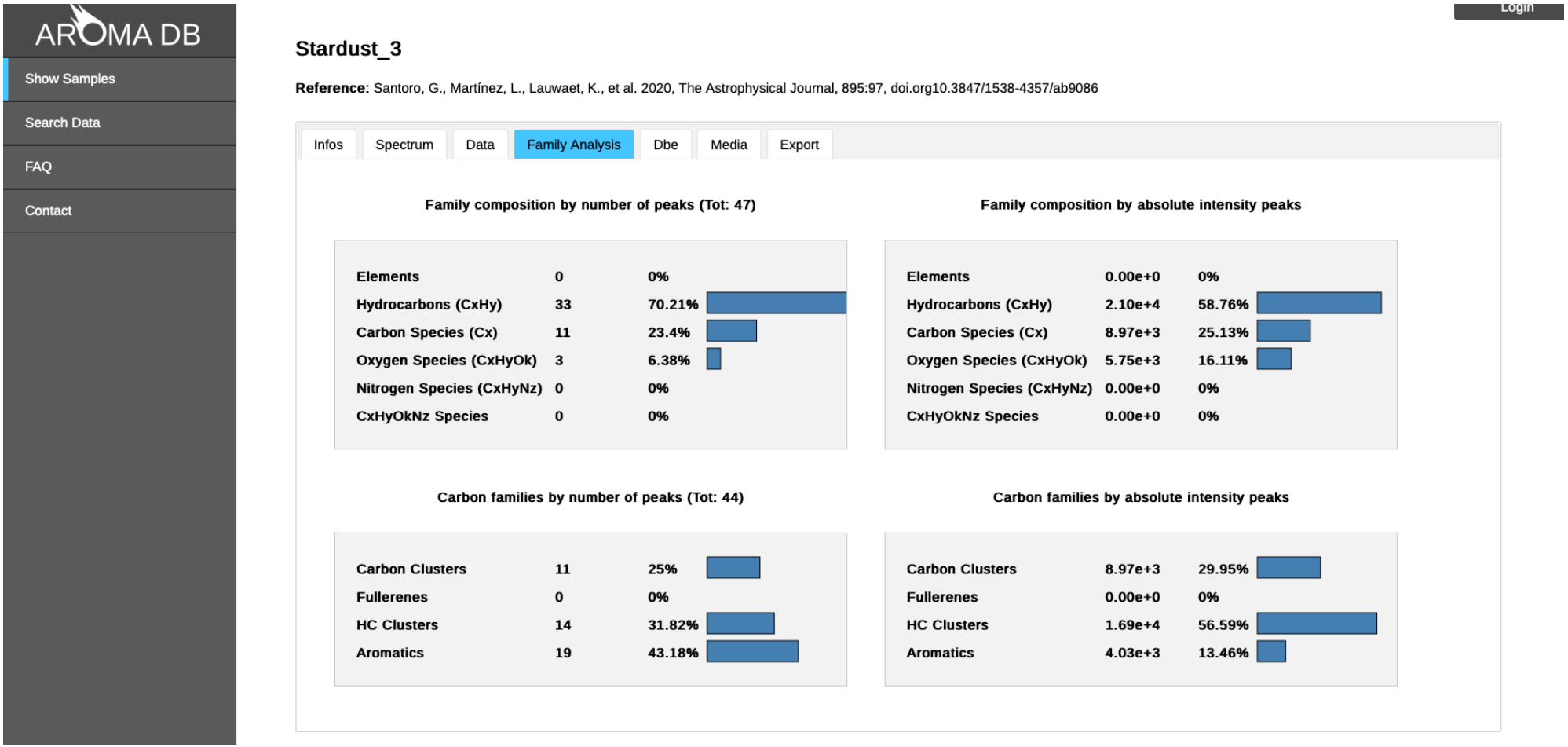




→ Different chemistries involved?

AROMA DB: family analysis

Analysis tools



AROMA DB: Status

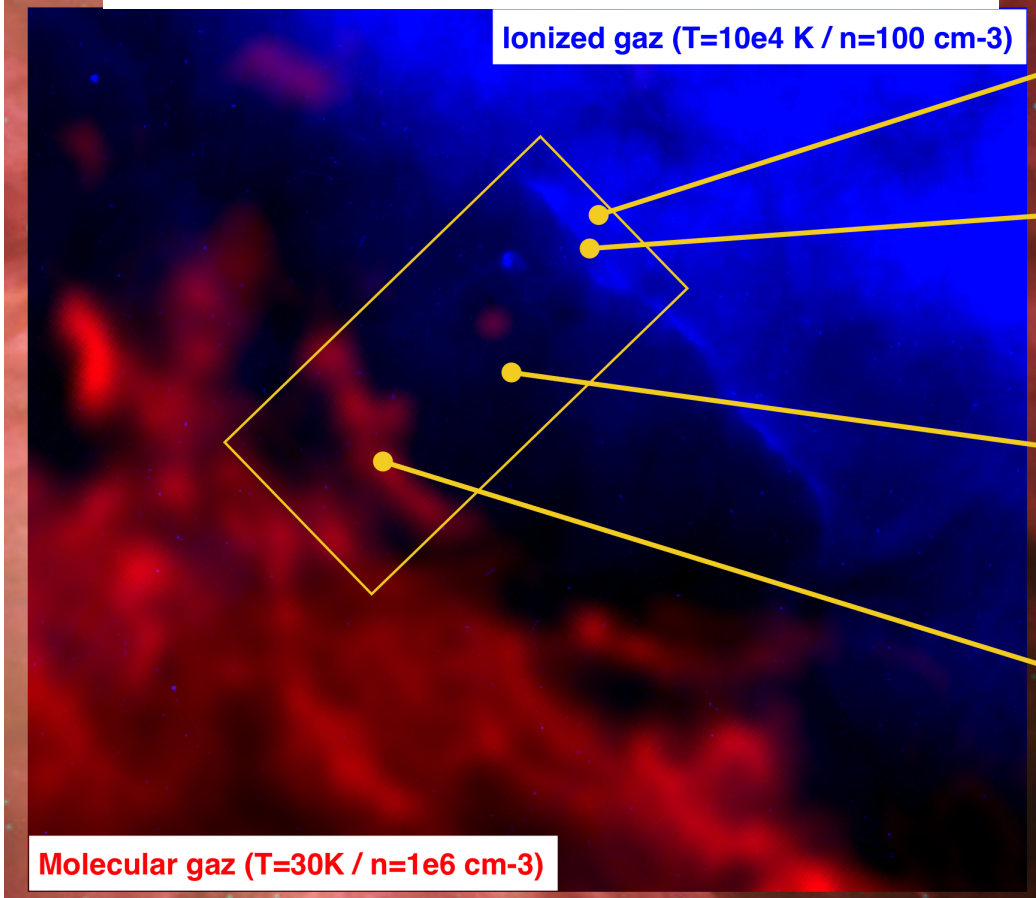
- Database publicly available on 10/2020
- Tools connected to the DB + mmass software (updated version mmass_IRAP)
- 05/2020 - 08/2020: mmass software development, upgrade for mac OS 64-bits. (Student project in OVGSO: E. Mauger)
- 11/2020 – 07/2021 : mmass software development by adding several functionalities 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.

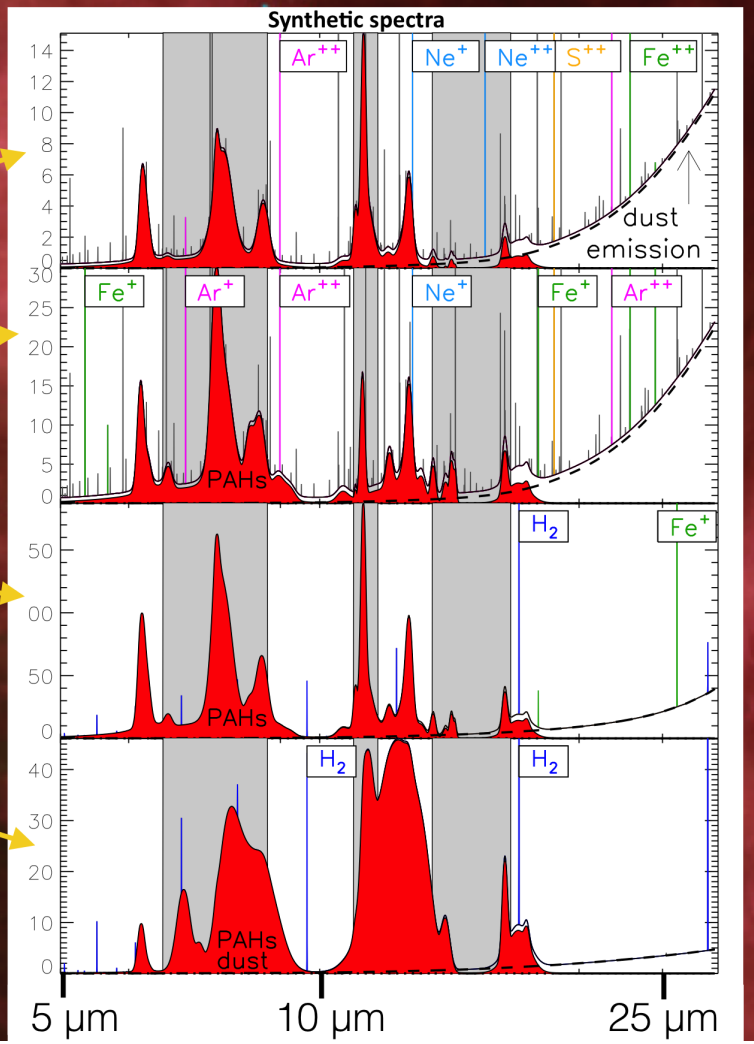
JWST Early Release Science program PDRs4All

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

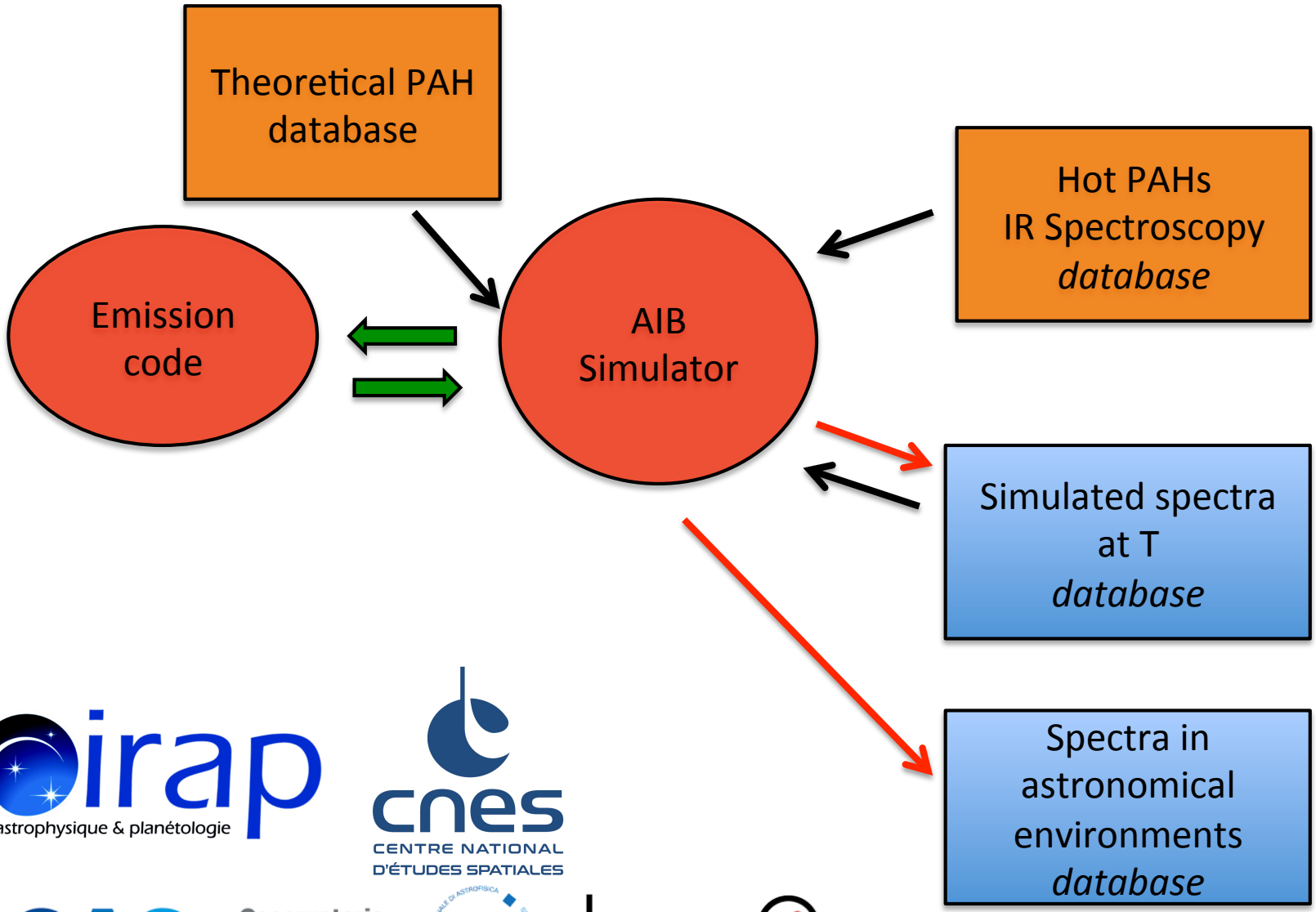
PI team: Olivier Berné (France), Emilie Habart (France), Els Peeters (Canada)
Core team of 19 members (Europe, Canada, US, Japan)
119 Science collaborators from 18 countries

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





LAIBrary: Library of simulated AIB spectra



irap astrophysique & planétologie

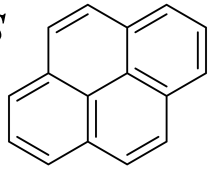
cnes CENTRE NATIONAL D'ÉTUDES SPATIALES

OAC Osservatorio Astronomico di Cagliari

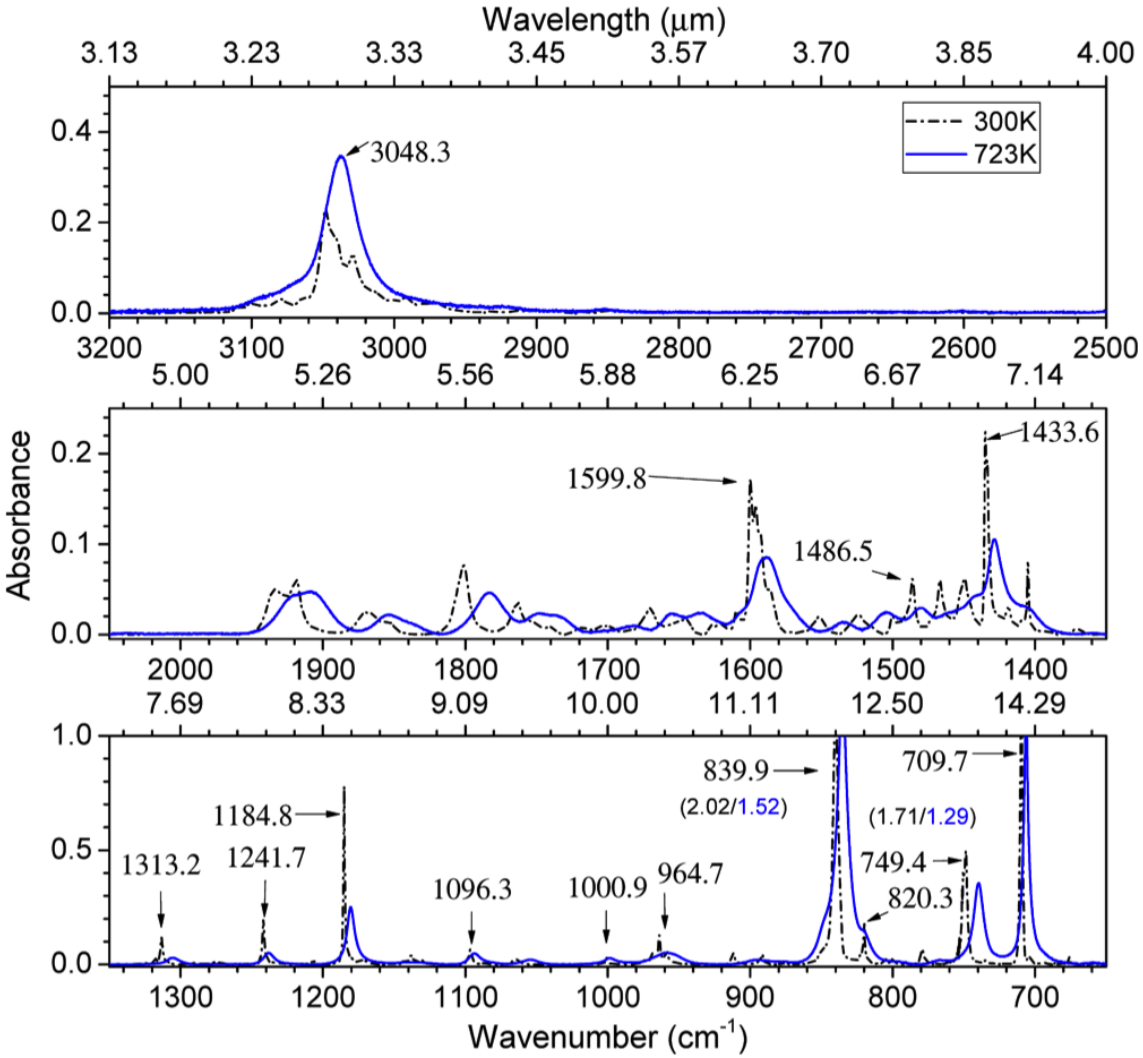
INAF

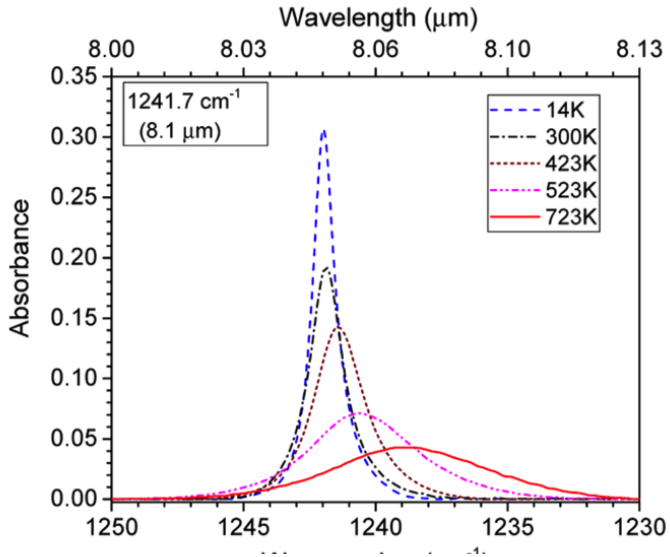
LCPQ Laboratoire de Chimie et Physique Quantiques

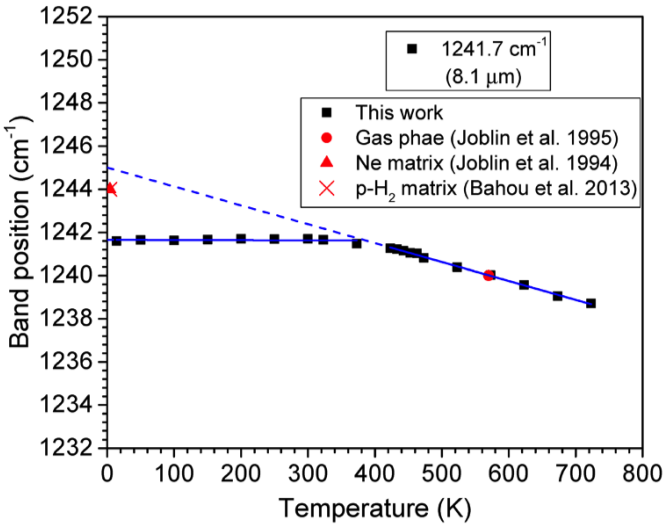
IR spectroscopy of hot neutral PAHs



Chakraborty et al., 2019, JPC A 123, 4139

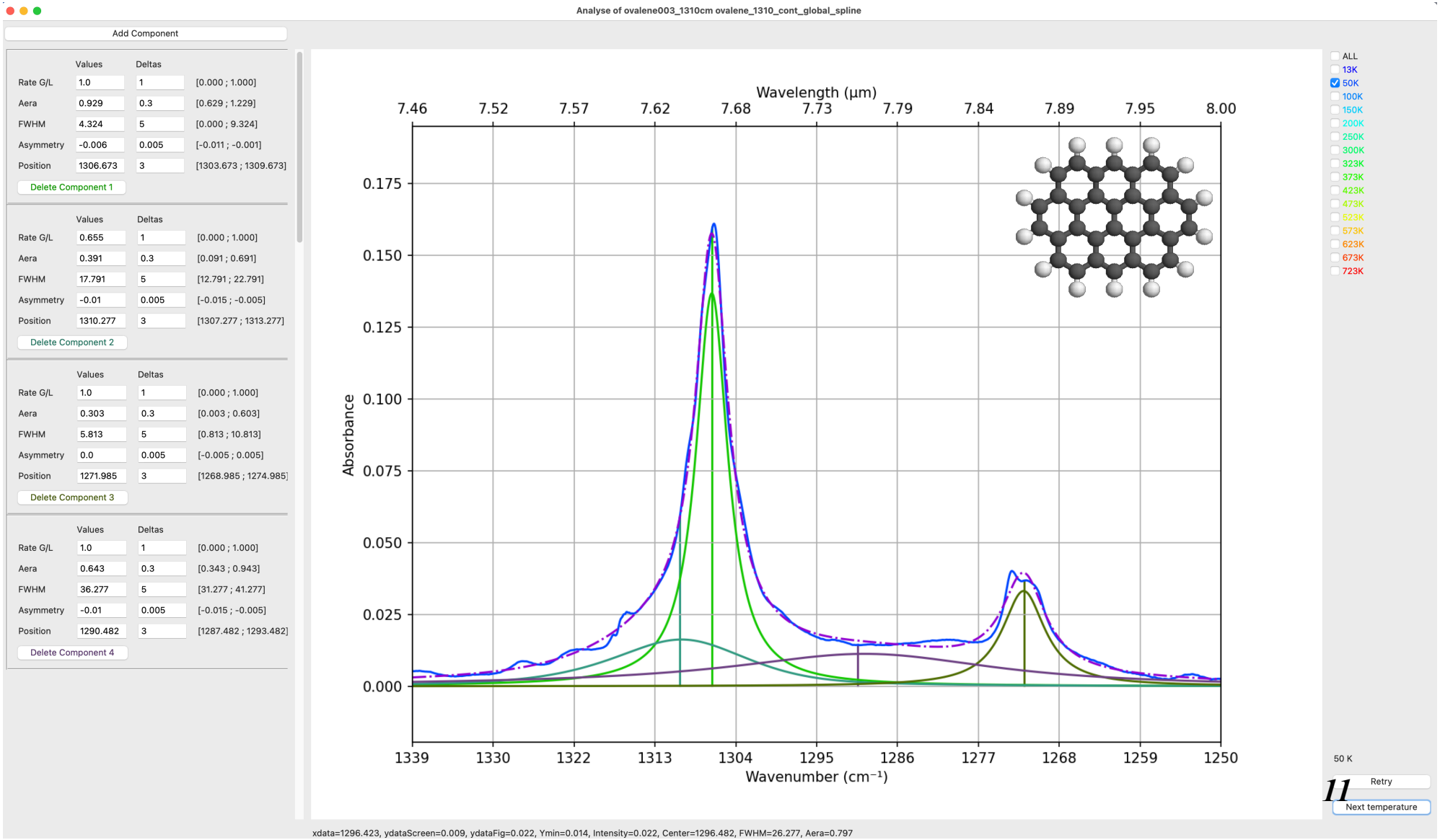






CosmicPAHmfit: multicomponent fitting tool

Python3 code
Asymmetric Gaussian + Lorenztian functions
Interactive definition of the components



Hot PAHs IR spectroscopy database

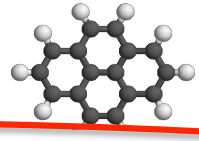
Hot PAHs IR

Show Samples

Profile

Log in

Pyrene : $C_{16}H_{10}$ - 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

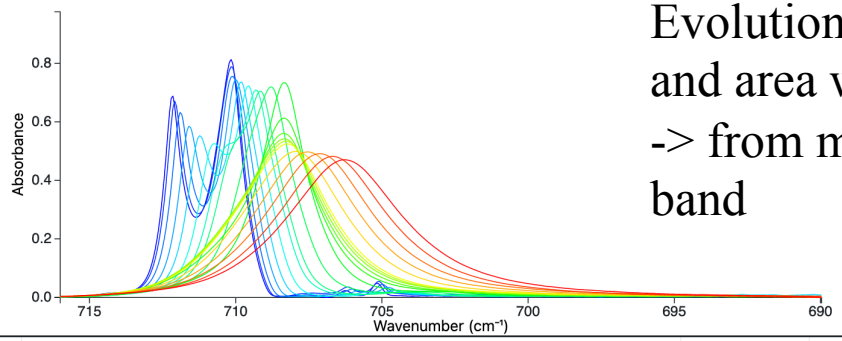
Profile

Log in

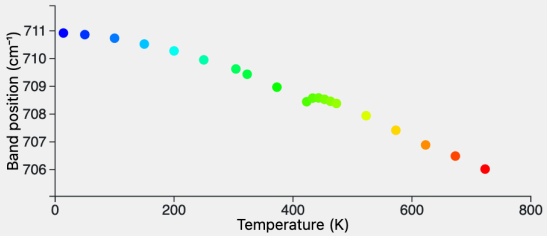
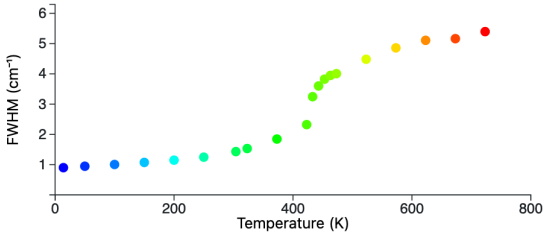
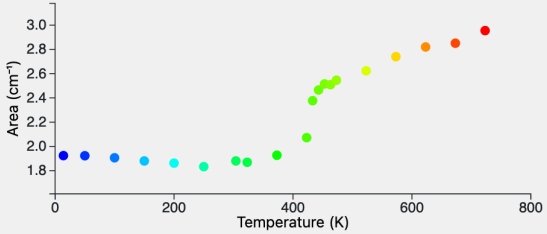
Study of mode 711 for Pyrene: $C_{16}H_{10}$

Download everything:

Pyrene $C_{16}H_{10}$ 711.zip



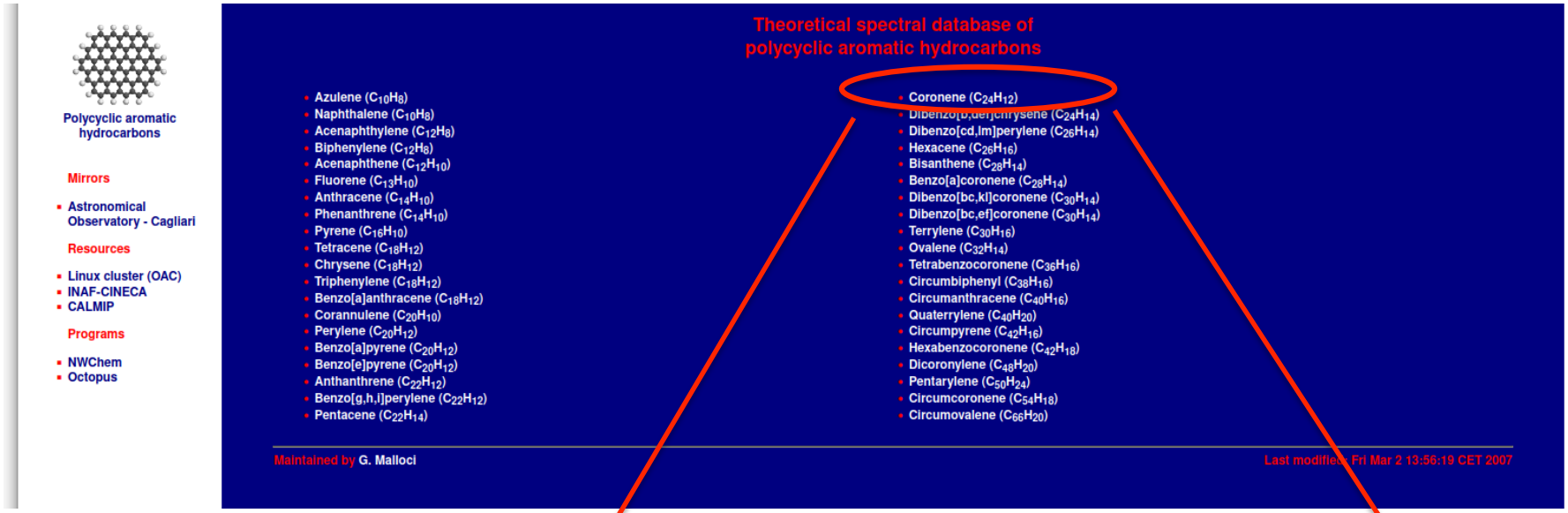
Evolution of peak position, FWHM and area with temperature
-> from multi-component fit of the band

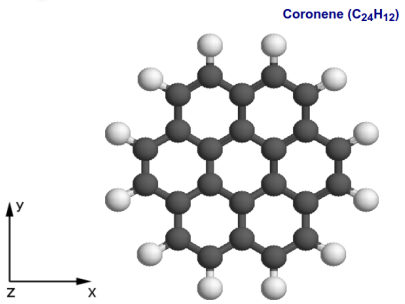
Method	Graph	Fit Range (K)	Empirical anharmonicity factors (×10⁻² cm⁻¹ K⁻¹)
Area weighted position		[150 ; 723] [14 ; 150]	-0.8 -0.3
Area weighted FWHM		[523 ; 723]	0.0071
Area evolution		---	---

Theoretical spectral database of PAHs (Cagliari/ Toulouse)

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

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



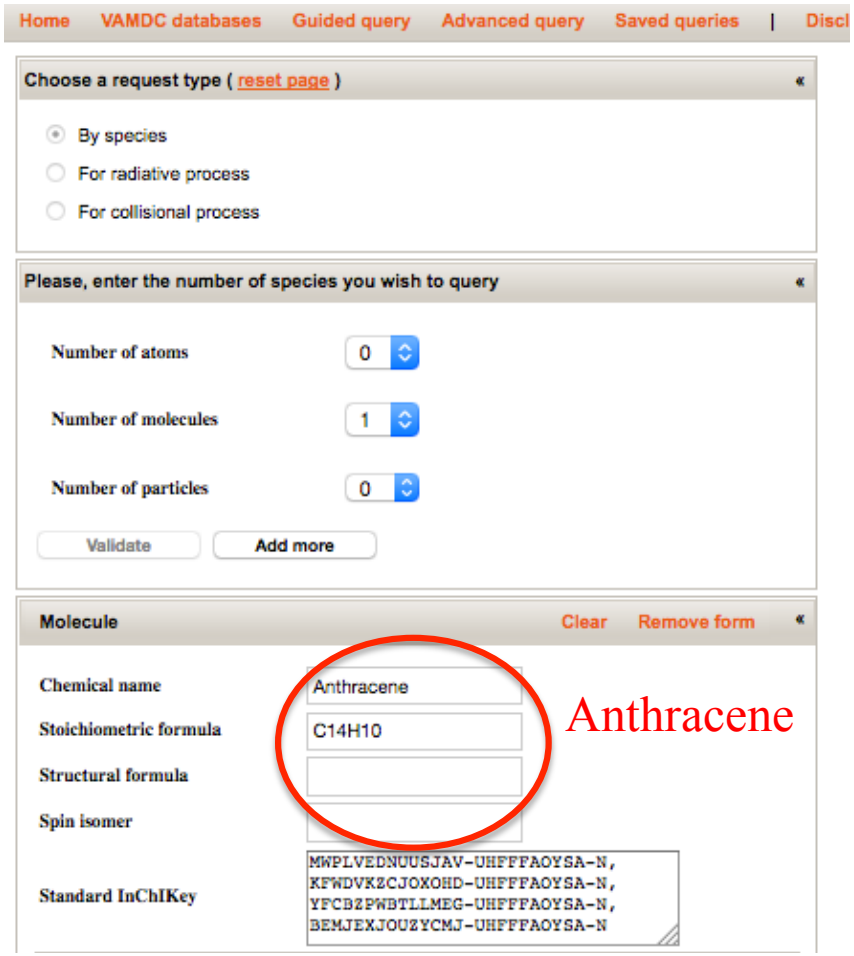


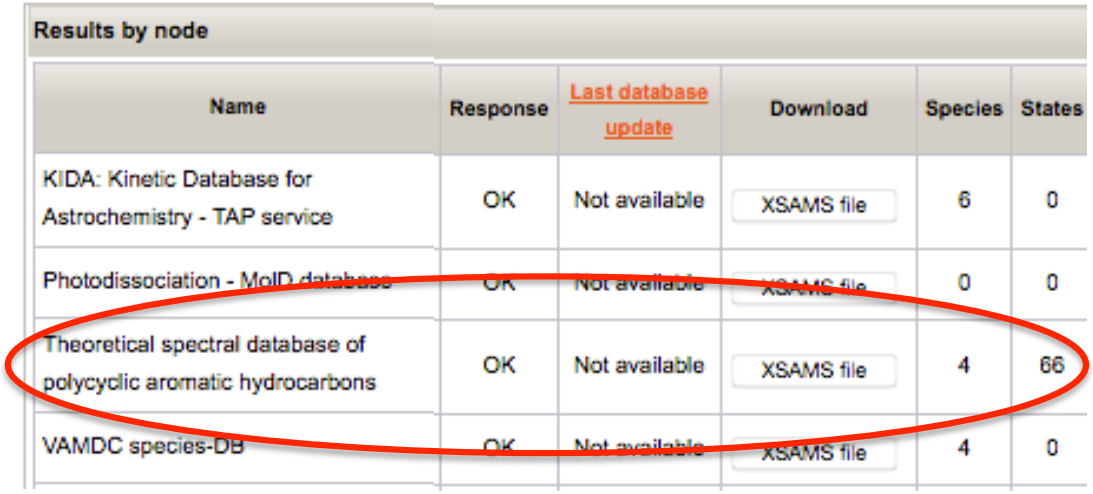
- NIST WebBook page
- General properties
- Ground-state optimized geometries
- Harmonic vibrational frequencies
- Anharmonic vibrational spectrum
- Photo-absorption cross-sections
- Bibliographic references

The fully relational database

- 2018: partly connected to the VAMDC portal

https://portal.vamdc.eu/vamdc_portal/home.seam





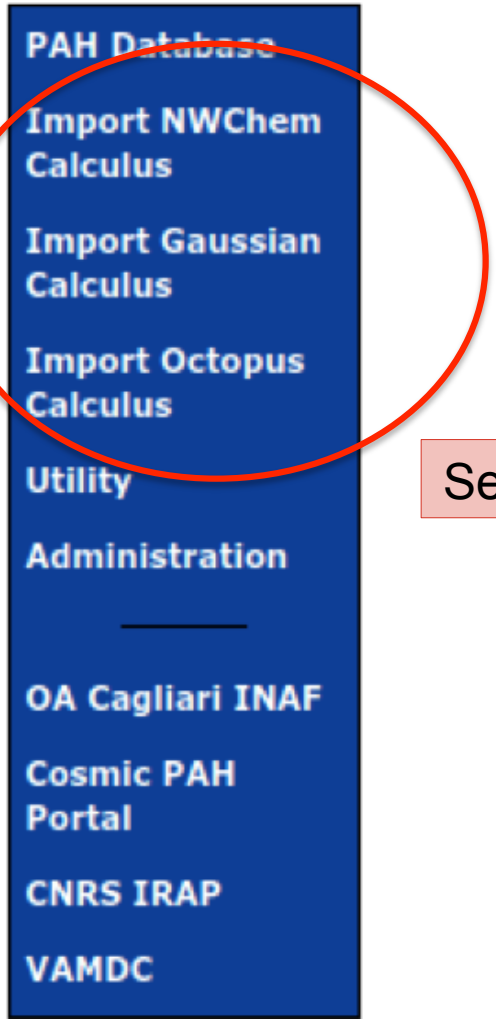
To be done:

- Develop tools for automatic (supervised) data ingestion (import from QChem codes) *https://qchitool-pah-dev.oa-cagliari.inaf.it/*

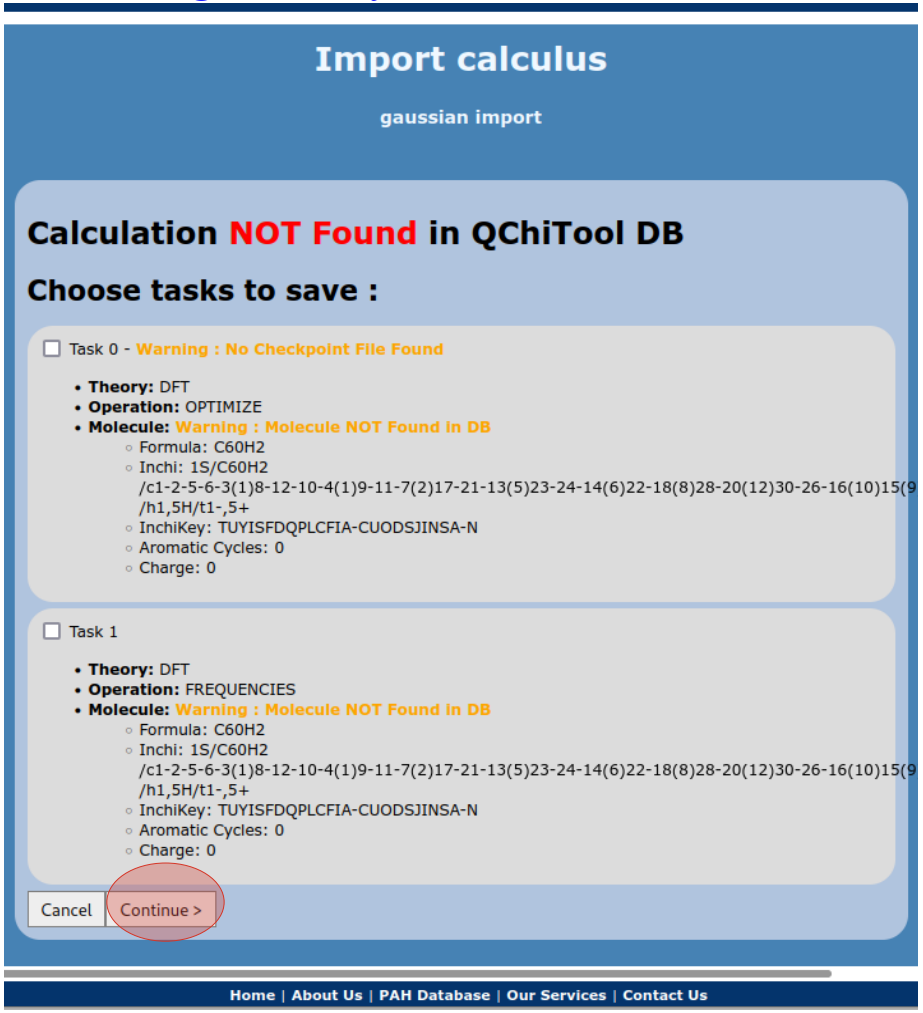
- Implement the new database at *astropah-qcalcs.oa-cagliari.inaf.it* and *astropah-qcalcs.irap.omp.eu*

Theoretical spectral database of Polycyclic Aromatic Hydrocarbons

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

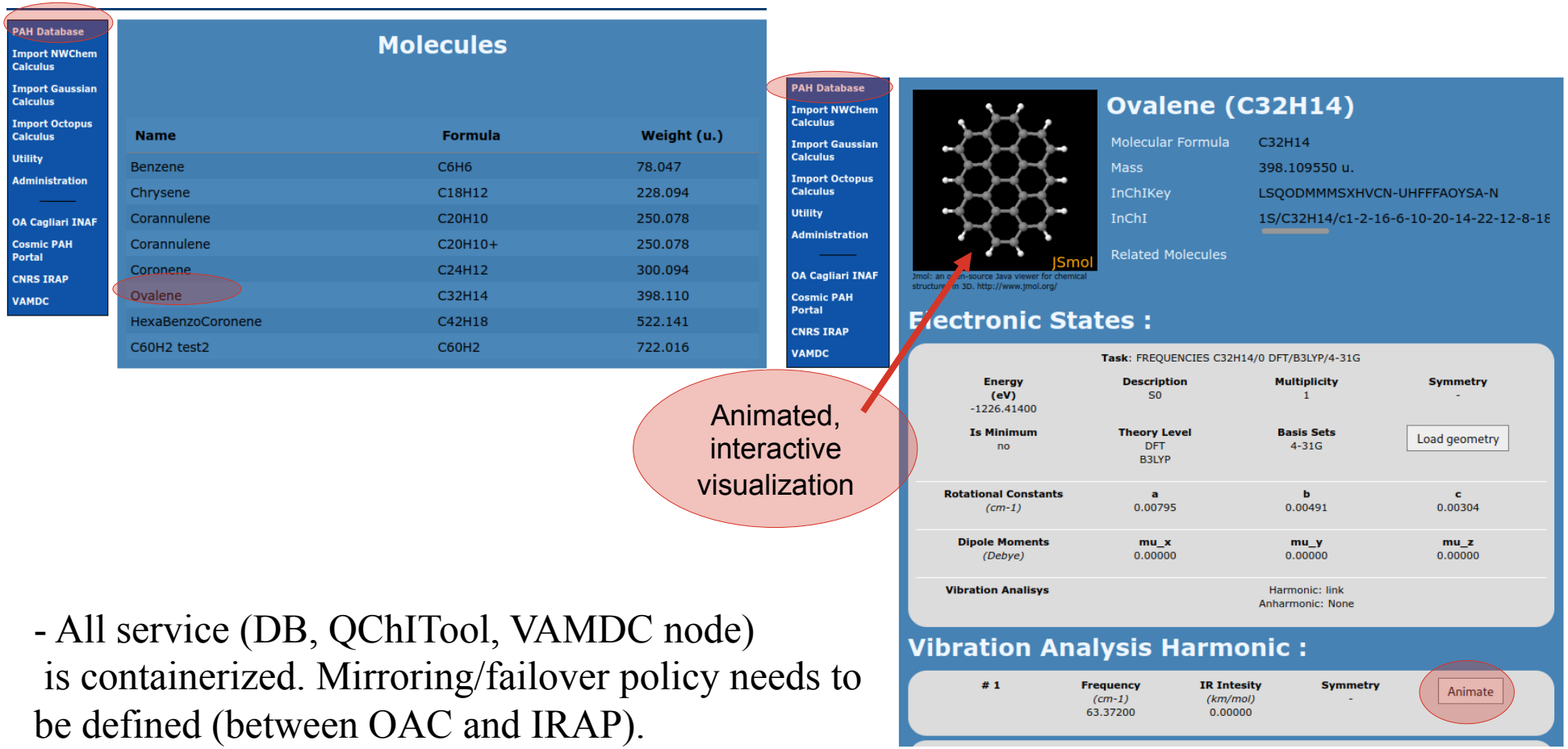


Select what to import...



Theoretical spectral database of Polycyclic Aromatic Hydrocarbons

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



- 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

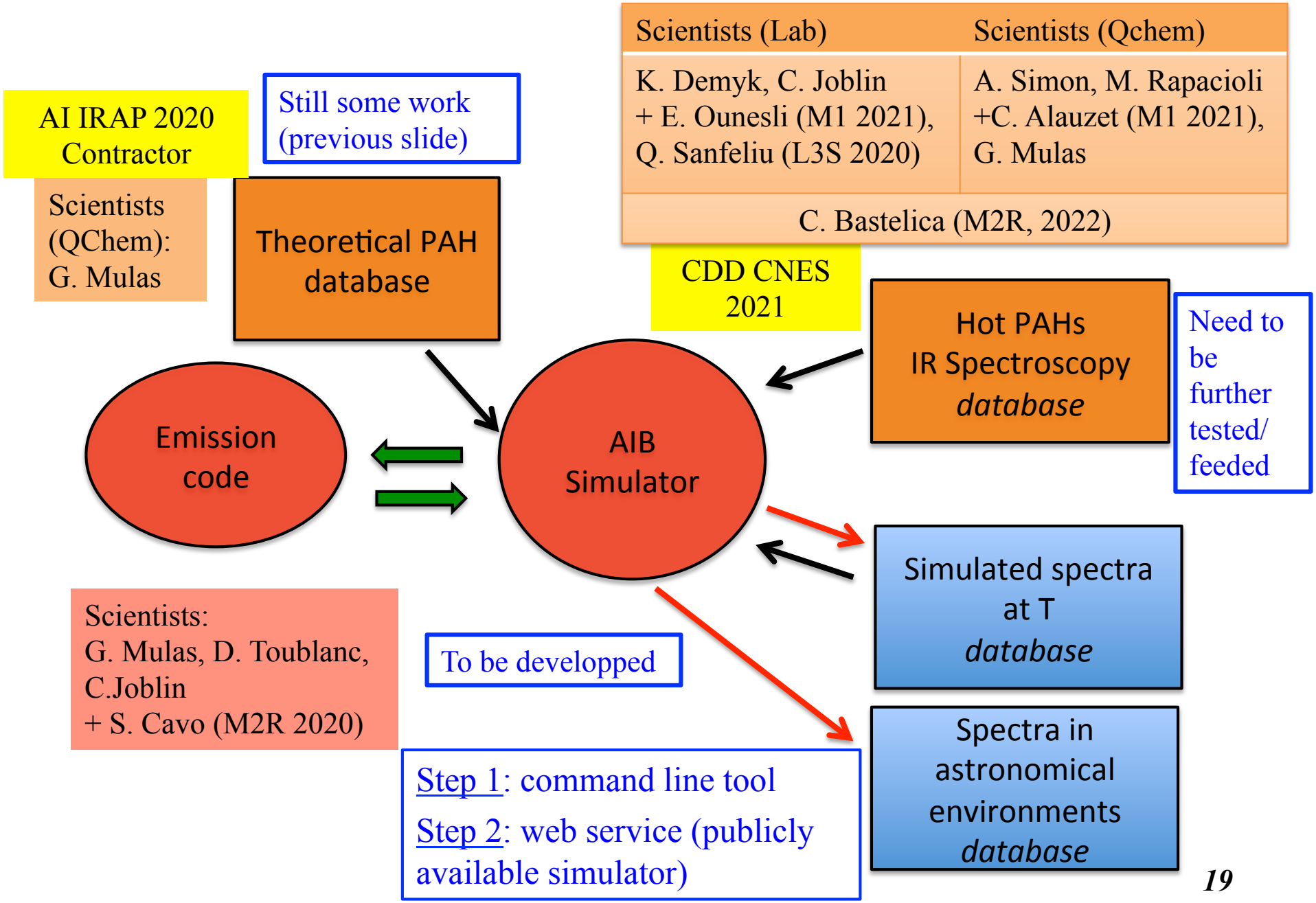
QChITool:

- 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



Logged in as: Christine Joblin (cjoblin) Update Profile Log Out

Cosmic PAH portal

Search Search

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: AROMA DB 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*

Table of Contents

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

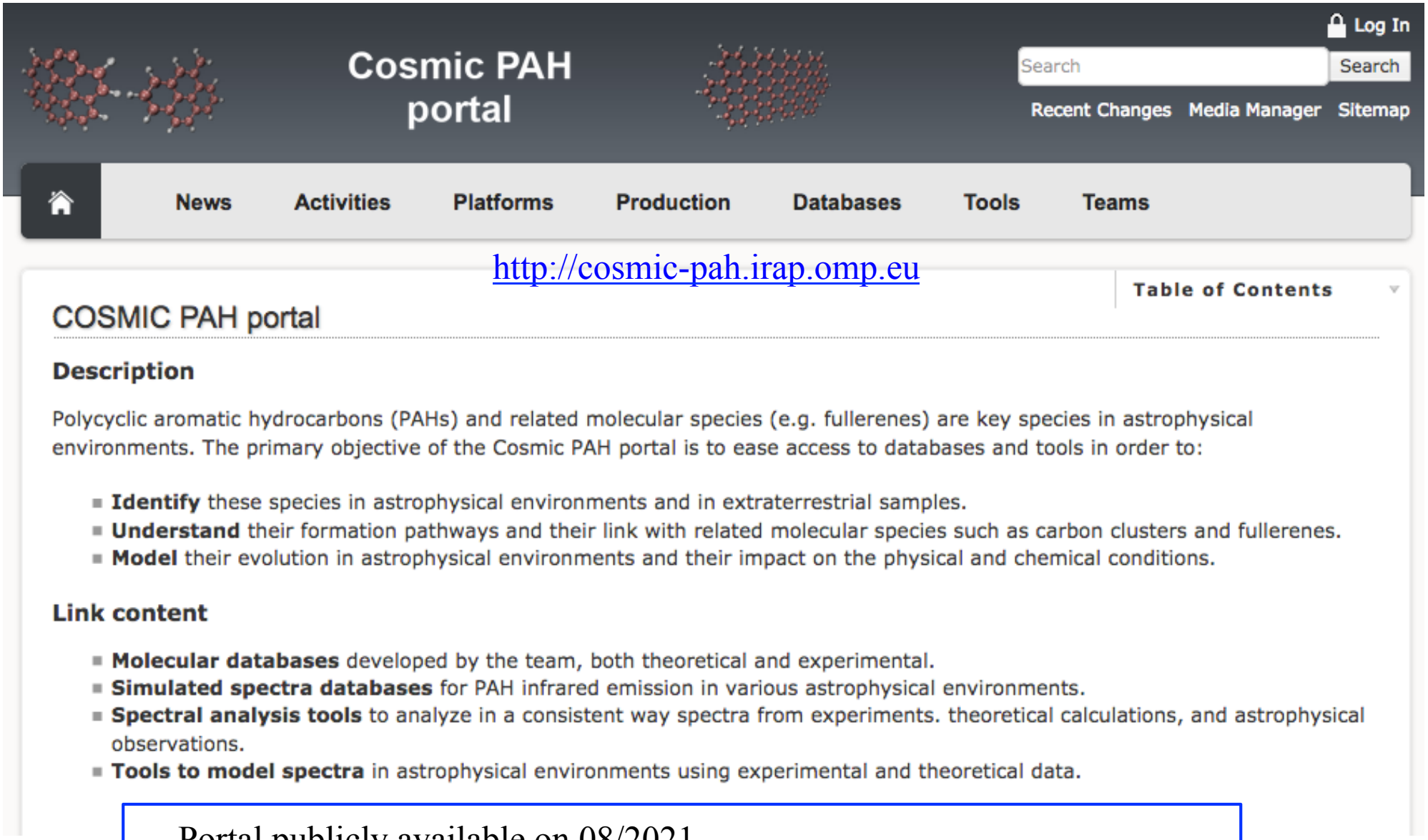
Description
QChITool is a web application for easy extraction of information from the log files of some quantum chemistry calculations, and import in the theoretical PAH database. More
Tool access https://qchitool-pah.oa-cagliari.inaf.it (restricted use of the tool to add data to the PAH database)

* cosmicPAHmfit → Hot PAHs IR spectroscopy

Description
cosmicPAHmfit provides a multi-component spectral fit and a graphical interface to derive area-weighed 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



- Portal publicly available on 08/2021

- Need to improve the design of the web portal

- Tools, DBs & services: Limited manpower. “Tâche de service” → “Labelisation”