Spectroscopic properties of cosmic dust analogues to support the interpretation of astronomical observations

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Data available at:

CosmicPAH-IRDB

Cosmic PAH portal

https://cosmic-pah.irap.omp.eu/doku.php

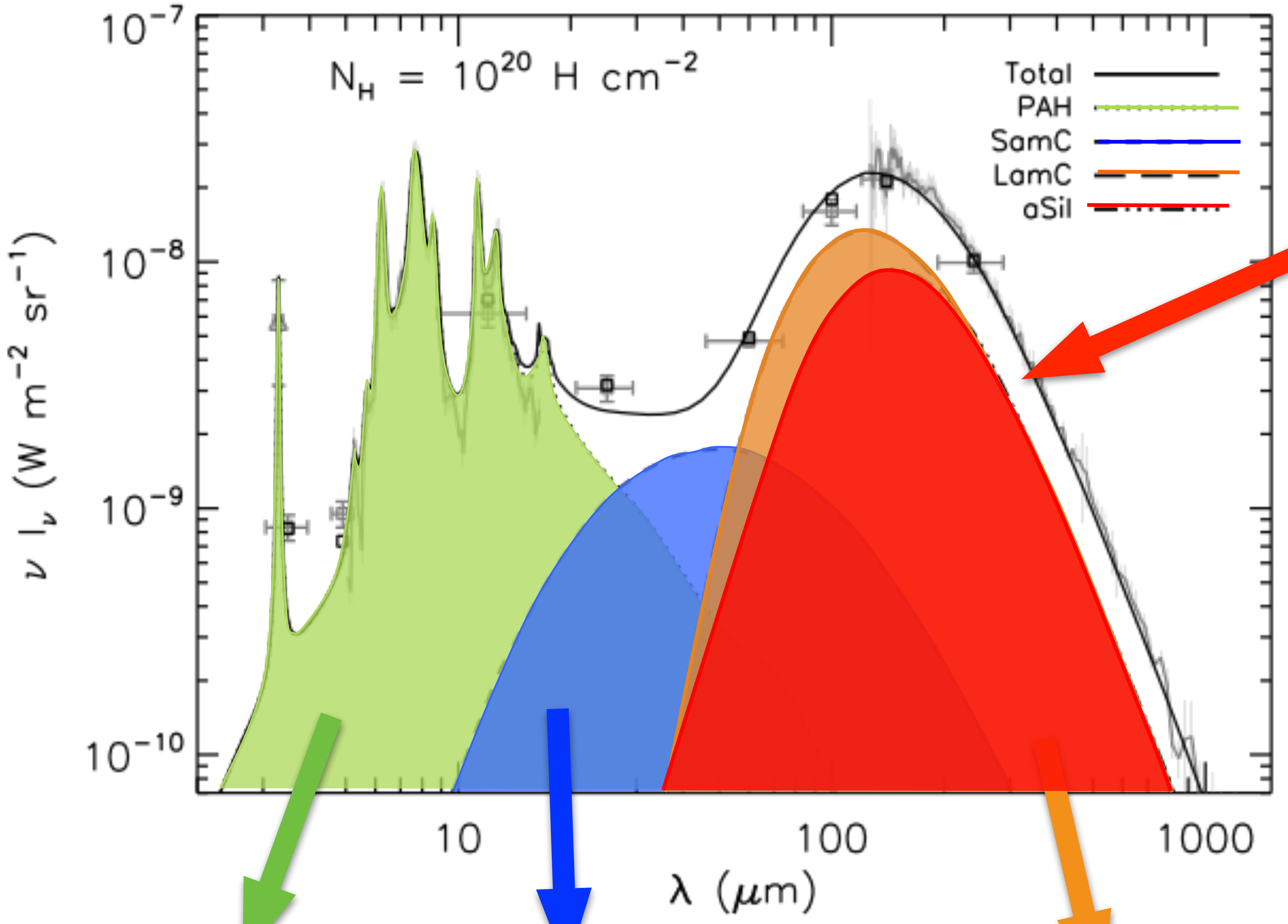
STOPCODA

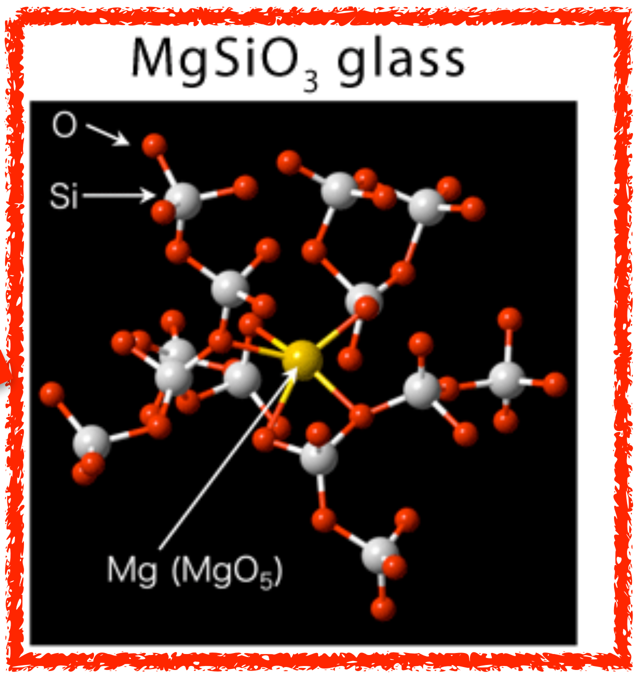
https://www.sshade.eu/db/stopcoda

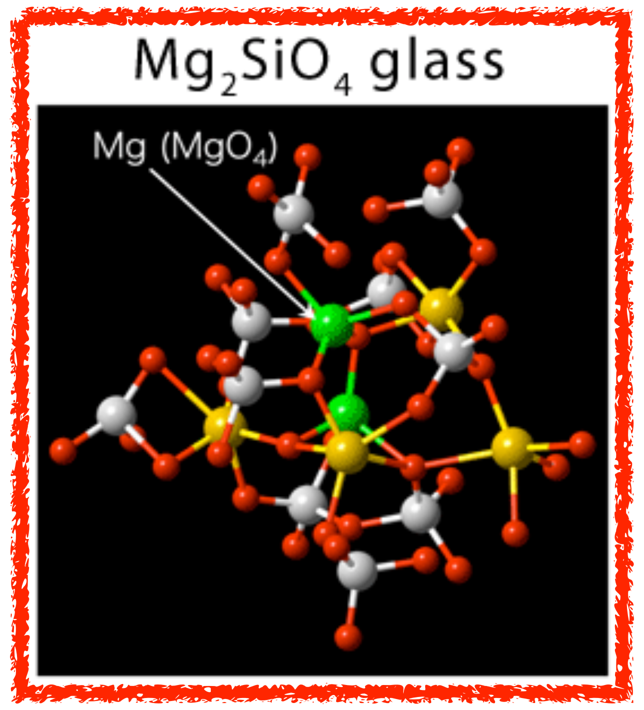
Dust emission in the ISM & cosmic dust models ingredients

Dust emission for the DISM at high galactic latitude

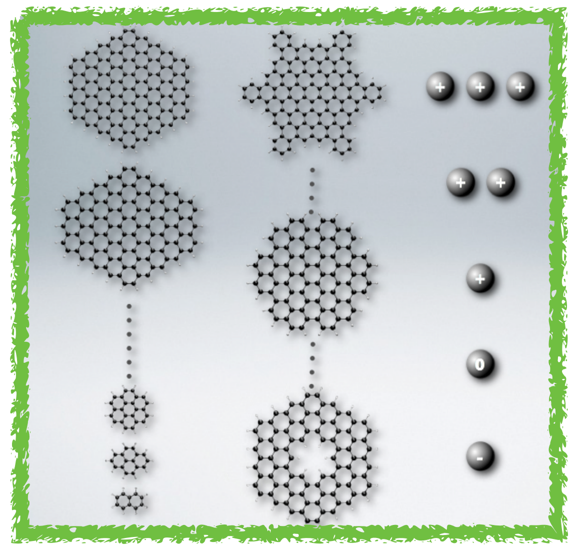
DustEm model [Compiègne et al. 2011]



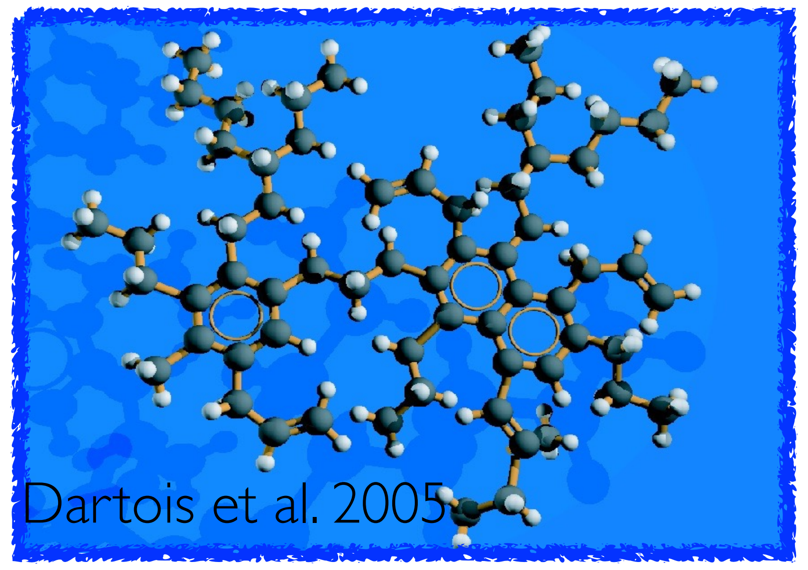




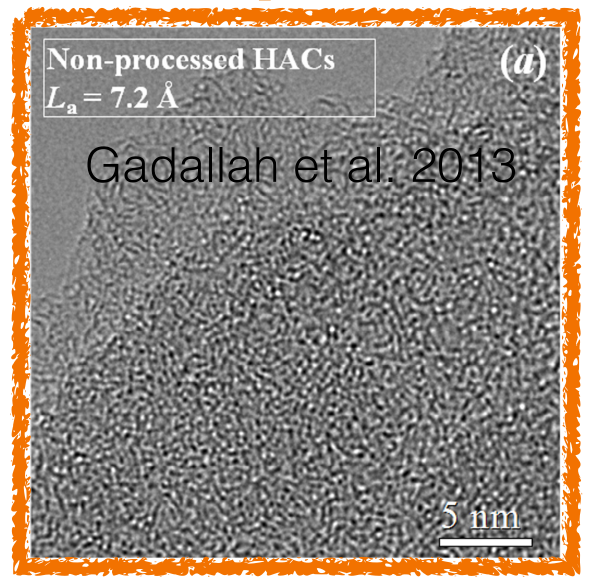
PAHs



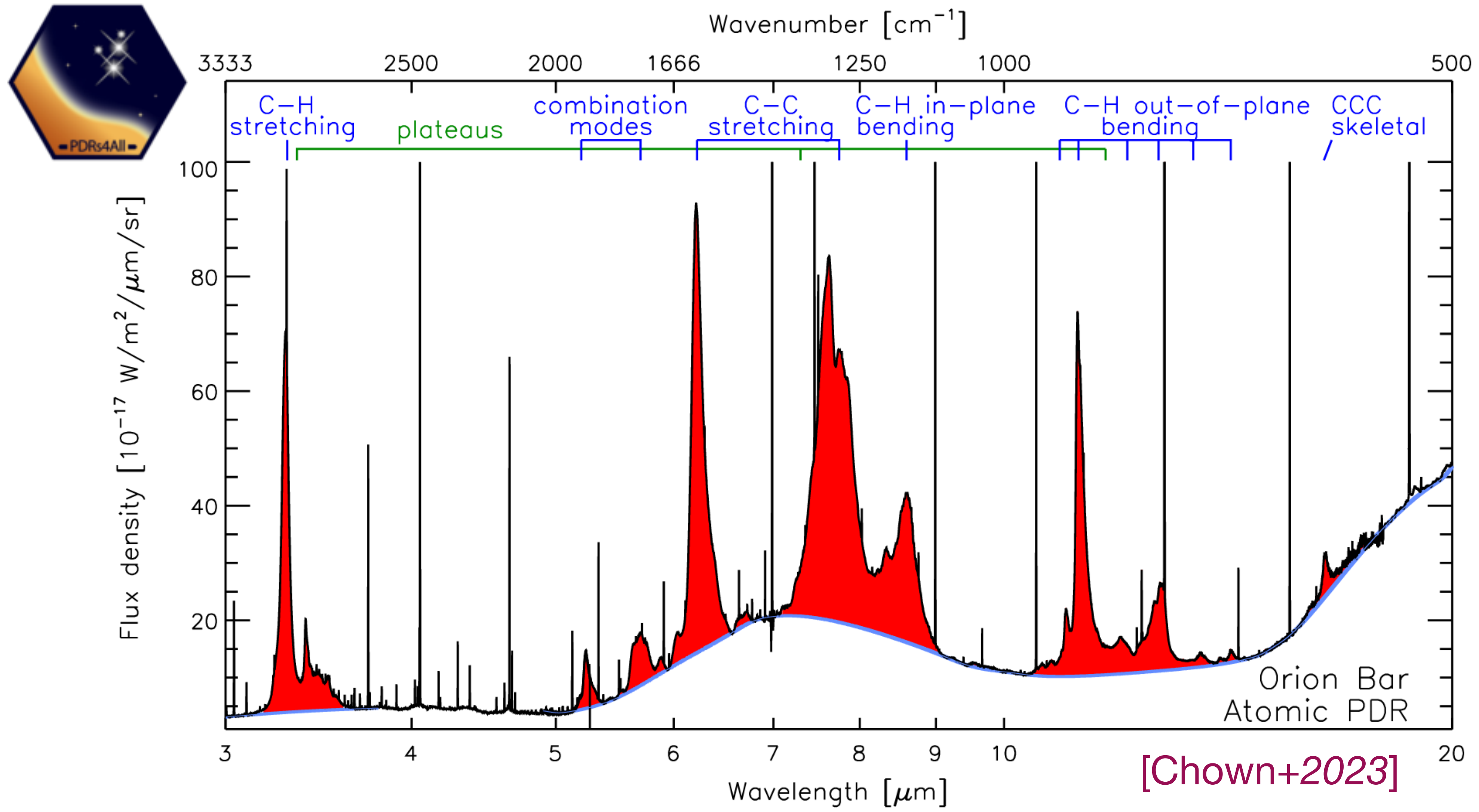
VSG



Amorphous carbon

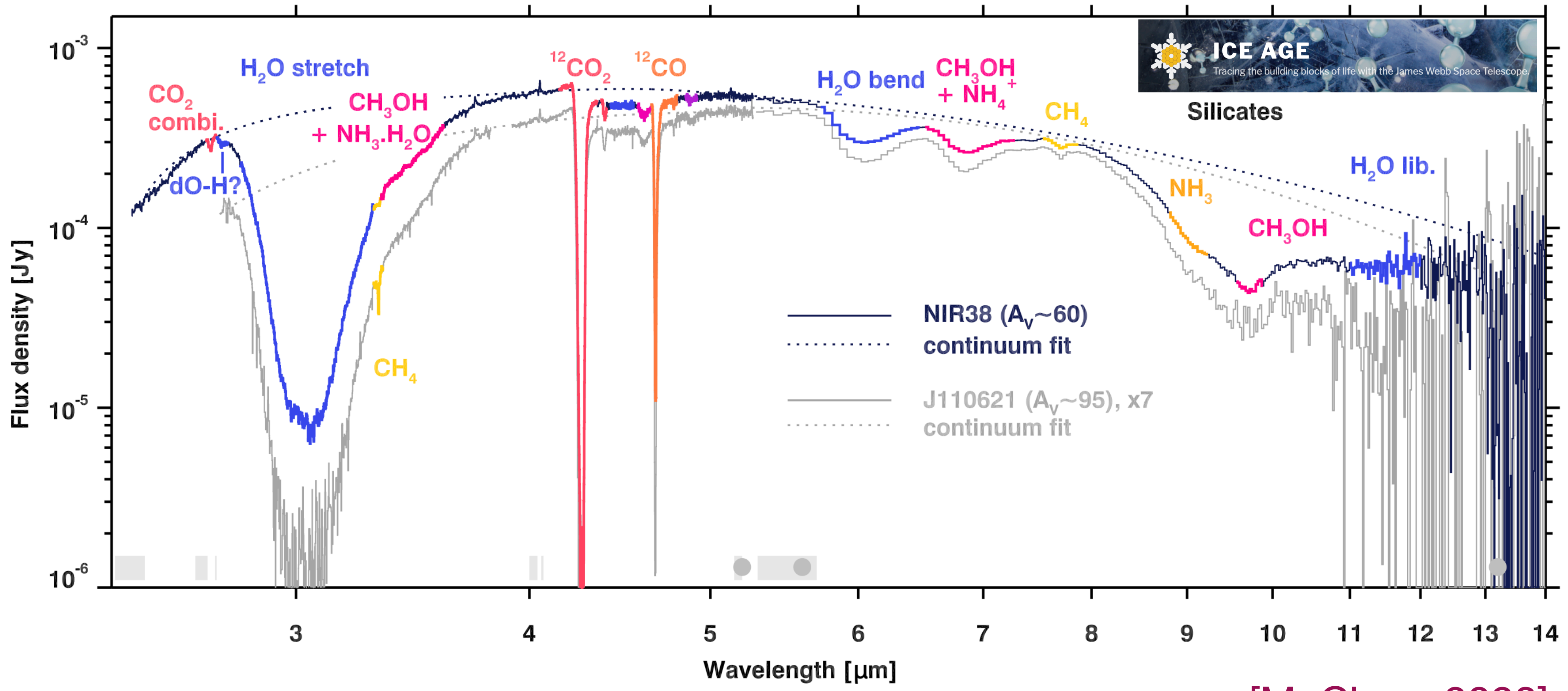


Orion Bar Atomic photo-dominated region



[Chown+2023]

Dense molecular clouds : protostellar envelopes

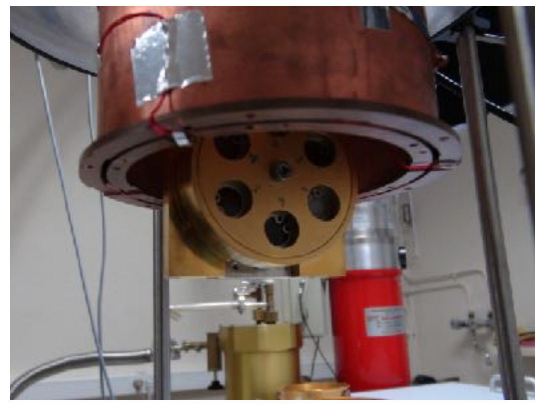


[McClure+2023]

The ESPOIRS setup

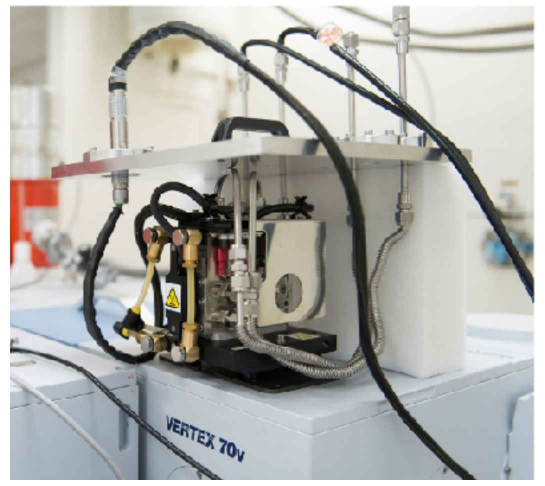
- Characterising optical properties of dust analogues to interpret astronomical observations : Herschel/Planck/ground based mm, JWST observations …
- Study dust properties and their evolution through the ISM cycle

Infrared Fourier Transform spectrometer covering from 0.9 µm to 1mm

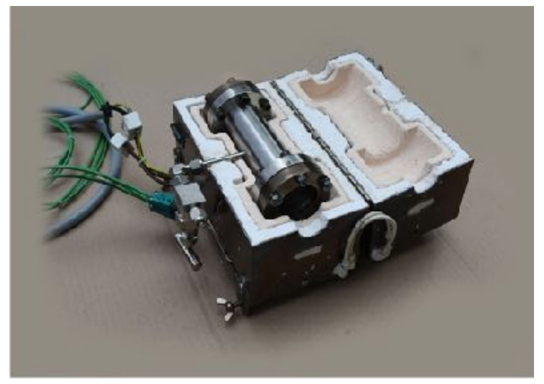


Cryostat for low temperature measurements :
- 10 - 300 K
- solid samples
- 2µm - 1mm

High temperature measurements :



HT/HP cell:
- 300 - 1100 K
- solid samples
- 2-20 µm



Gas cell + oven:
- 300 - 850 K
- gas species
- NIR to FIR

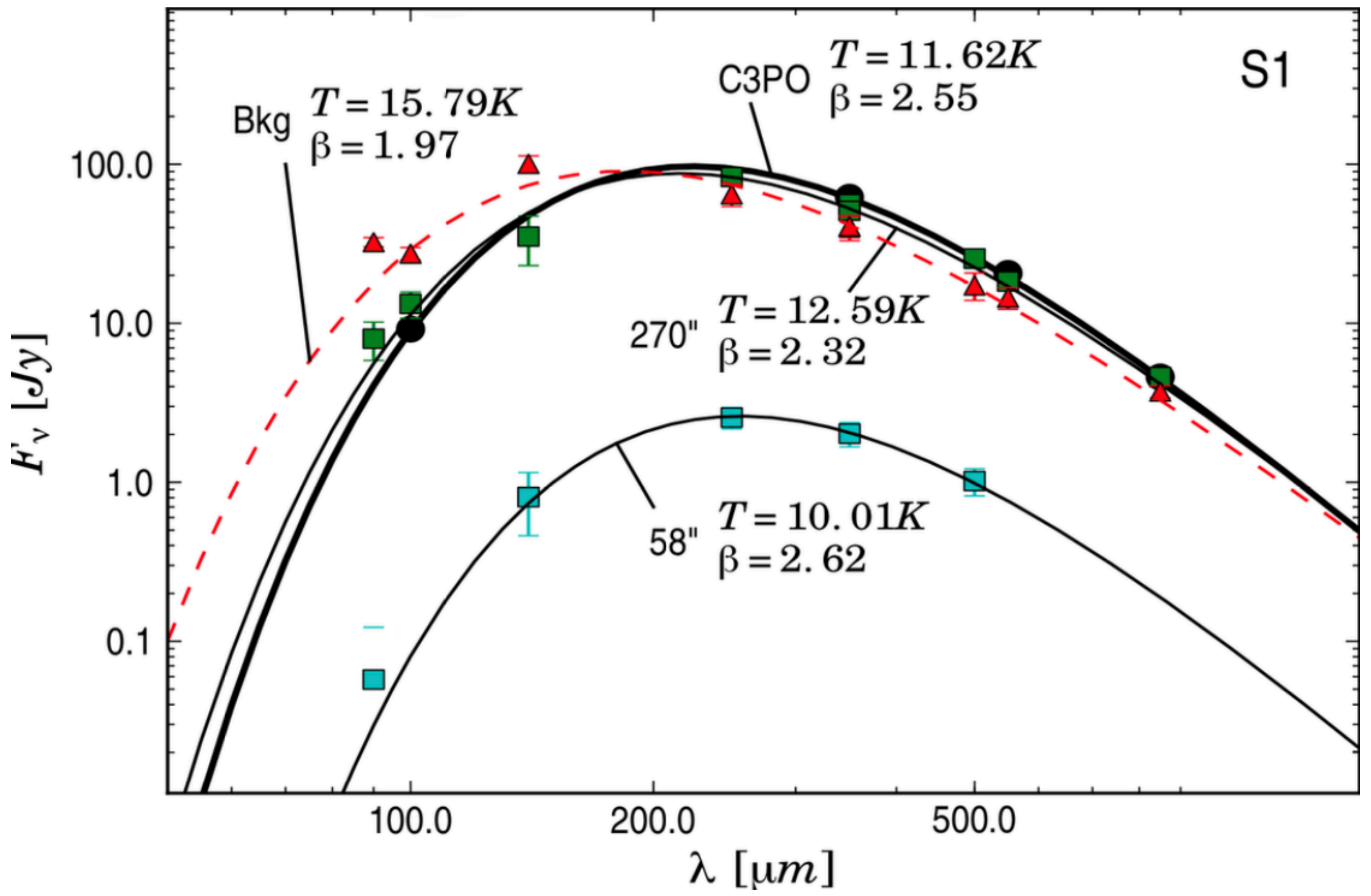
Big grains : Variation of their properties in the ISM

Modified black body model:

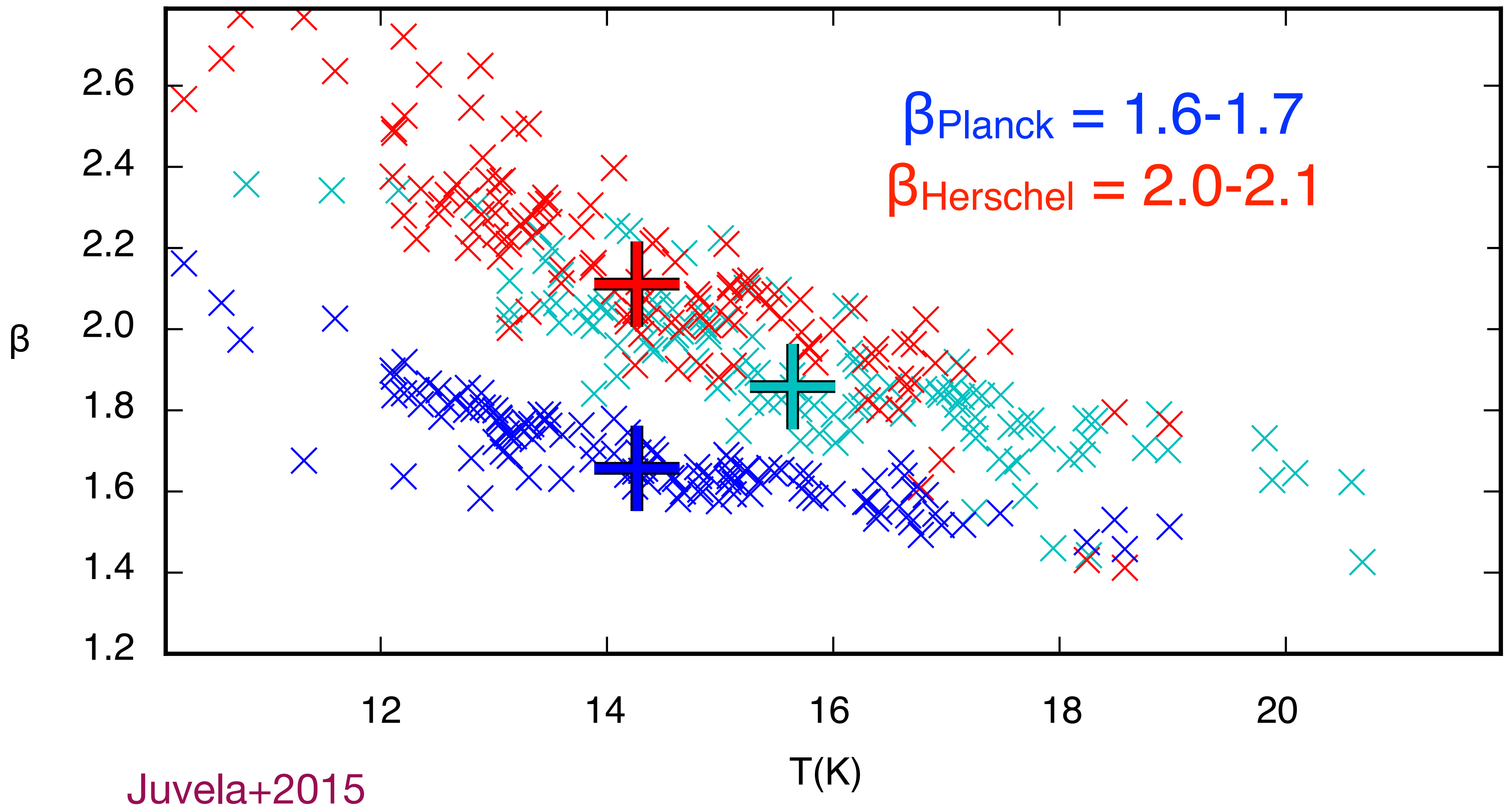
$$I_\nu \approx \tau B_\nu(T) = \frac{M_{dust} B_\nu(T)}{d^2\Omega} \kappa_0 \left(\frac{\nu}{\nu_0}\right)^\beta$$

Mass Absorption Coefficient

- β independent of T_d and λ
- β = 1 to 2



Variation of dust properties in cold cores



Juvela+2015

➡ not an effect of noise, temperature mixing along the line of sight, bias from the fitting method, not likely mixing of dust populations

➡ variation of the intrinsic properties of dust grains with temperature and/or the environment

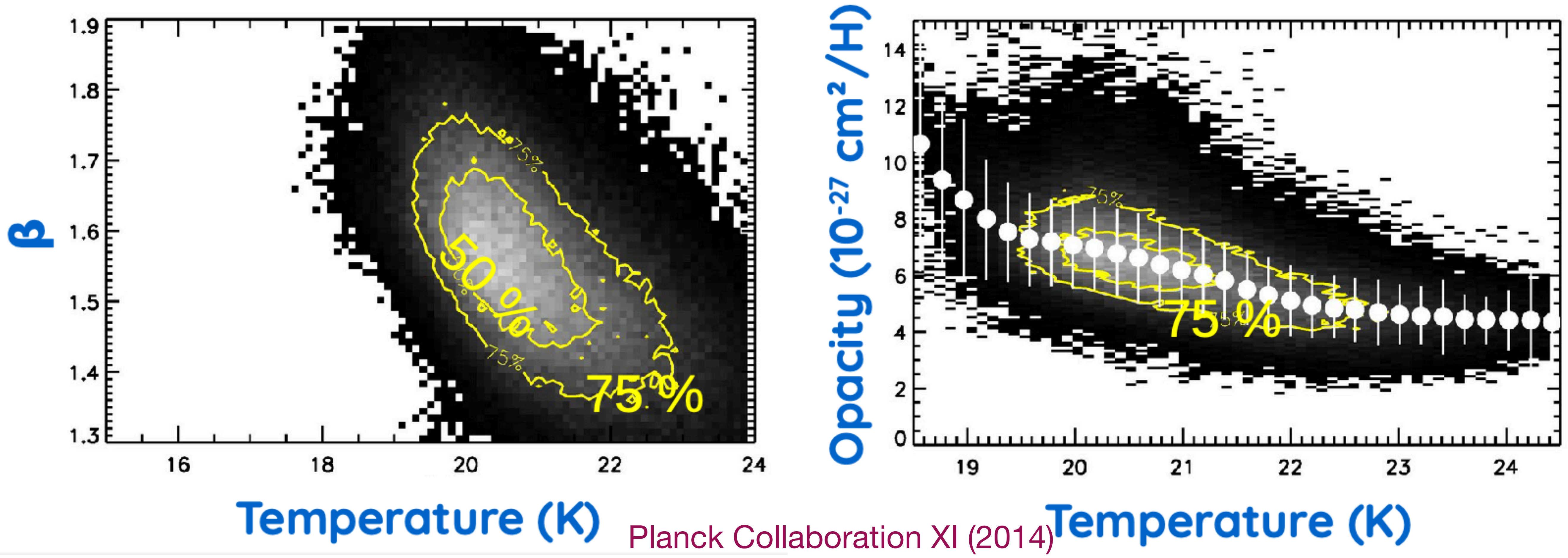
What about lab data?

➡ Most of the measurements at room temperature and for λ < 100/300 μm

➡ Some showed that κ varies with T and λ [Mennella+1998, Boudet+2005]

➡ Do a more systematic study

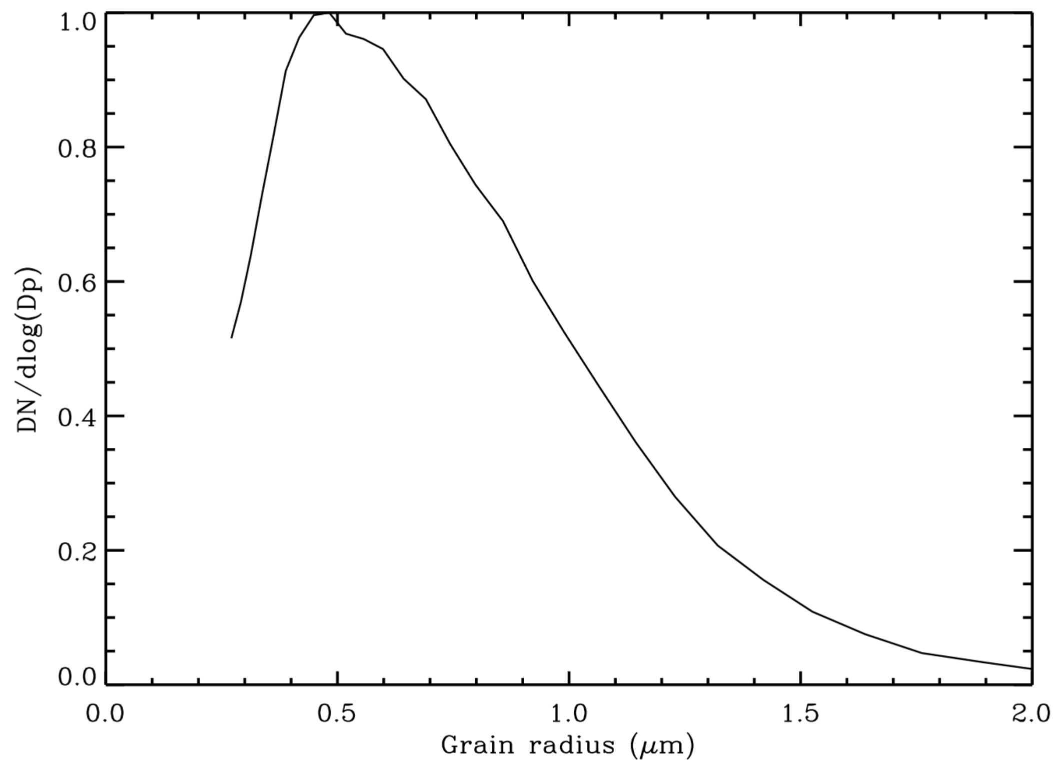
Variation of dust properties in diffuse ISM



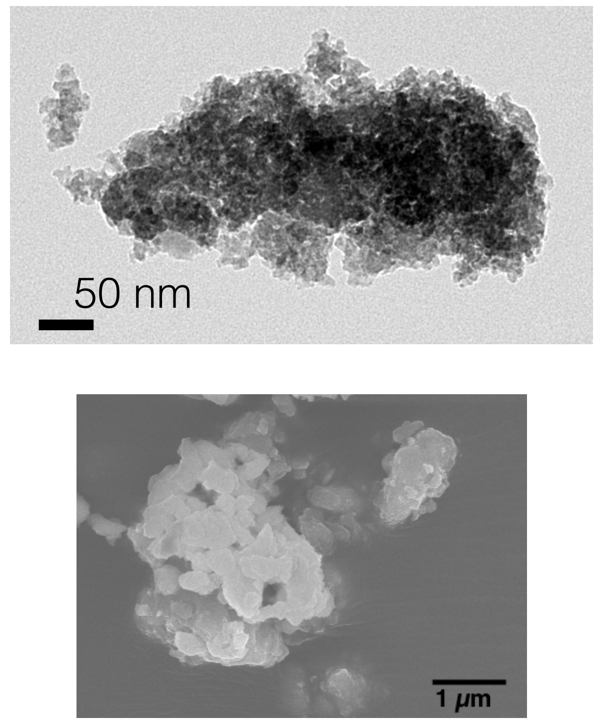
Planck Collaboration XI (2014)

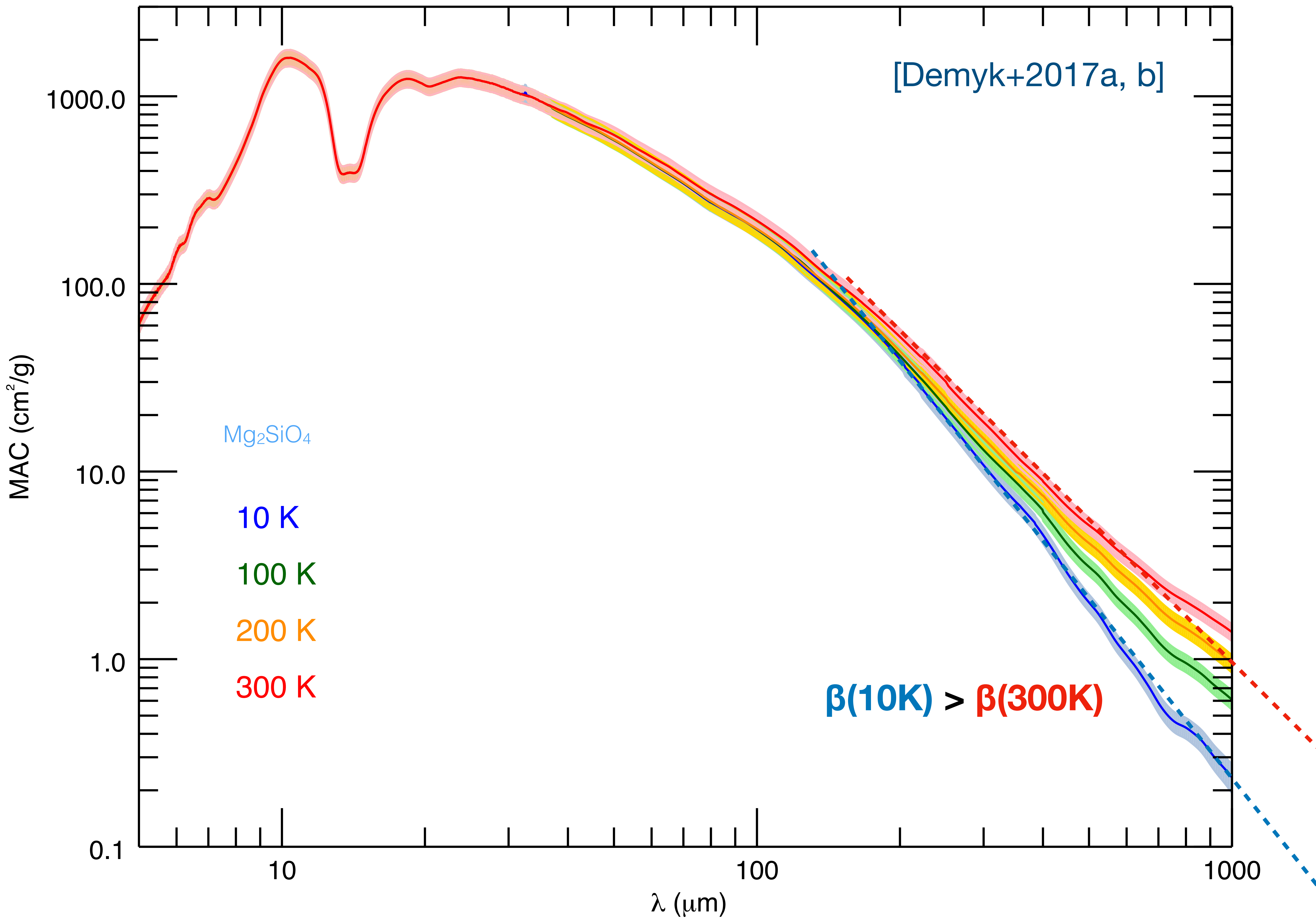
Temperature variation of the mass absorption coefficient of silicates analogues

- 4 Mg-rich glassy silicates Mg2SiO4 → MgSiO3
- 8 (Mg,Fe) chaotic silicates $Mg_{(1-x)}Fe_xSiO_3$, x= 0.1- 0.4
- Submicronic grains
- 10 - 300 K
- 5 - 600/1000 µm



$MgSiO_3$ amorphous silicates

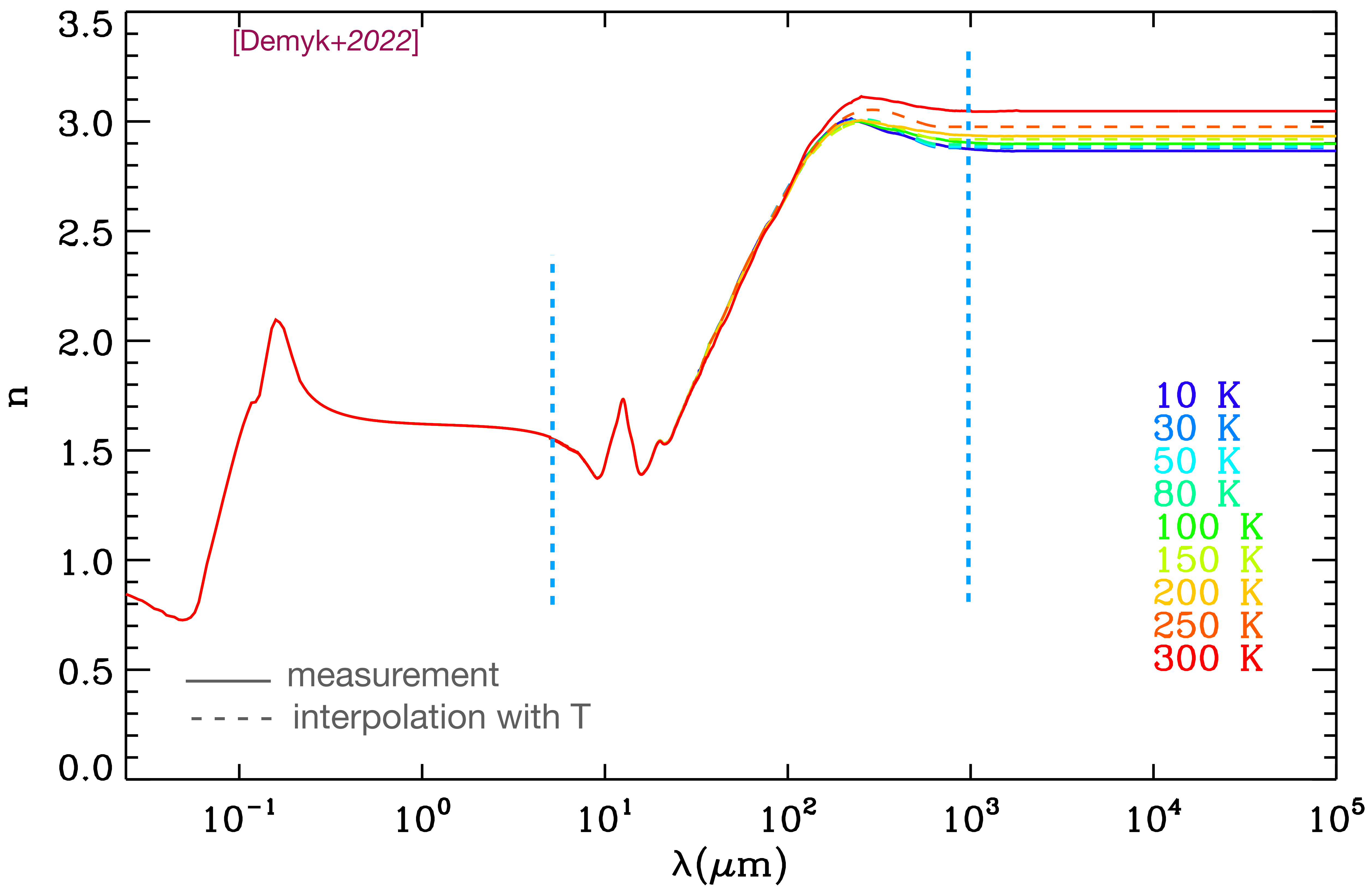


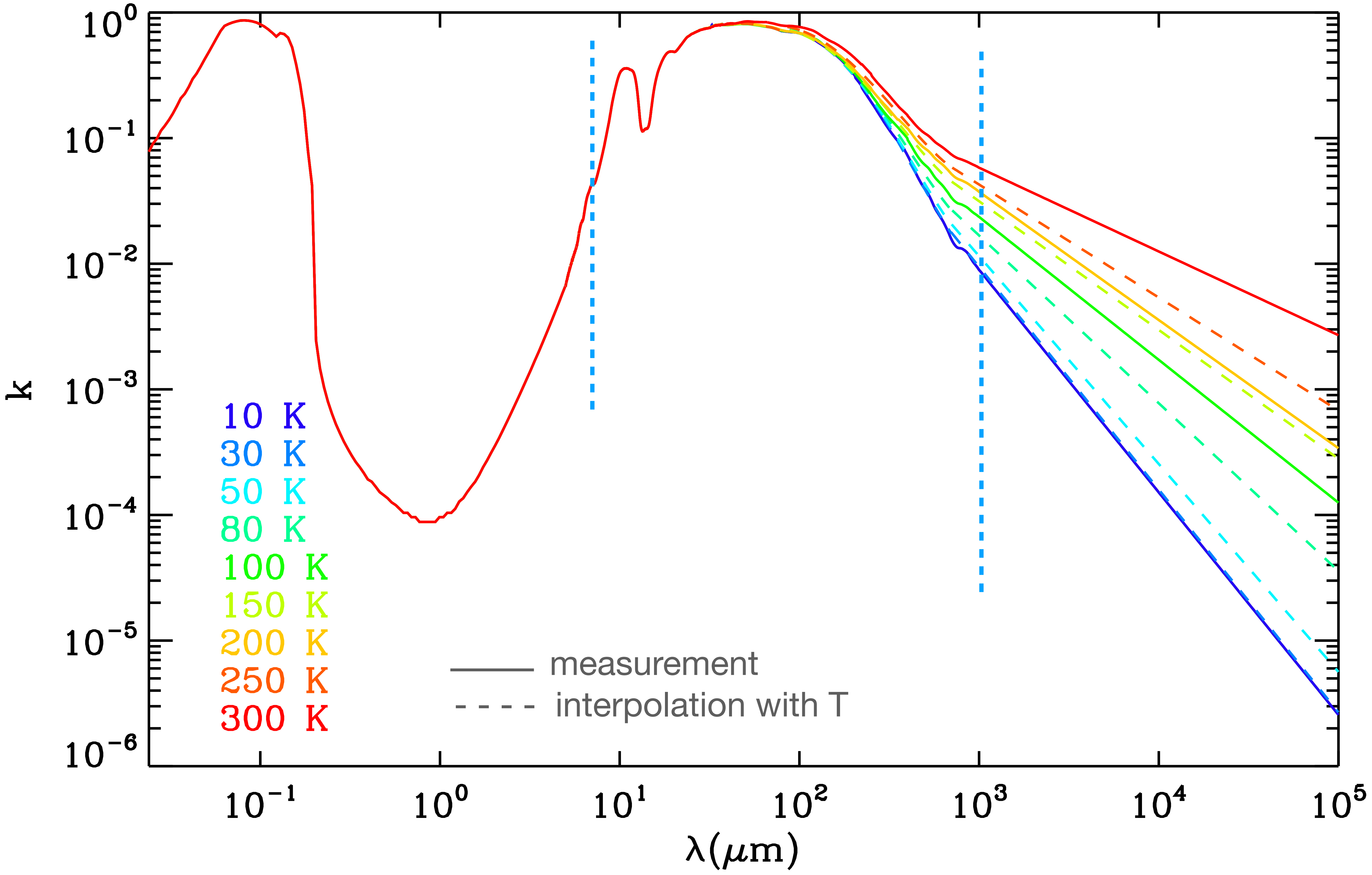


- **MAC ↗ when T ↗**
- **β varies with λ and T**
- **β(λ) ↗ when T ↘**

[See also: Coupeaud+11, Boudet+05, Mennella+98, Agladze+96 and Mény+07]

New temperature-dependent optical constants





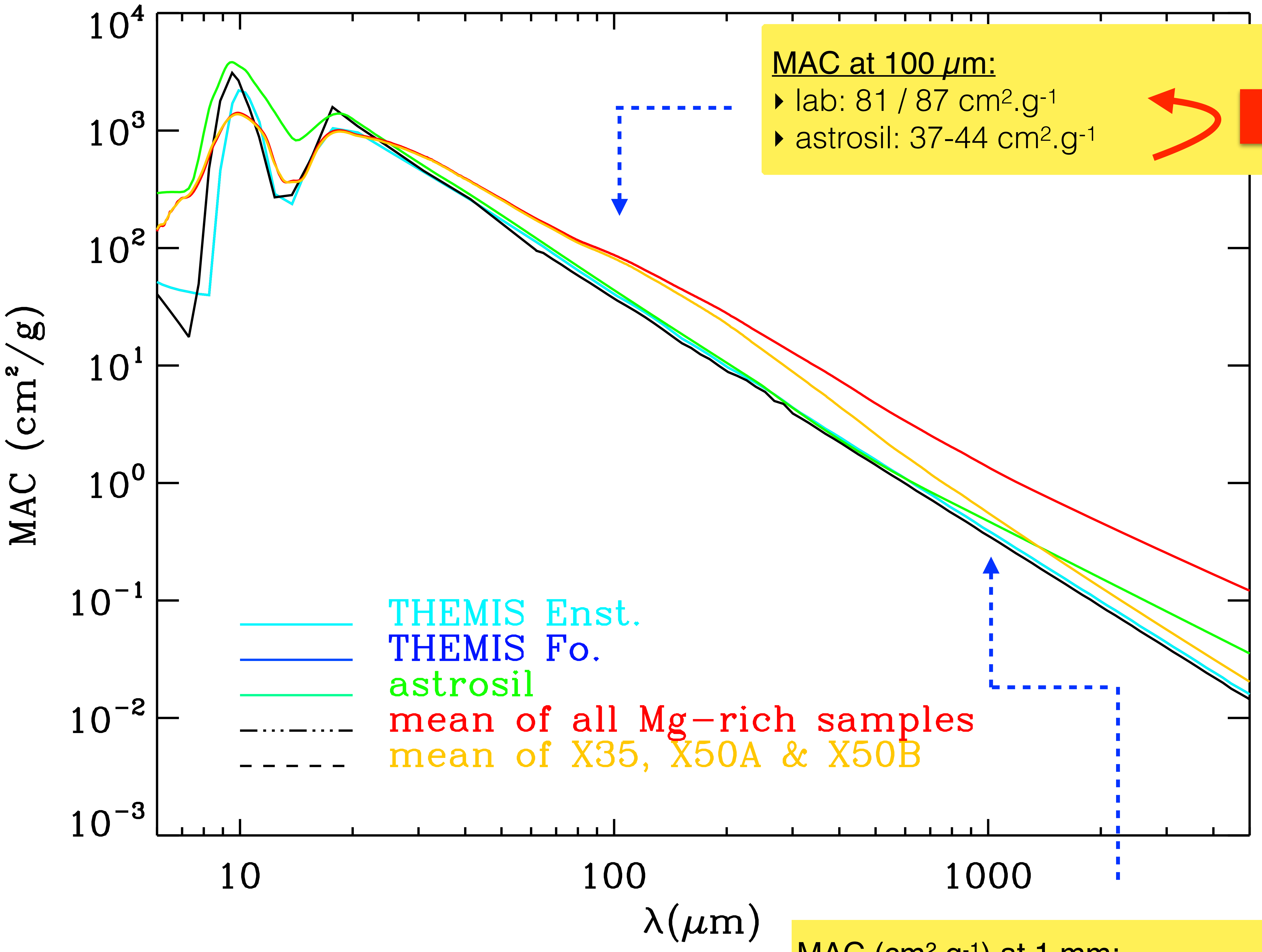
Data (MAC and optical constants) available on the **stopcoda database** for the 12 species and all temperatures

STOPCODA

https://www.sshade.eu/db/stopcoda

Comparison with silicates in cosmic dust models

MAC of small prolate grains (a/b=1.5)



MAC at 100 μm:
- lab: 81 / 87 $cm^2.g^{-1}$
- astrosil: 37-44 $cm^2.g^{-1}$

× 2-2.3

MAC ($cm^2.g^{-1}$) at 1 mm:
- lab: 0.56 - 1.36 at 10K
- astrosil: 0.35 - 0.47

× 1.6 - 3.9 at 10K

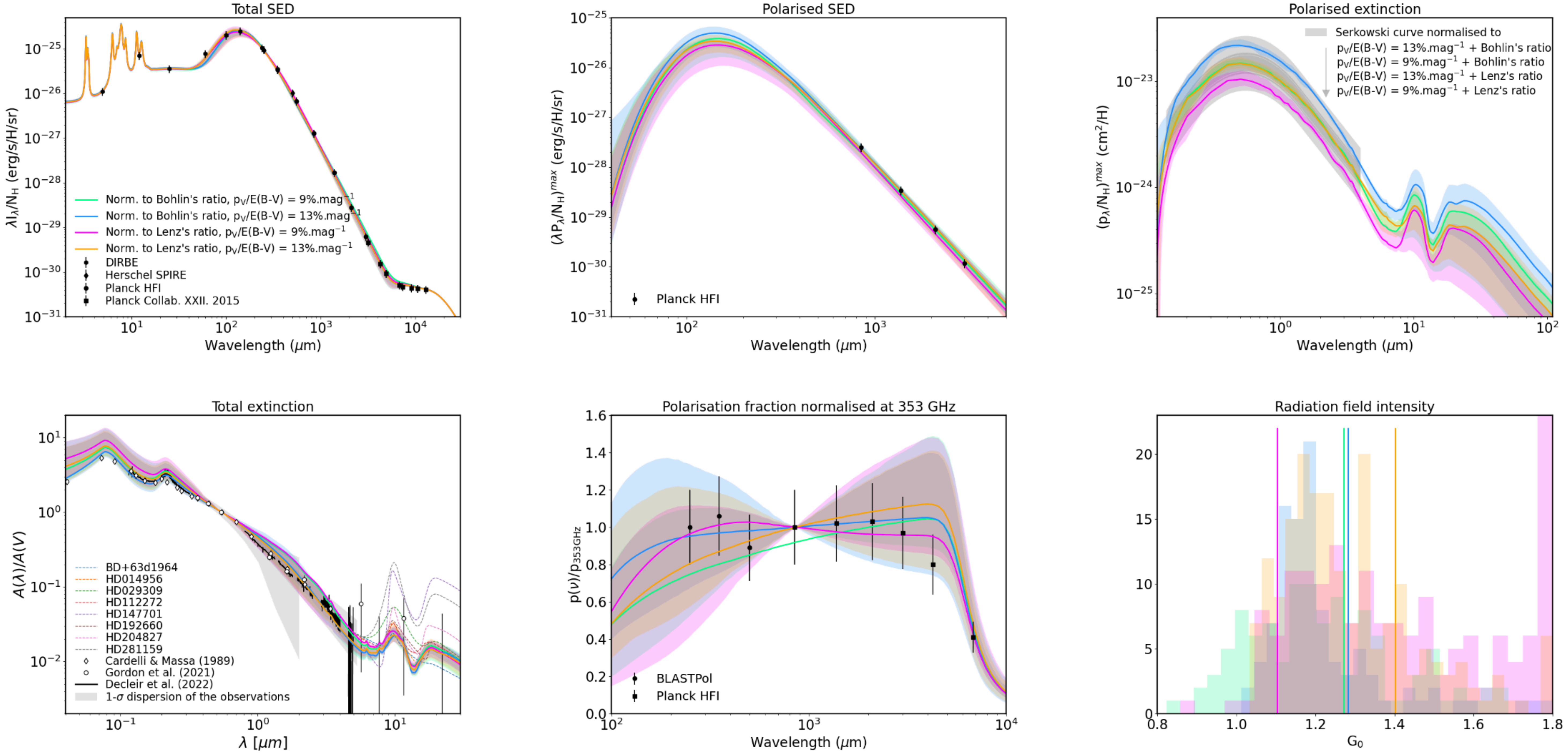
Themis 2 : the only model based on silicate low temperature data

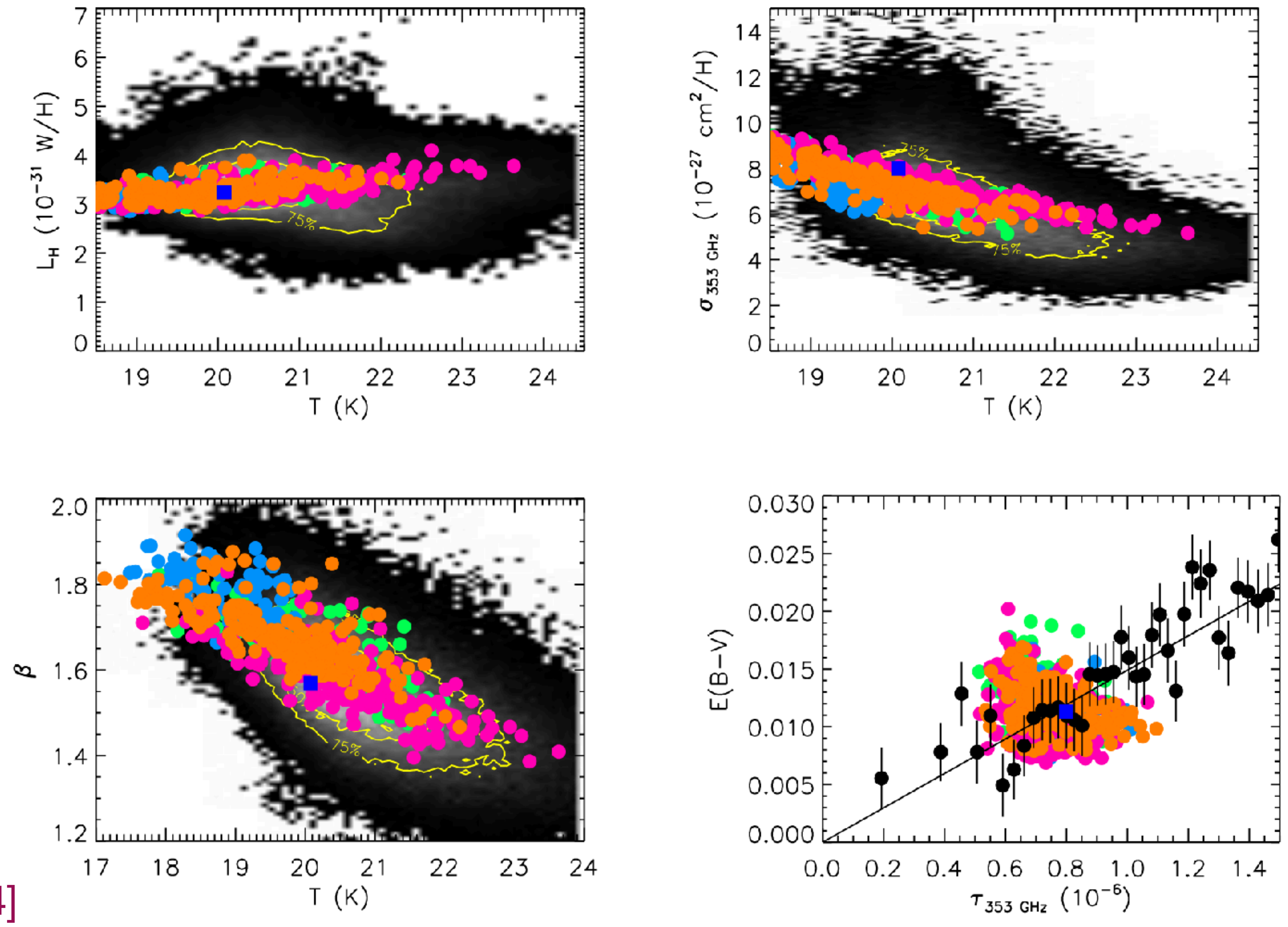
- A versatile model:
  - Various silicate mixtures (olivine vs pyroxene)
  - various mantle descriptions (aromatic vs aliphatic carbon)

  - All can explain the observations (intensity and polarisation)

Composition	$\beta_{200-500\mu m}$	β_{1-3mm}	$r_{850\mu m}$	r_{2mm}
THEMIS I	2.00	1.94	1.00	1.00
aSil-1/a-C$^{2.5nm}$	2.80	2.09	0.58	0.48
aSil-2/a-C$^{2.5nm}$	2.47	2.25	0.87	0.64
aSil-3/a-C$^{2.5nm}$	2.20	2.25	1.24	0.91
aSil-4/a-C$^{2.5nm}$	2.02	2.26	1.62	1.20
aSil-5/a-C$^{2.5nm}$	2.97	1.85	0.61	0.60
aSil-6/a-C$^{2.5nm}$	2.88	1.77	0.76	0.85
aSil-7/a-C$^{2.5nm}$	2.79	1.73	0.92	1.11

Different olivine/ pyroxene ratio → Different β values ← Different silicate/ nano-C ratio





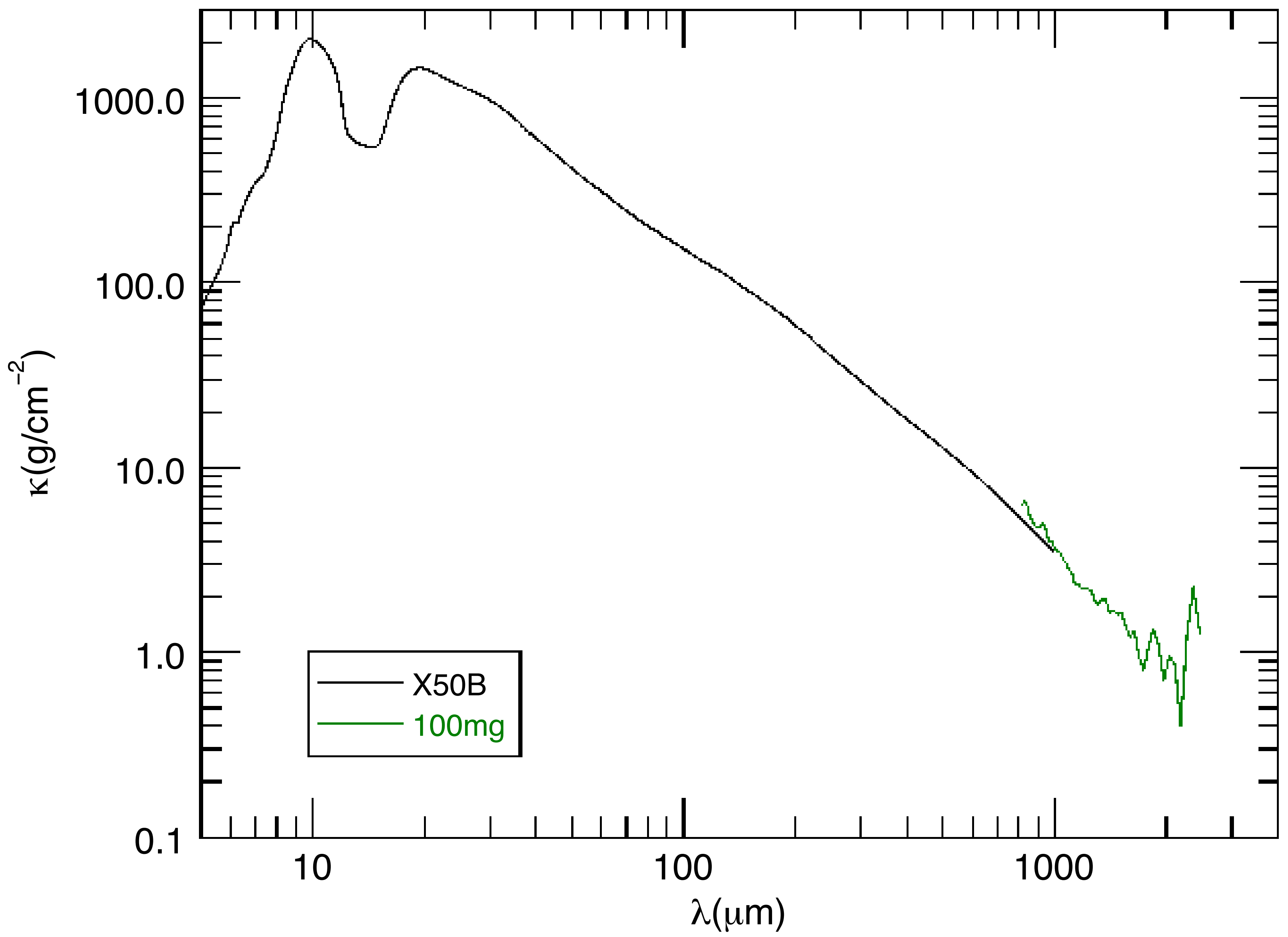
[Ysard+2024]

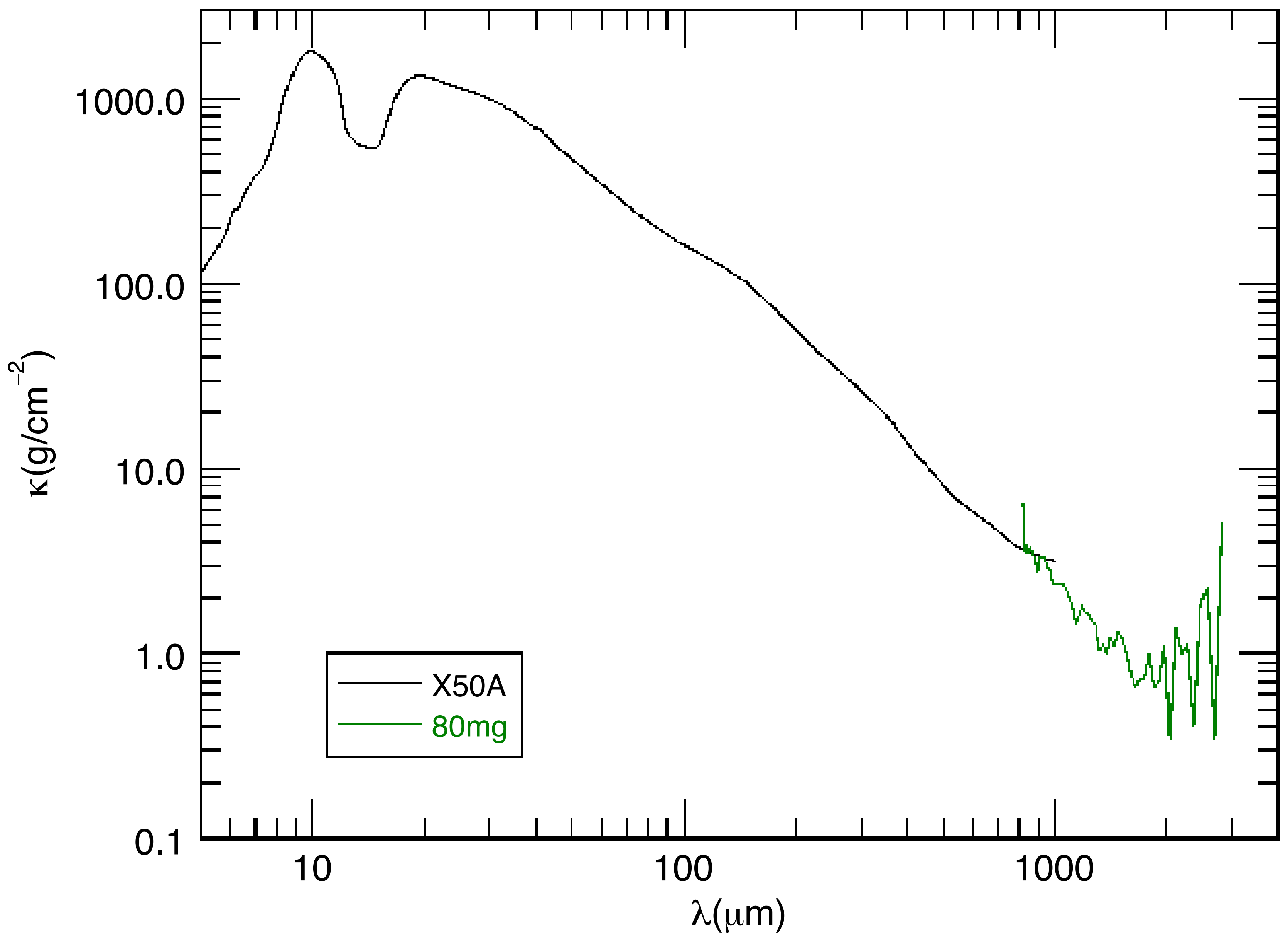
THEMIS
The Heterogeneous dust Evolution Model for Interstellar Solids

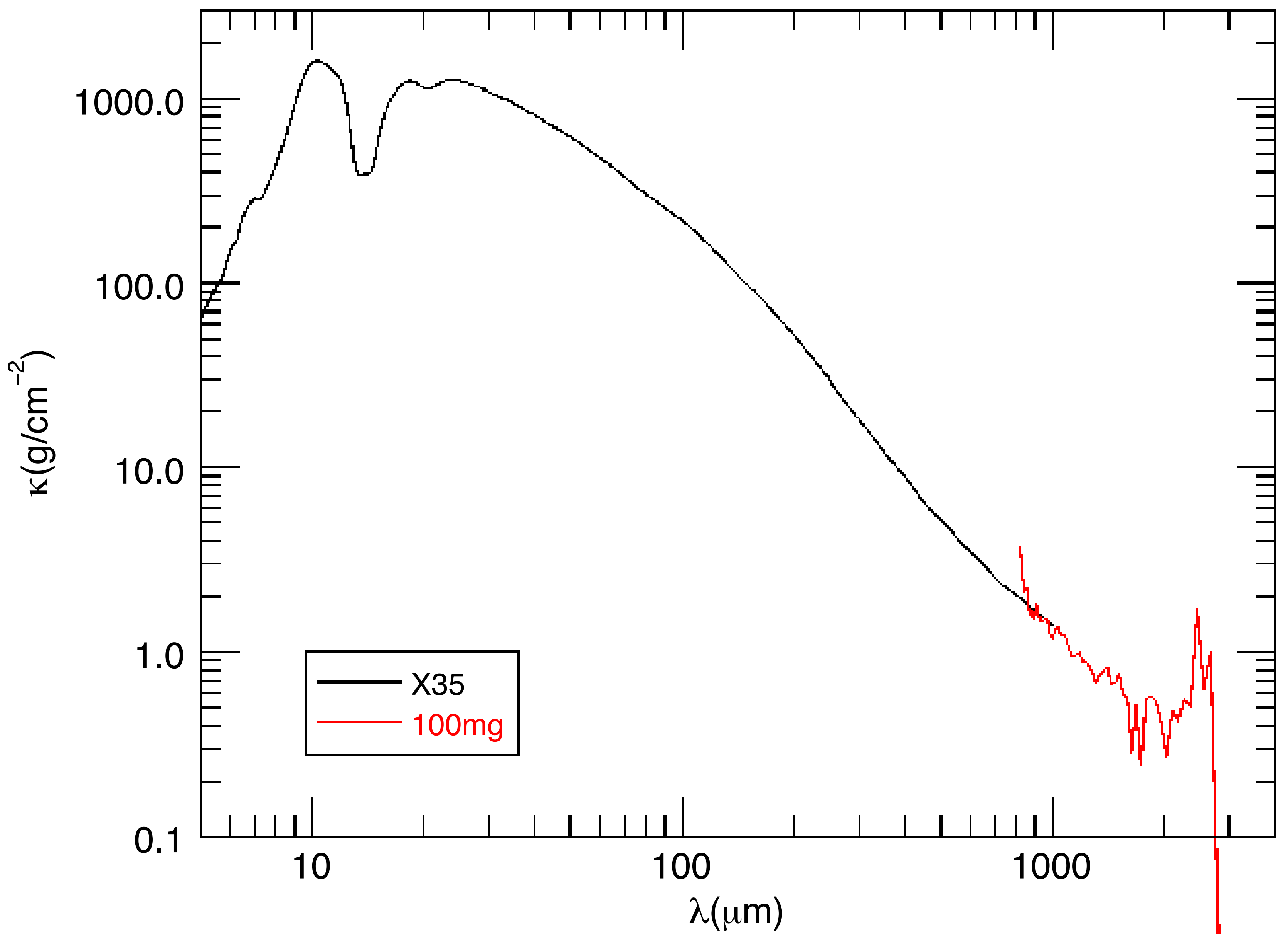
https://www.ias.u-psud.fr/themis/THEMIS_model.html

Perspectives : new measurements beyond 1 mm :

- At Institut Néel & IPAG [F.X. Désert, A. Monfardini, M. Calvo]
- 370 - 100 GHz, measured with the NIKA1.5 cryostat, 1mm kids array and a Martin-Puplett interferometer
- room temperature
- data at 10K coming soon

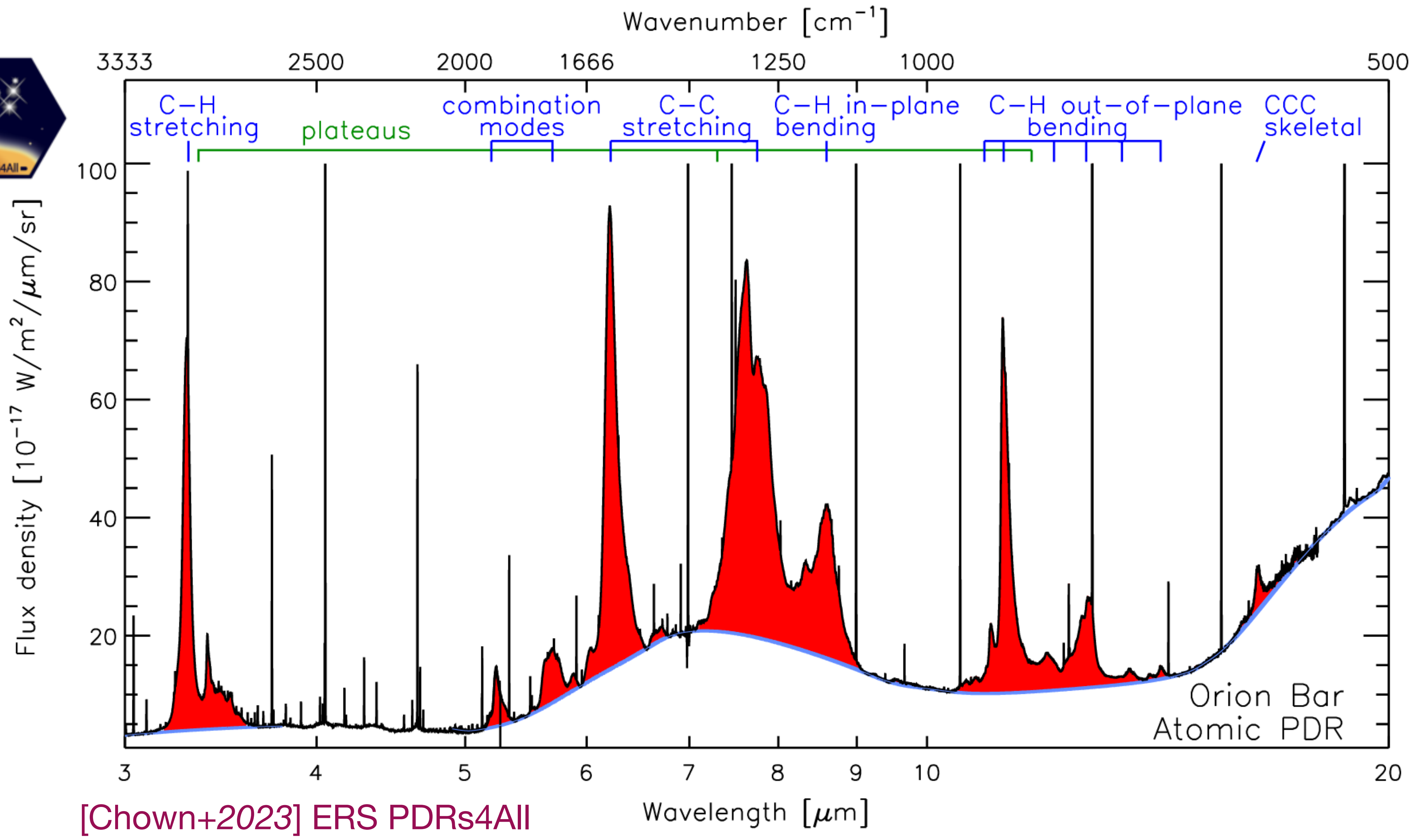






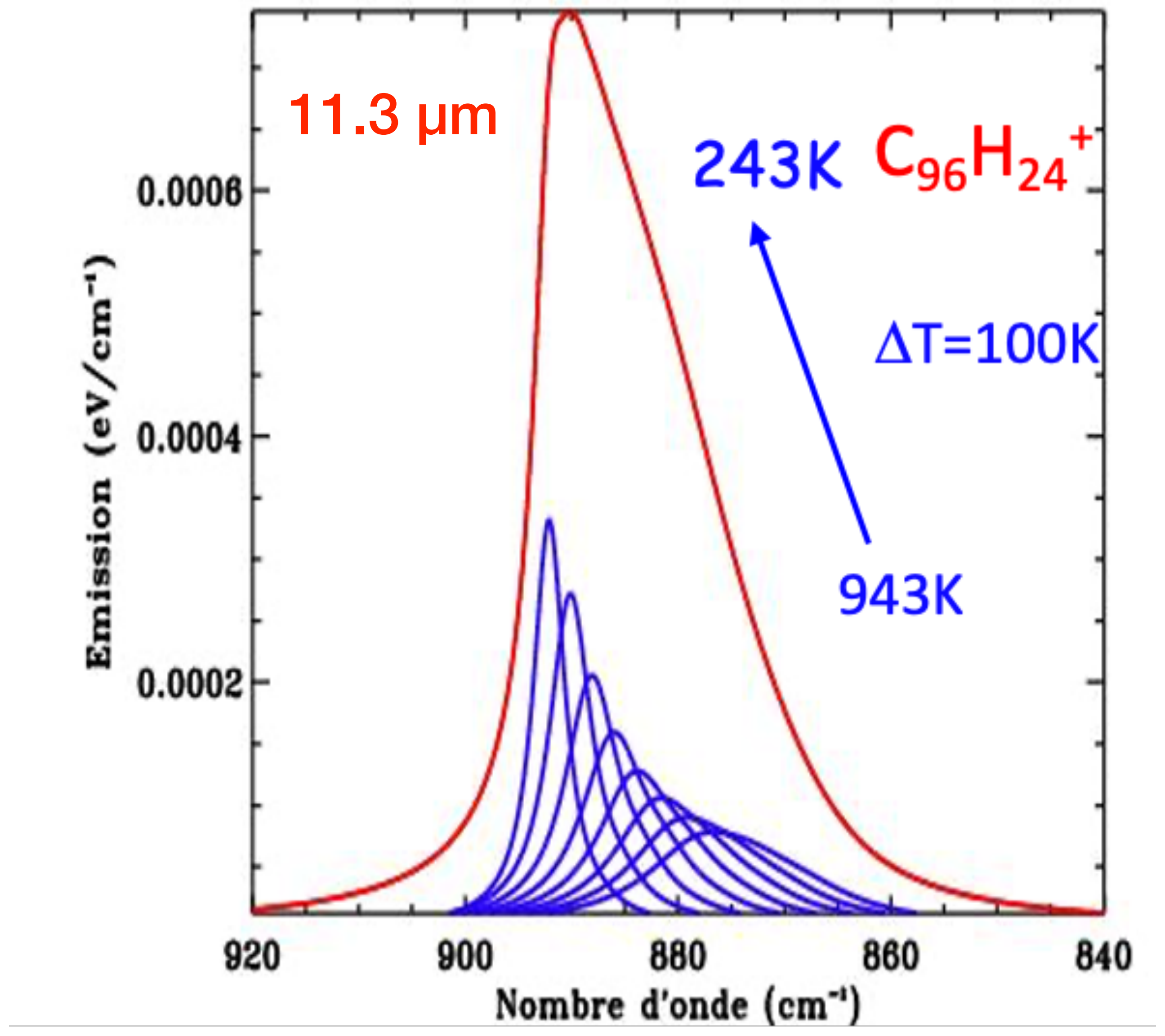
➜ Very good agreement with shorter wavelength studies
➜ Reliability of the long wavelength extrapolations

The Aromatic Infrared bands : modelling the emission of hot PAHs



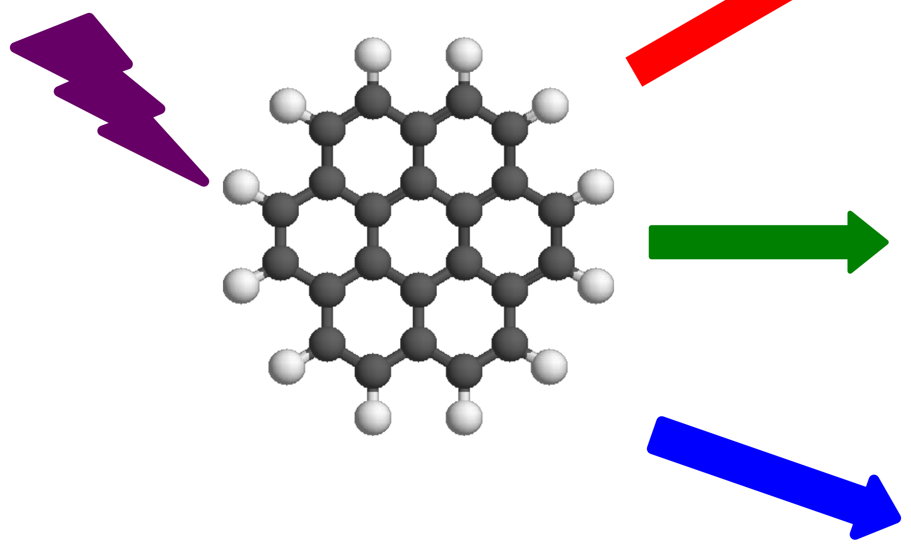
[Chown+*2023*] ERS PDRs4All

[Pech+2002]



Simulation with UV radiation field of PN IRAS 21282+5050 :

VUV photon

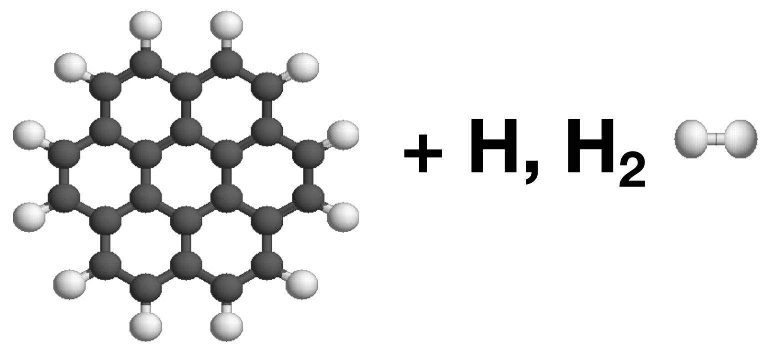


Radiative cooling

The Aromatic Infrared Bands (AIBs)

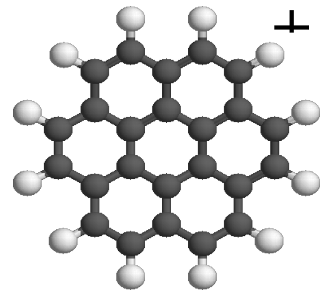
Photodissociation

PAH lifetime



Ionization

Photoelectric effect/ Gas heating

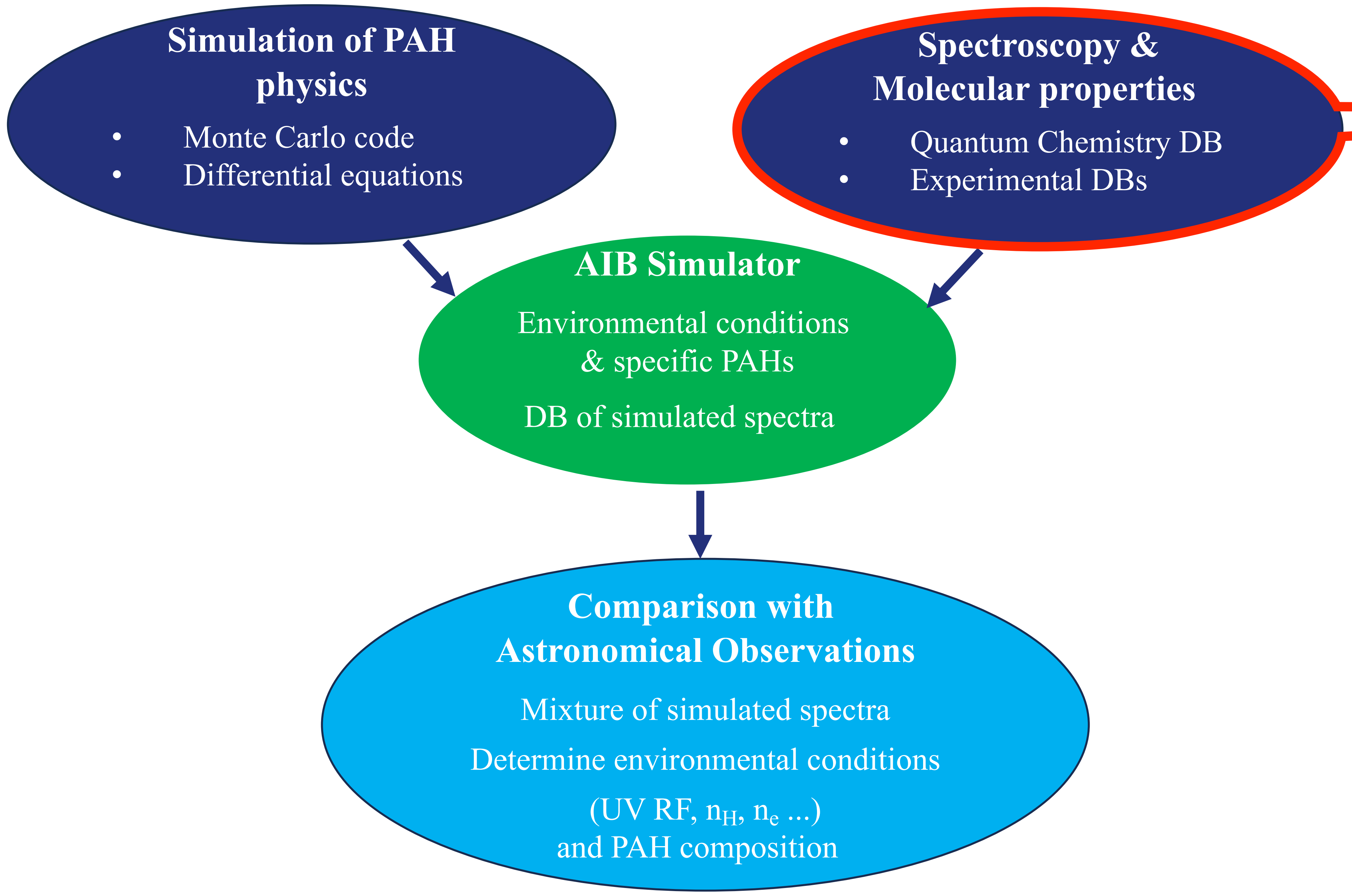


➡ Requires to simulate the spectrum of *a family of PAH* in a given radiation field knowing :

- the excitation conditions (physical conditions, UV) and molecular complexity
- photo-absorption cross-sections
- **vibrational modes**
- **IR band positions and widths as a function of T**

The Aromatic Infrared bands : modelling the emission of hot PAHs

The LAIBrary project :
Library of simulated AIB spectra



Cosmic PAH portal

https://cosmic-pah.irap.omp.eu

See L. de Bentzmann et al. poster

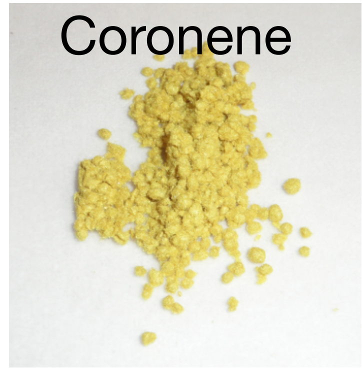
New tools to simulate the infrared emission of PAHs in astrophysical environments:

MIR spectroscopy of solid state and gas phase PAHs as a function of temperature :

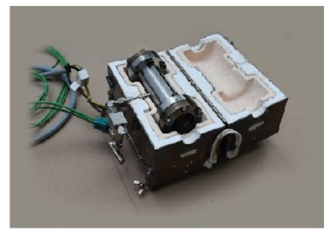
- Transmittance measurements
- Solid state: 14K - 300K & 300K - 723K
- Gas phase: 300K - 673K

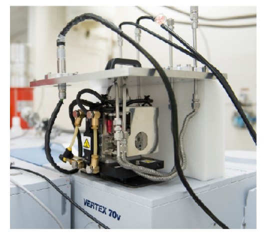
PAHs and fullerene :

- Anthracene ($C_{14}H_{10}$)
- Pyrene ($C_{16}H_{10}$)
- Coronene ($C_{24}H_{12}$)
- Ovalene ($C_{32}H_{14}$)
- Dicoronylene ($C_{48}H_{20}$)
- Fullerene C_{60}



Gas | Solid | Gas & Solid





Decorated species:

Anthracene ($C_{14}H_{10}$) series :

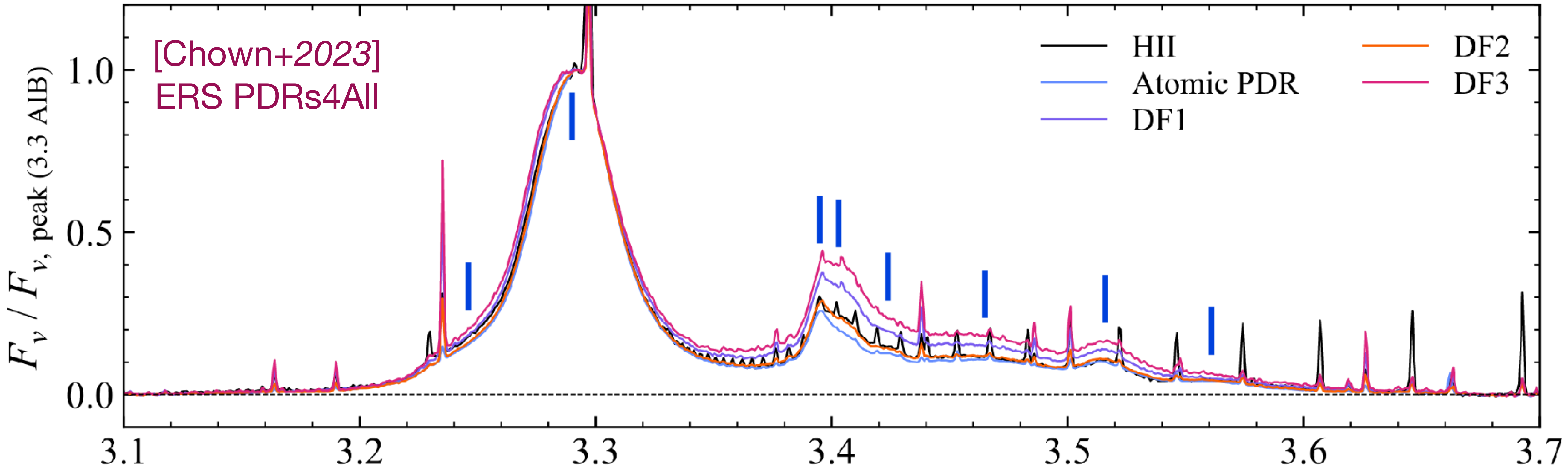
- Anthracene ($C_{14}H_{10}$)
- 2-Methyl Anthracene ($C_{15}H_{12}$)
- 9-Methyl Anthracene ($C_{15}H_{12}$)

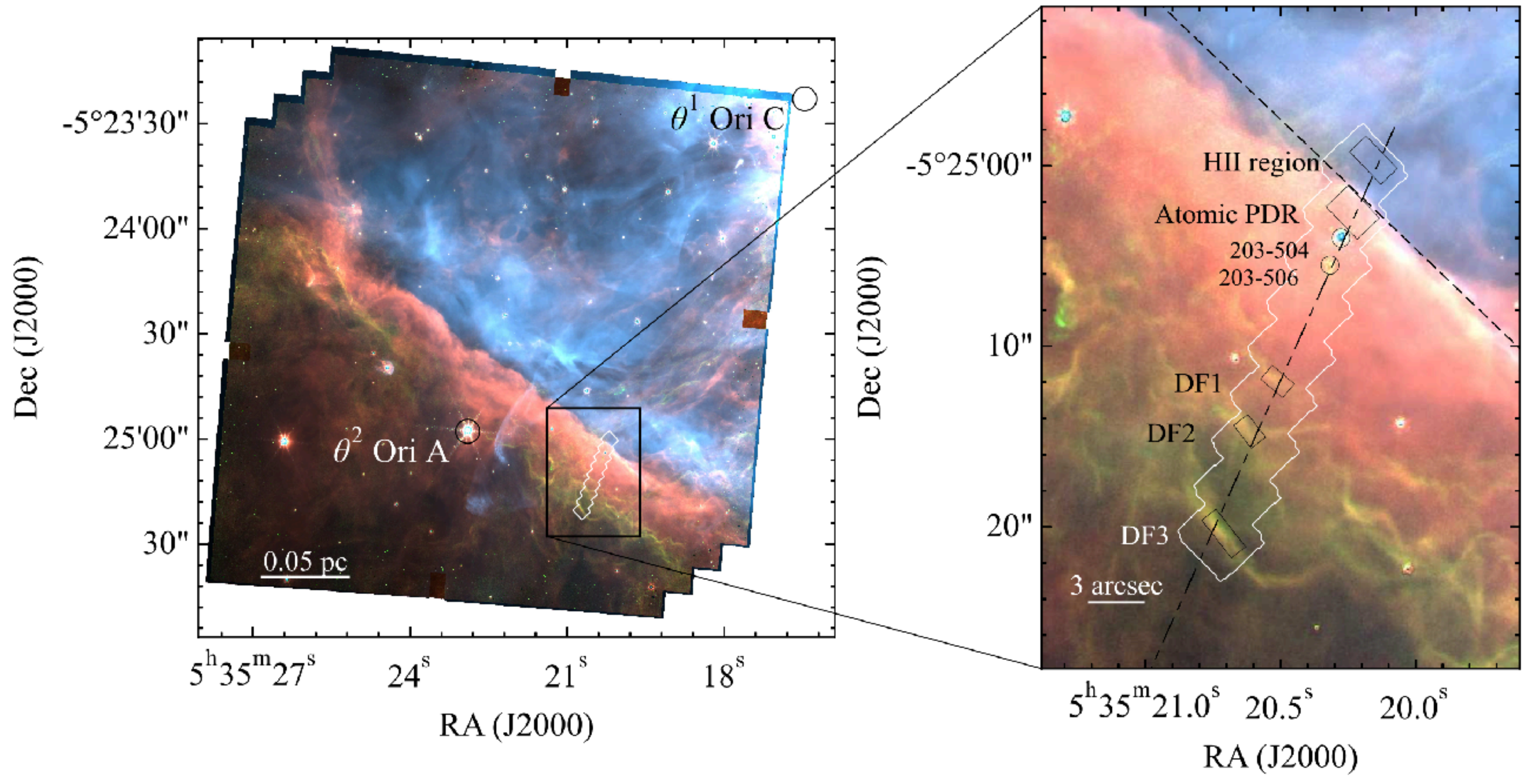
Pyrene ($C_{16}H_{10}$) series :

- 1-Methyl Pyrene ($C_{17}H_{12}$)
- 2-hydropyrene ($C_{16}H_{12}$)
- 4-hydropyrene ($C_{16}H_{14}$)
- 6-hydropyrene ($C_{16}H_{16}$)

The 3.4 µm bands

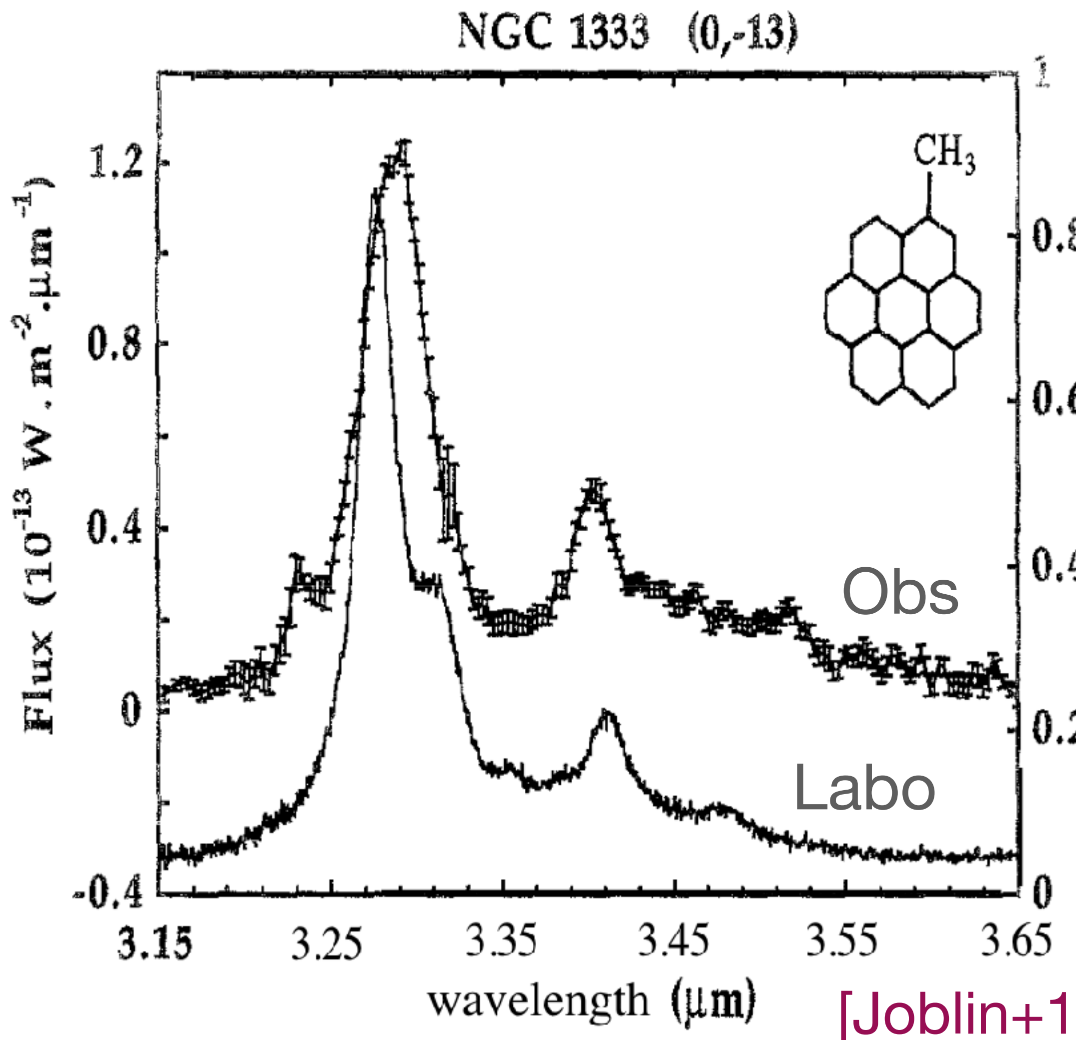
- 3.3 µm band : aromatic CH stretching vibration
- 3.4 µm massif : aliphatic CH stretching vibrations
  - several bands at 3.40, 3.46, 3.51, 3.57 µm
- $I_{3.4}$ / $I_{3.3}$ ↘ when G_o ↗ [eg. Geballe+1989, Pilleri+2015, Chown+2023]





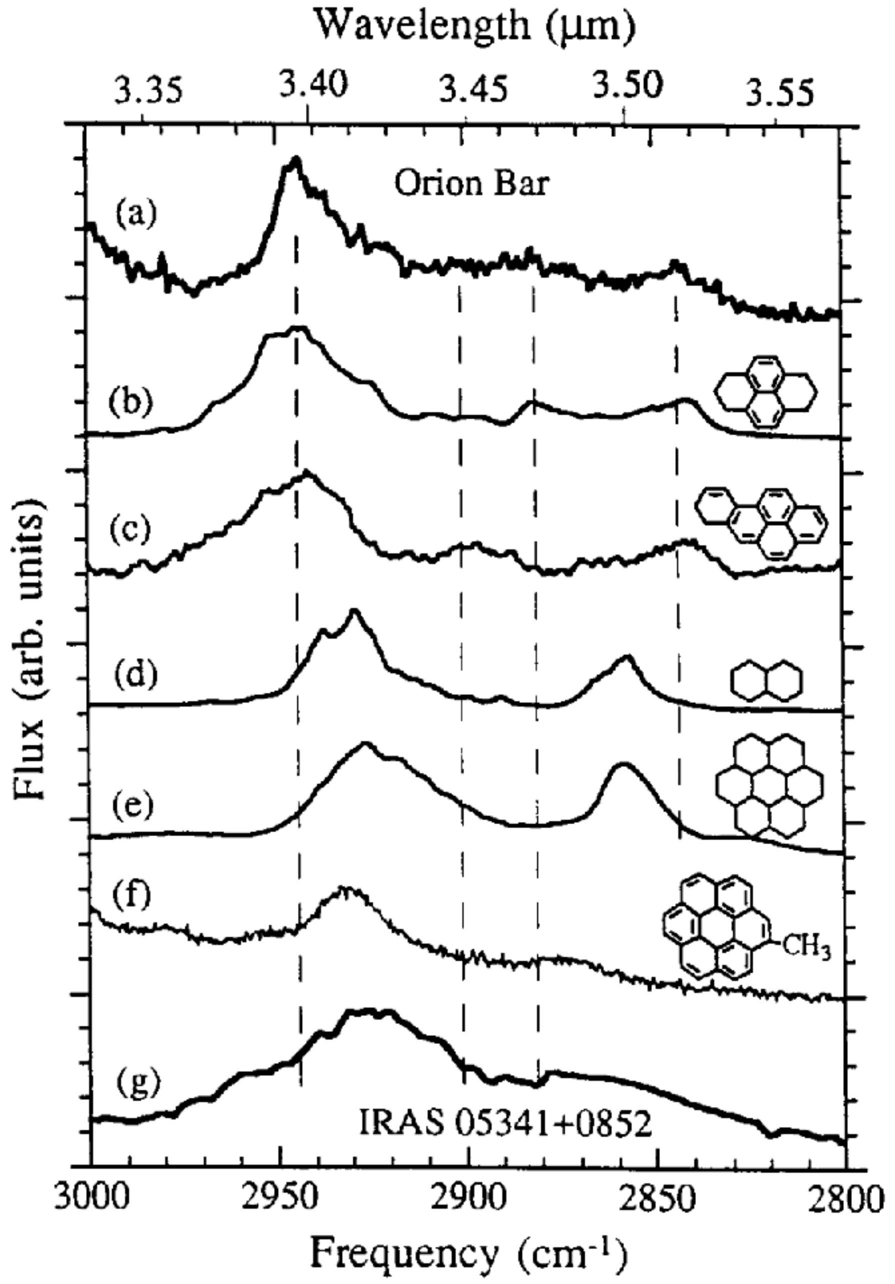
➡ Decorated PAHs (methylated, hydrogenated)

methylated coronene
gas phase spectrum
high temperature



[Joblin+1996]

matrix spectra
low temperature
methylated coronene
hydrogenated PAHs

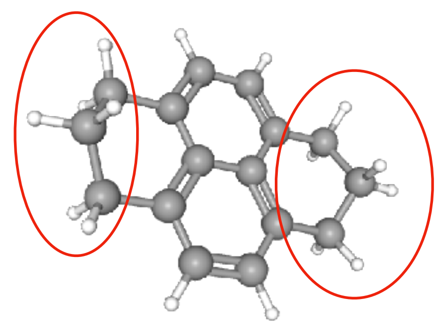


[Berstein+1996]

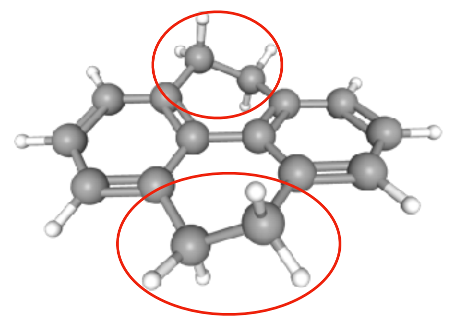
➡ Hydrogenated carbonaceous nanograins (THEMIS model), see Elyajouri+2024

Gas phase methylated and hydrogenated pyrene

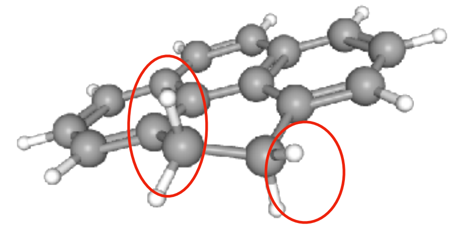
Hexahydropyrene



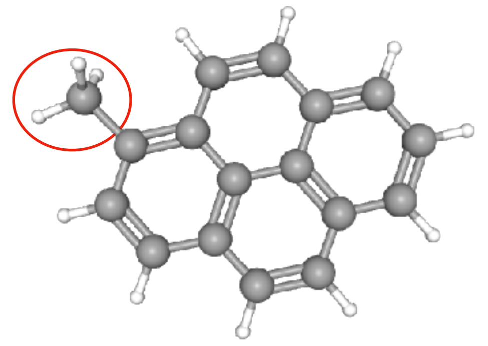
Tetrahydropyrene



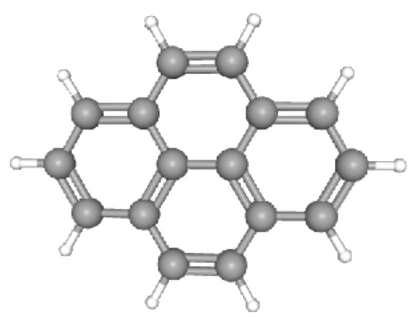
Dihydropyrene



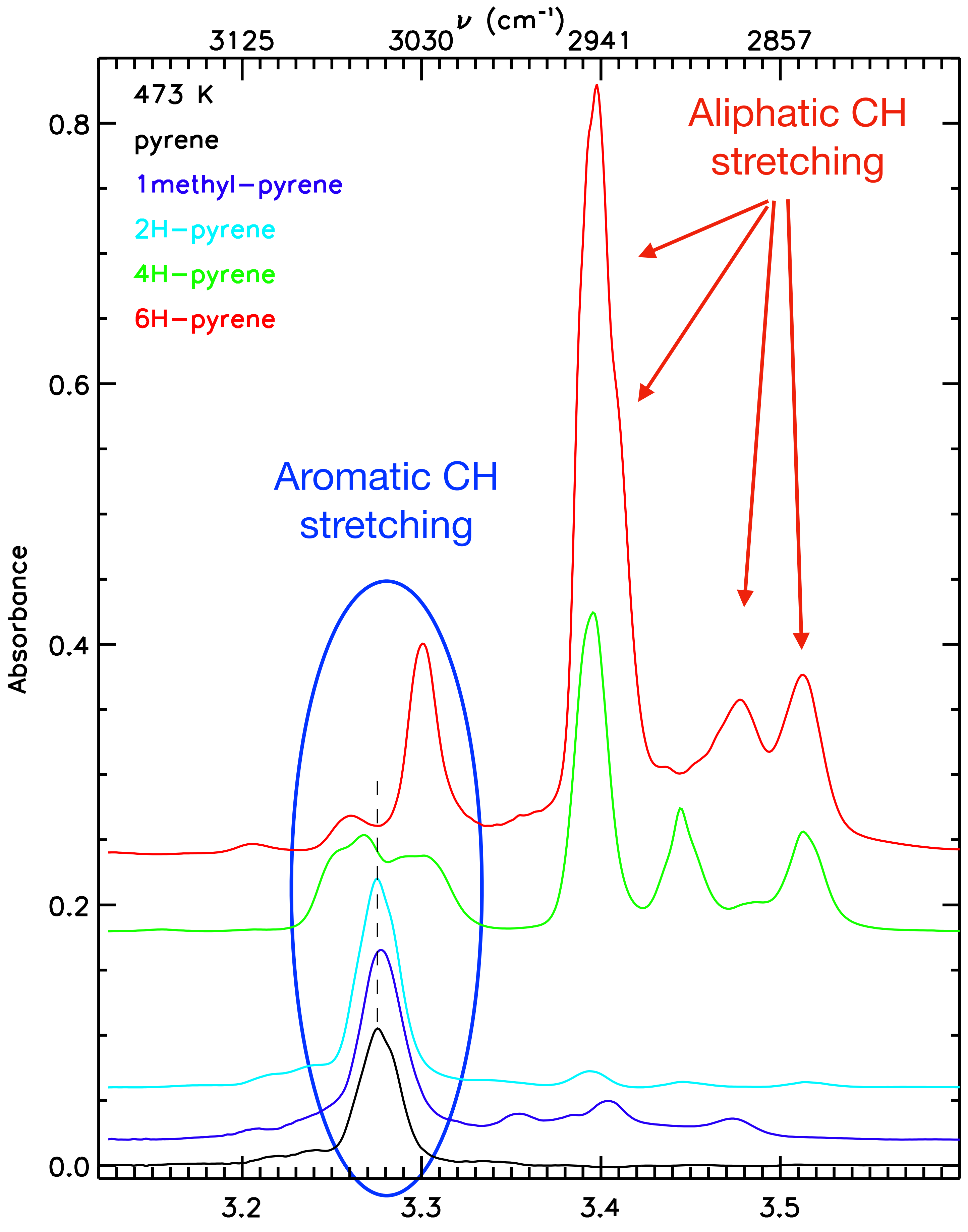
Methylpyrene

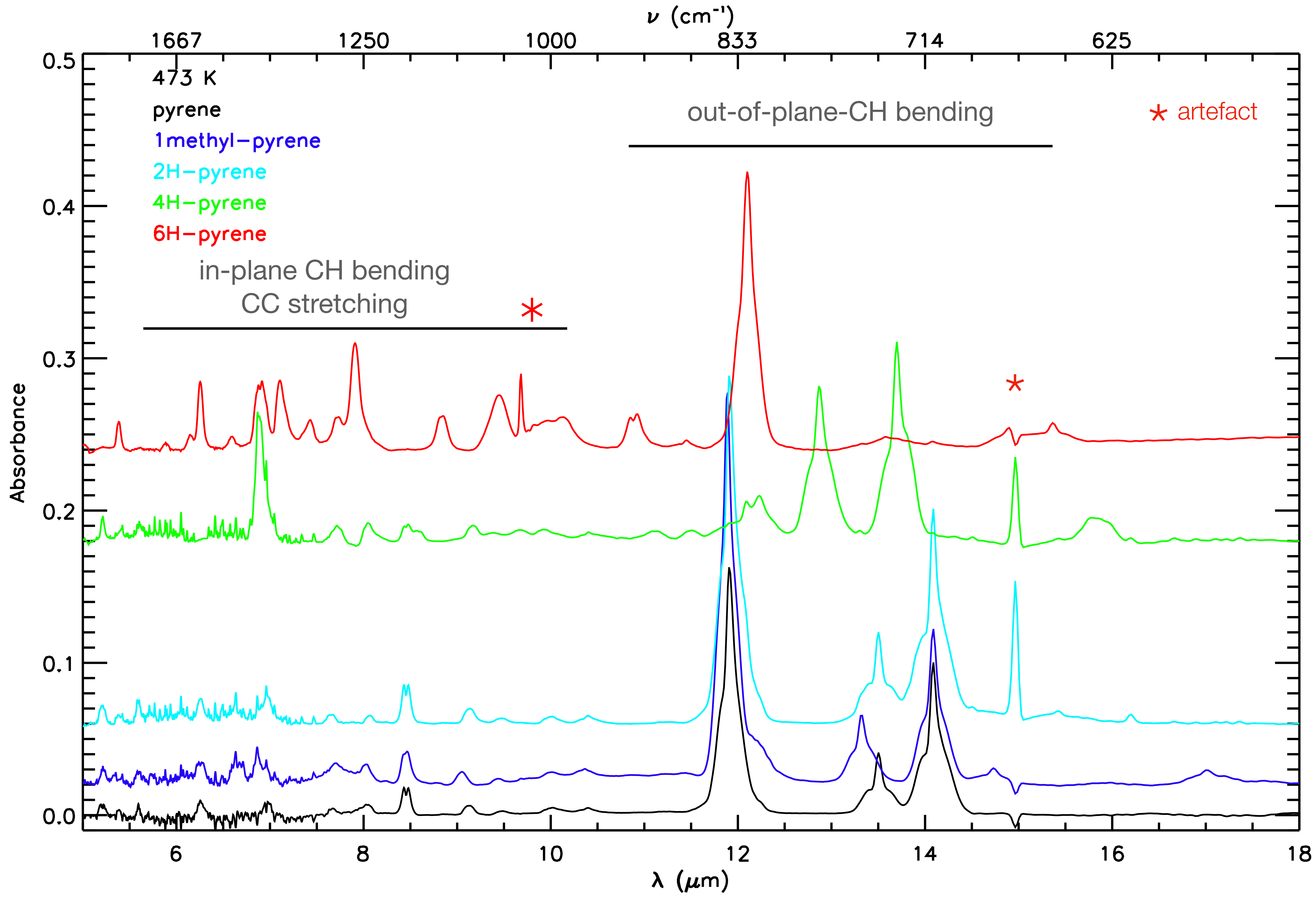


Pyrene



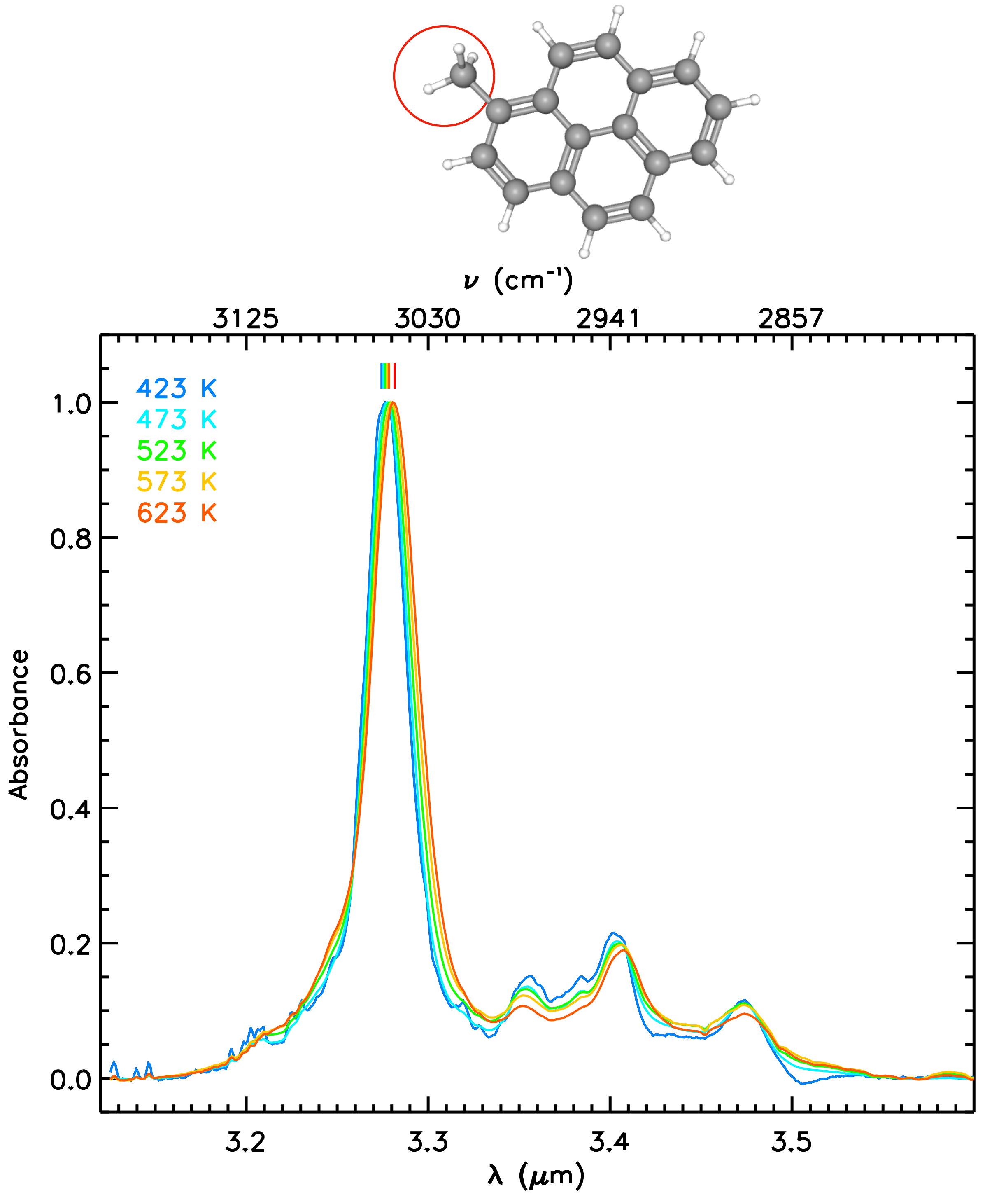
- @ 3µm good agreement with low temperature data from Maltseva+18 (molecular jet) and Sandford+13 (Ar matrix)



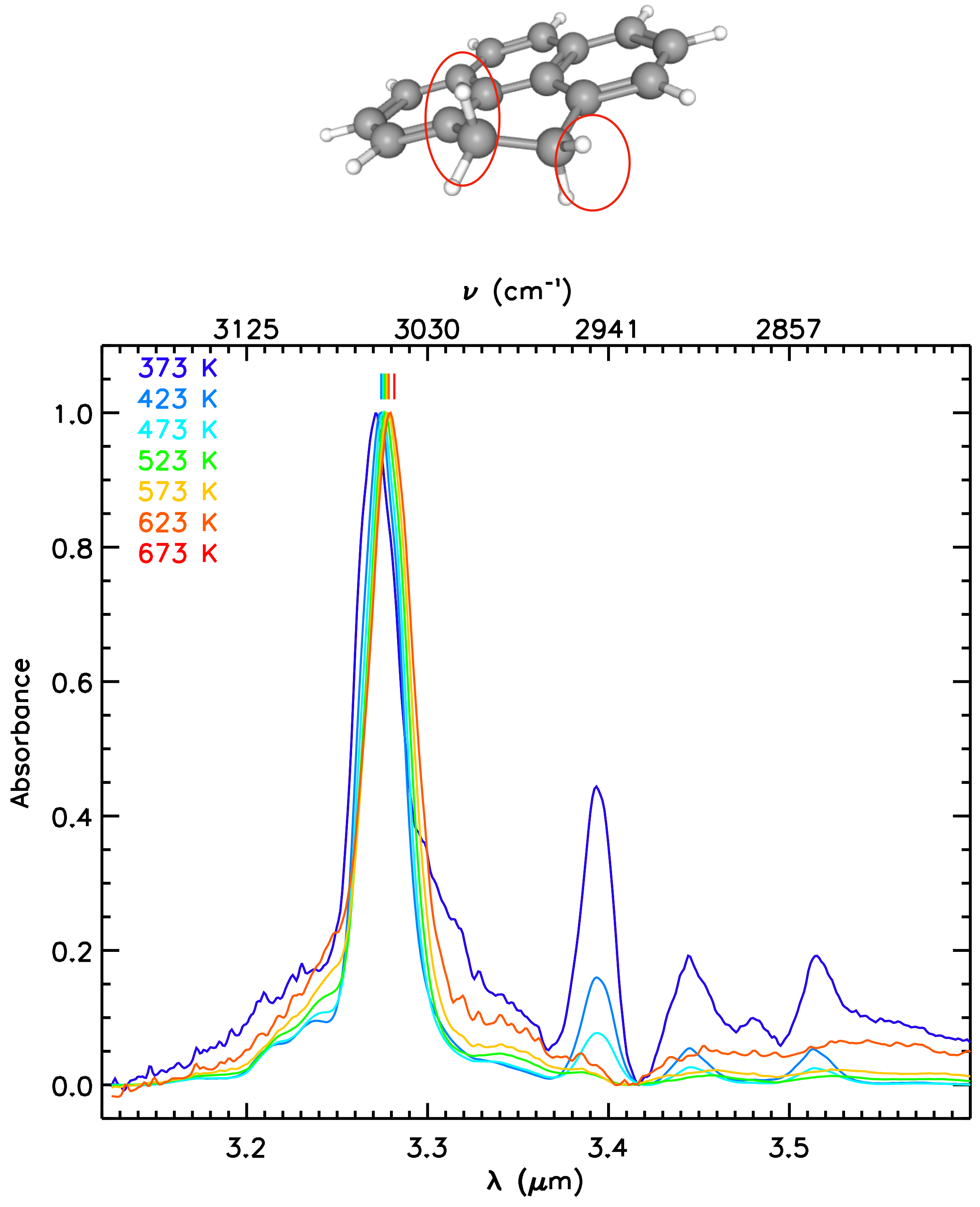


CH stretching evolution with temperature

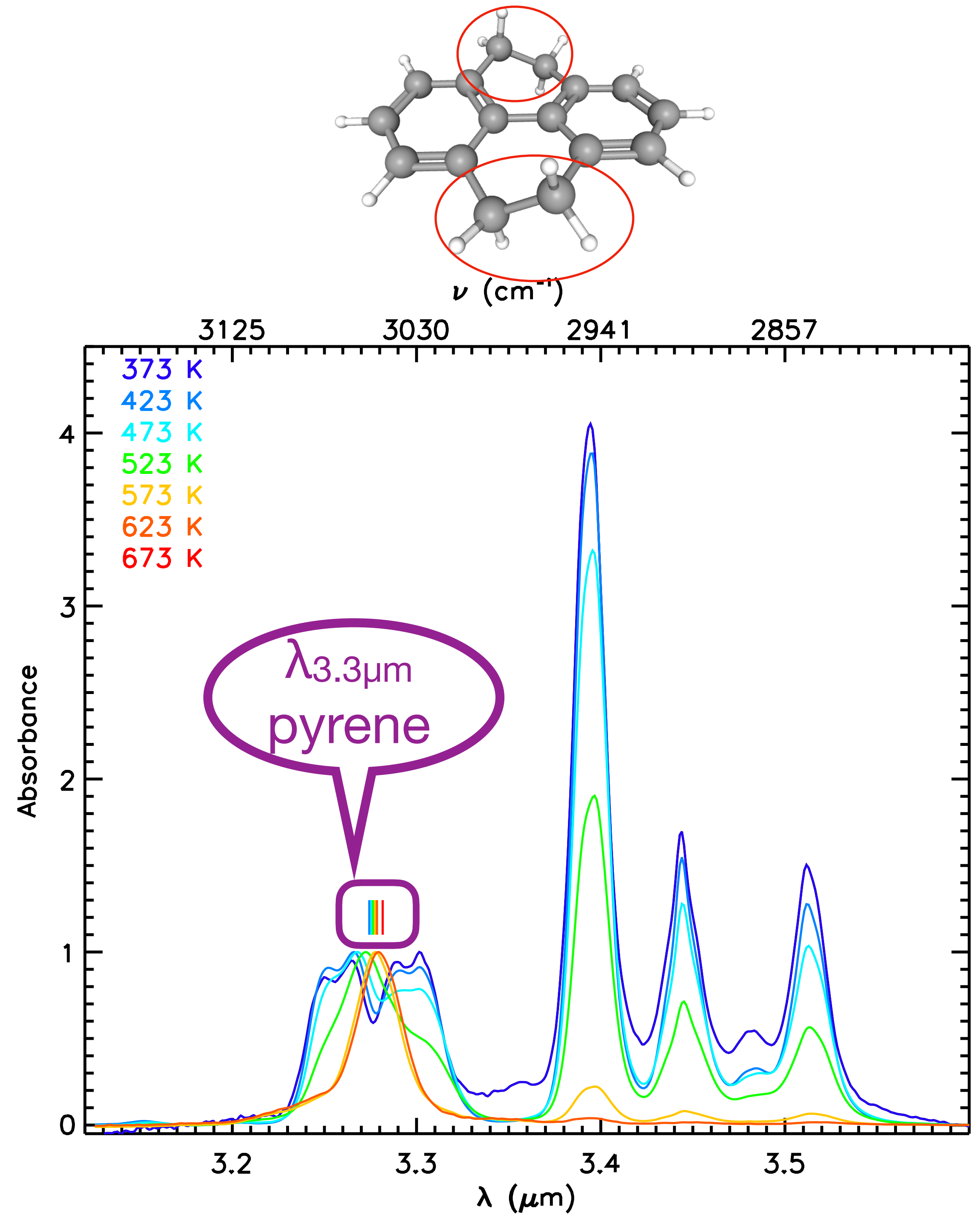
Methylpyrene



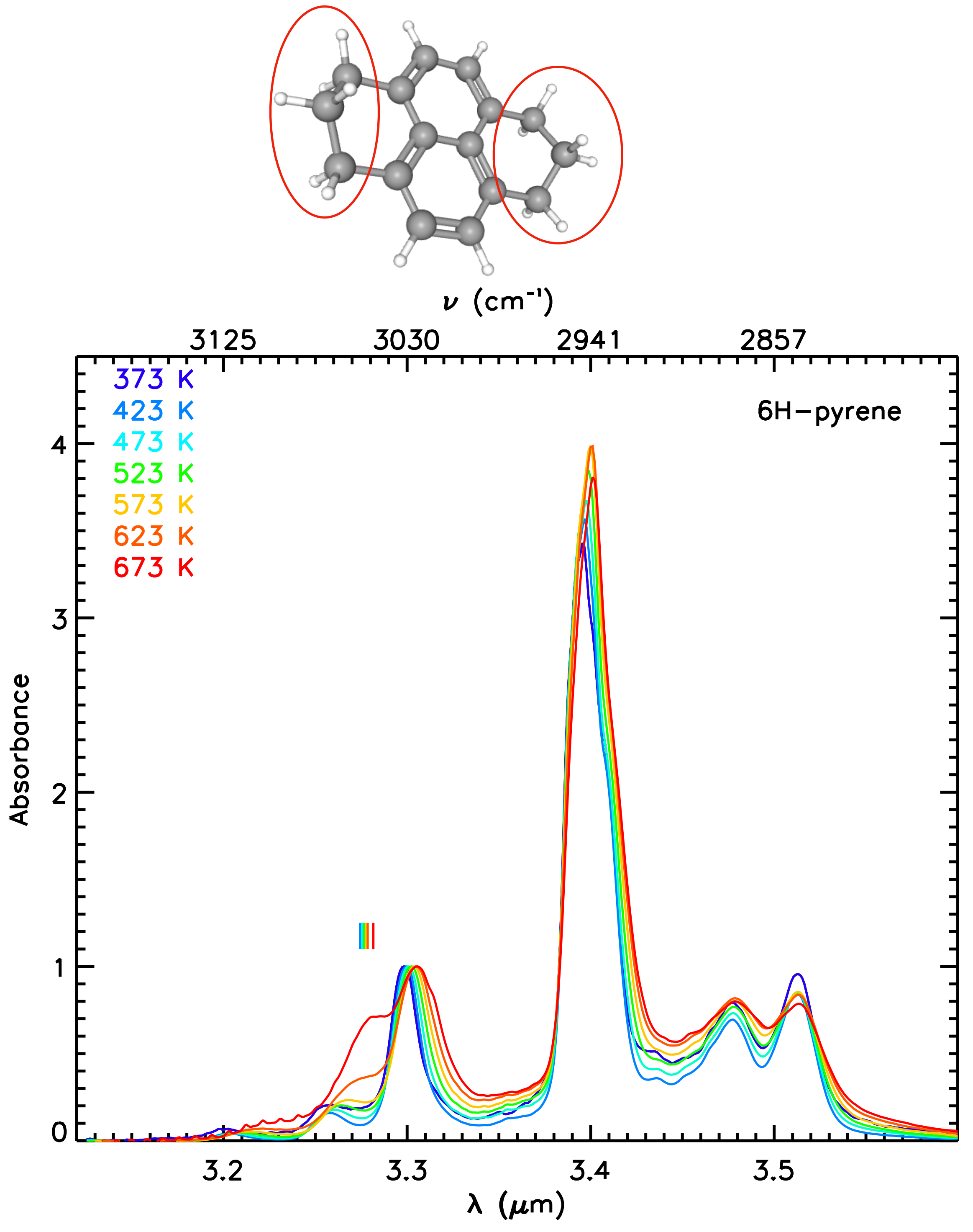
Dihydropyrene



Tetrahydropyrene



Hexahydropyrene



➡ Variation of the band position and intensity with temperature

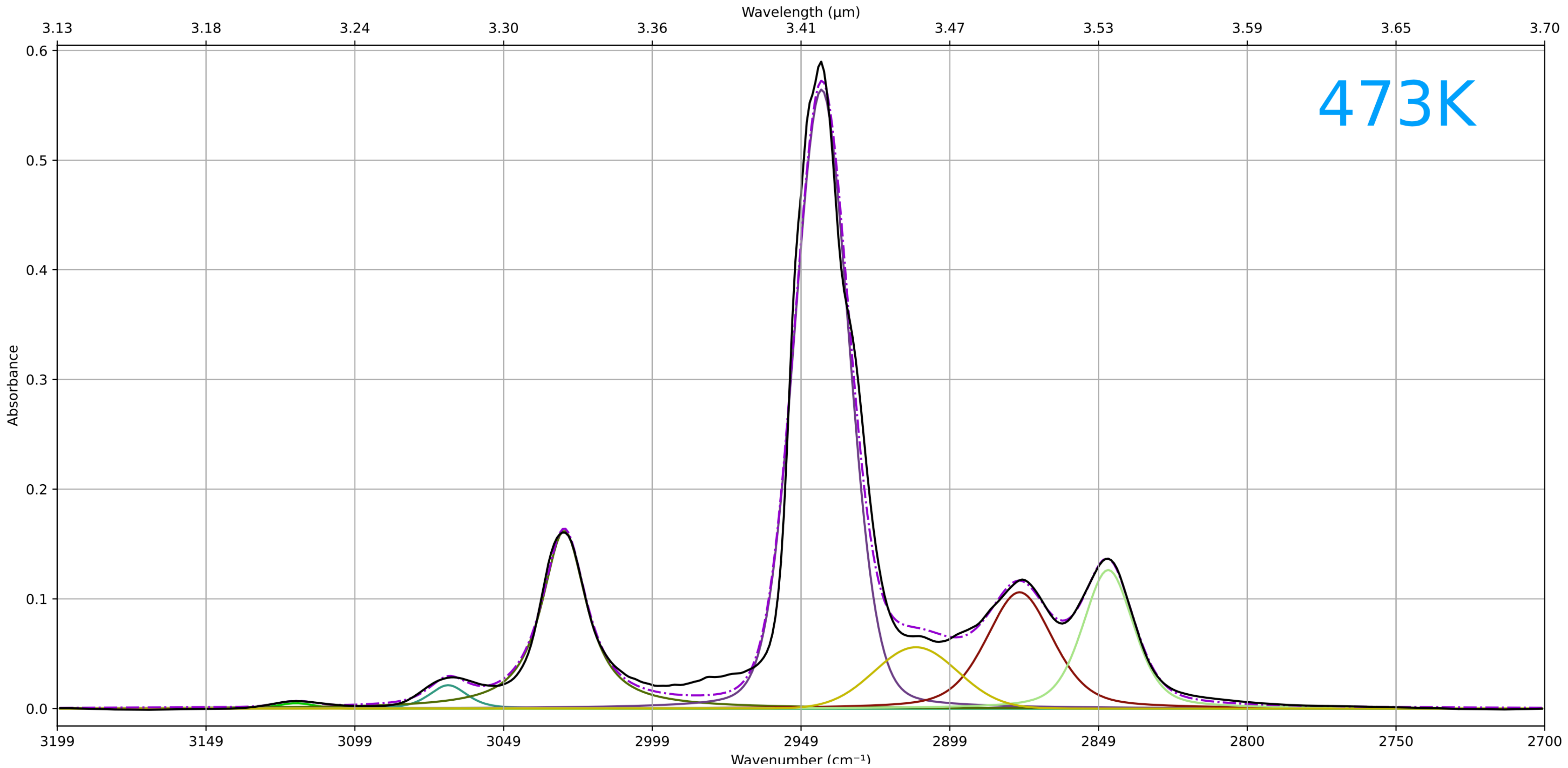
- Di- and tetra-hydropyrene disappear at T ≥ 423 - 473 K
- Methyl-pyrene and hexa-hydropyrene are present up to T ≥ 623 K
  - ➡ Related to our experimental conditions (high pressure)

Data available on the cosmicPAH-IRDB database

See L. de Bentzmann et al. poster
New tools to simulate the infrared emission of PAHs in astrophysical environments:

Analysing the spectra : characterising the anharmonicity

- Spectral decomposition at each temperature with the CosmicPAHmfit tool (see Louan de Bentzman poster)
  - pseudo-Voigt profil



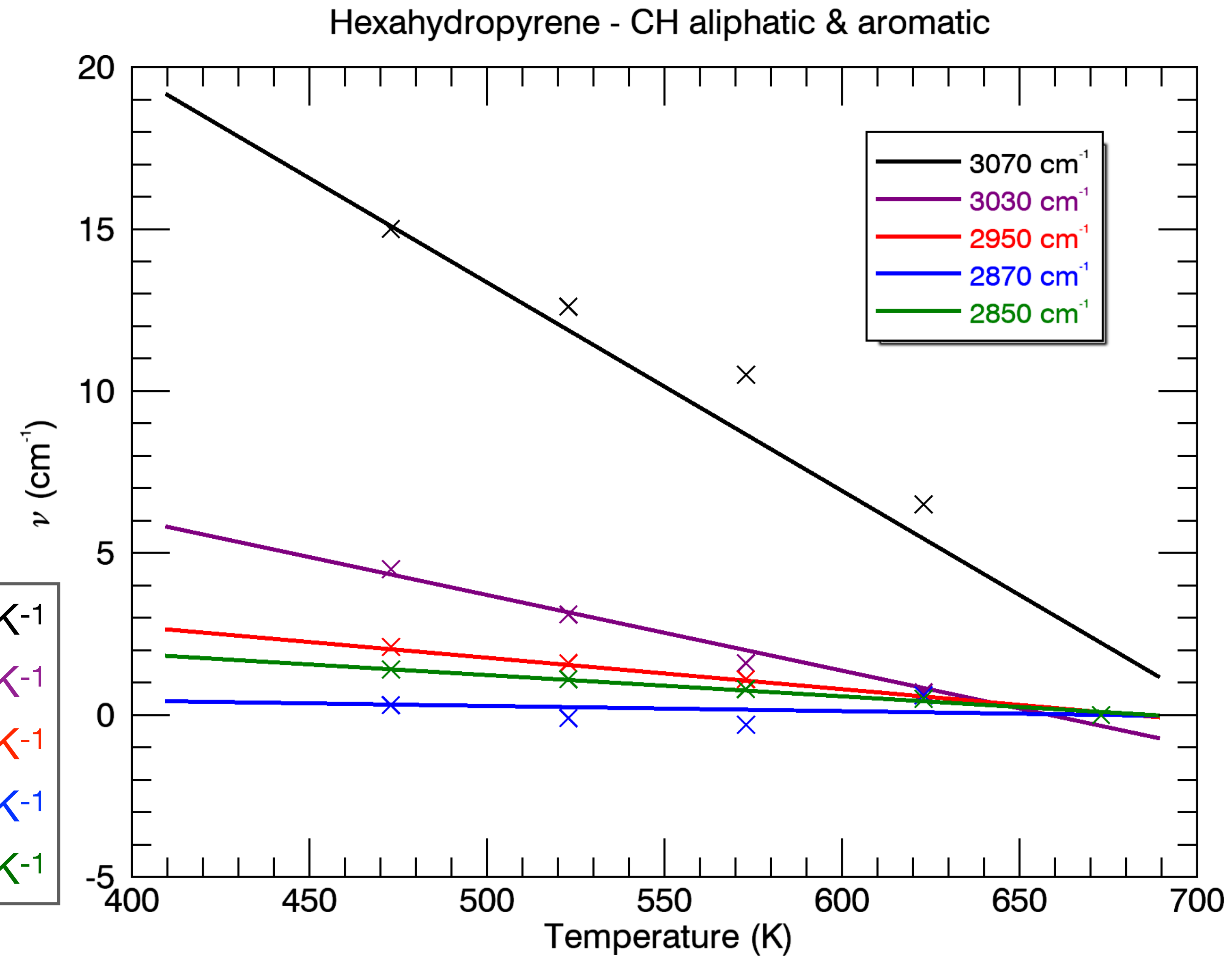
χ_{pos} = -6.43E-2 cm^{-1}.K^{-1}

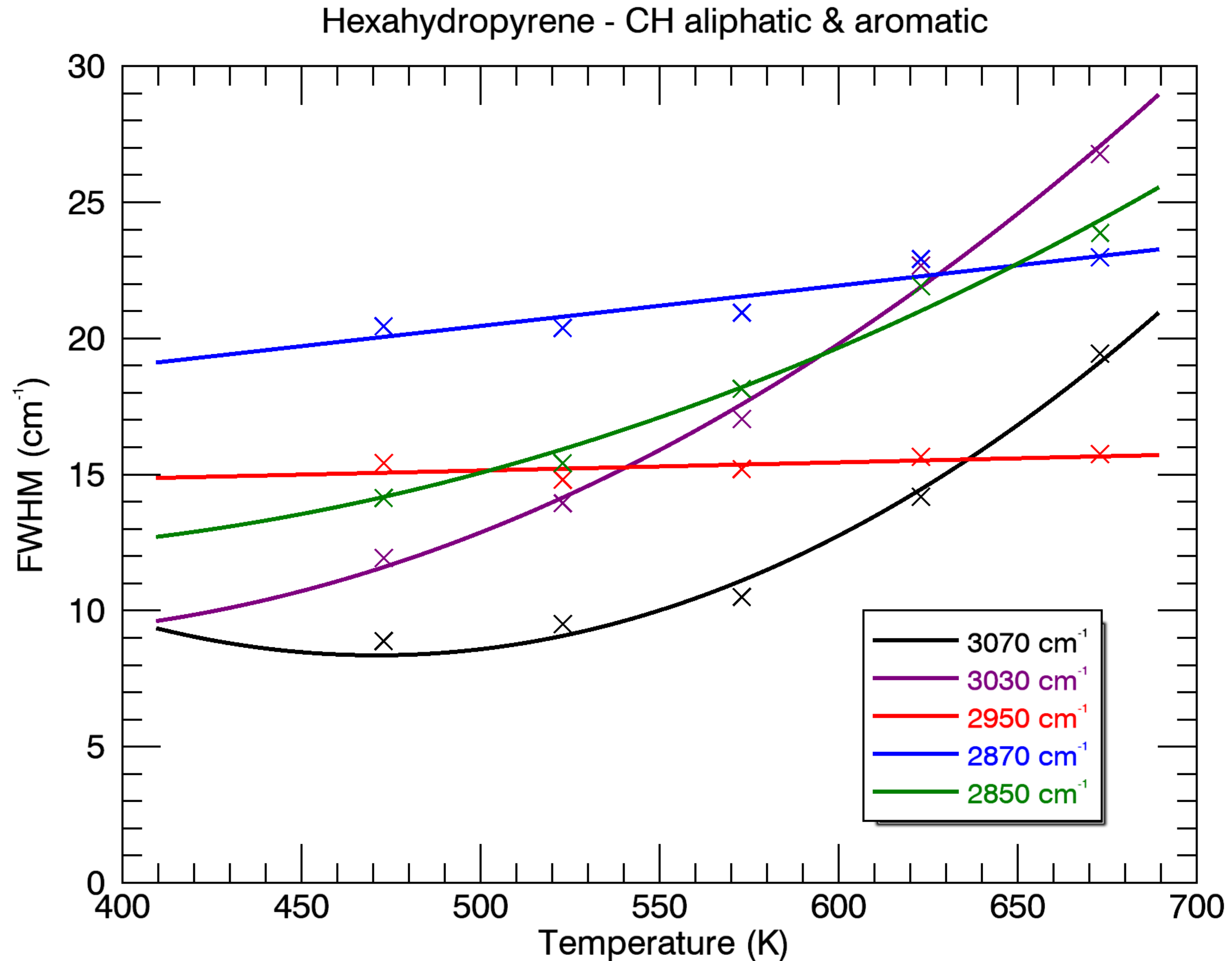
χ_{pos} = -2.33E-2 cm^{-1}.K^{-1}

χ_{pos} = -0.97E-2 cm^{-1}.K^{-1}

χ_{pos} = -0.16E-2 cm^{-1}.K^{-1}

χ_{pos} = -0.65E-2 cm^{-1}.K^{-1}





- Correct for rotational broadening
- Linear or polynomial fit of the pos, width vs T $\Rightarrow \chi_{pos}, \chi_{width}$ on the measured range

- Outside the studied temperature range :
  - combine with solid state and gas phase data if possible
  - find the best extrapolation

cosmicPAH-IRDB

cosmicPAH
IRDB

- Show samples
- Help
- Update User
- New Species
- Edit Instruments
- Log out

WORK IN PROGRESS of The Toulouse cosmicPAH database of anharmonic infrared spectra

CosmicPAH_IRDB is a spectroscopic database providing infrared spectra of molecular species, in solid or gas phase, as a function of temperature. It also provides the empirical anharmonicity functions that characterise the temperature evolution of the band position and width.

Targeted molecules include polycyclic aromatic hydrocarbons (PAHs), fullerenes and derivative species.

The experimental data presented were obtained with the ESPOIRS setup at IRAP, which has been developed in the framework of the COLD DUST ANR project and the Nanocosmos ERC synergy project (https://nanocosmos.iff.csic.es).

ESPOIRS consists of a Bruker infrared Fourier transform spectrometer 70V equipped with a set of sources, detectors and beamsplitters allowing for measurements from 0.9 µm to about 1mm. It is equipped with a cryostat for measurements of solid state samples from 10 to 300 K, a high-temperature cell for solid state samples (300 - 1000 K) and a high-temperature gas cell (300 - 800K).

The recorded infrared spectra are analysed using the multi-component fitting tool, CosmicPAHmfit, to decompose the vibrational bands with pseudo-Voigt profiles and derive empirical anharmonicity functions which quantify the evolution of the band positions and widths with temperature.

Contacts

Scientific Contacts

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Contributions by Giacomo Mulas (OAC, INAF) and Dominique Toublanc (LCAR, UT3, CNRS) are acknowledged.

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Molecules

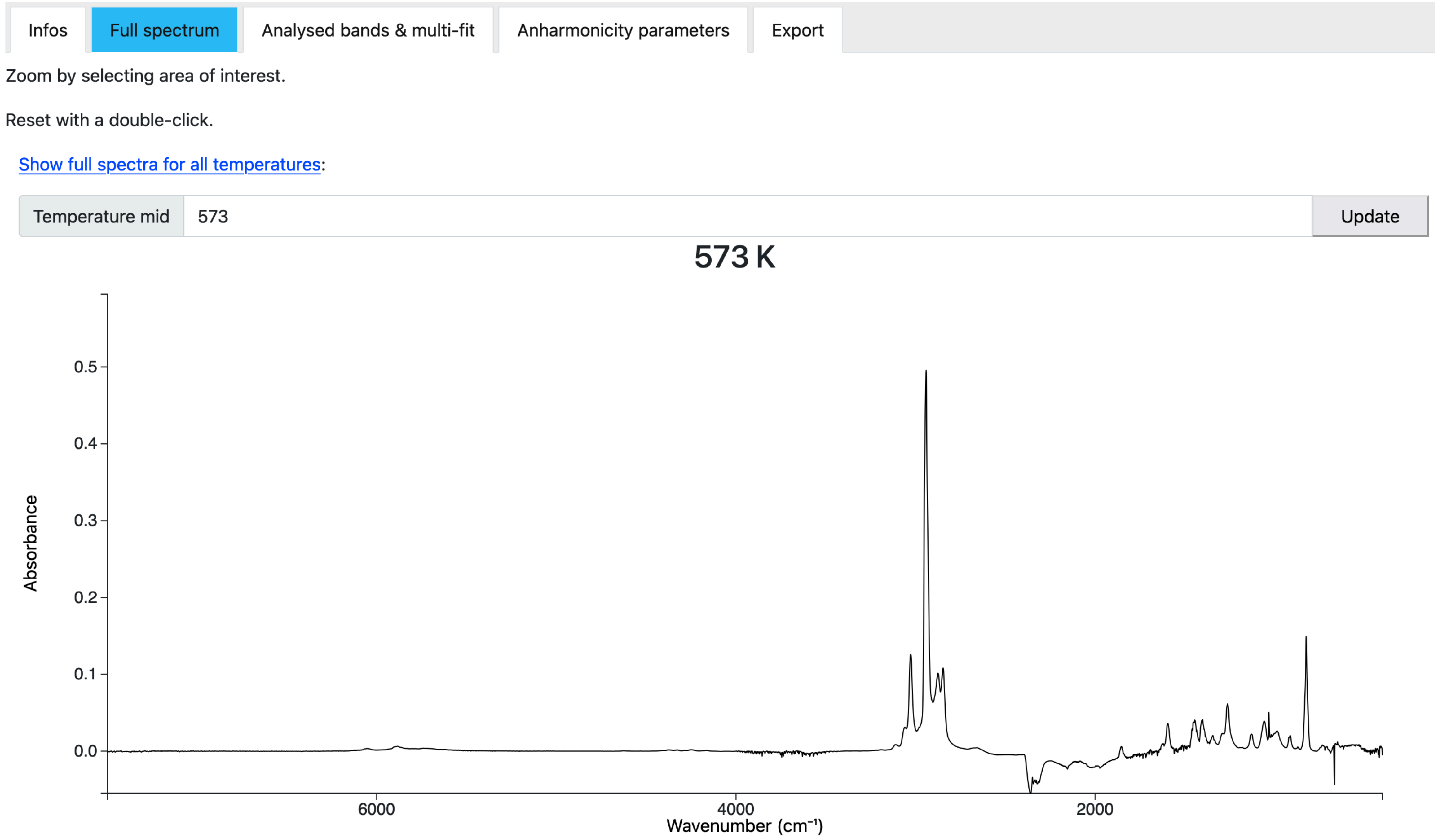
List of species in the database

Formula/Name... | Category... | Phase... | Visibility... | Date... | Id...

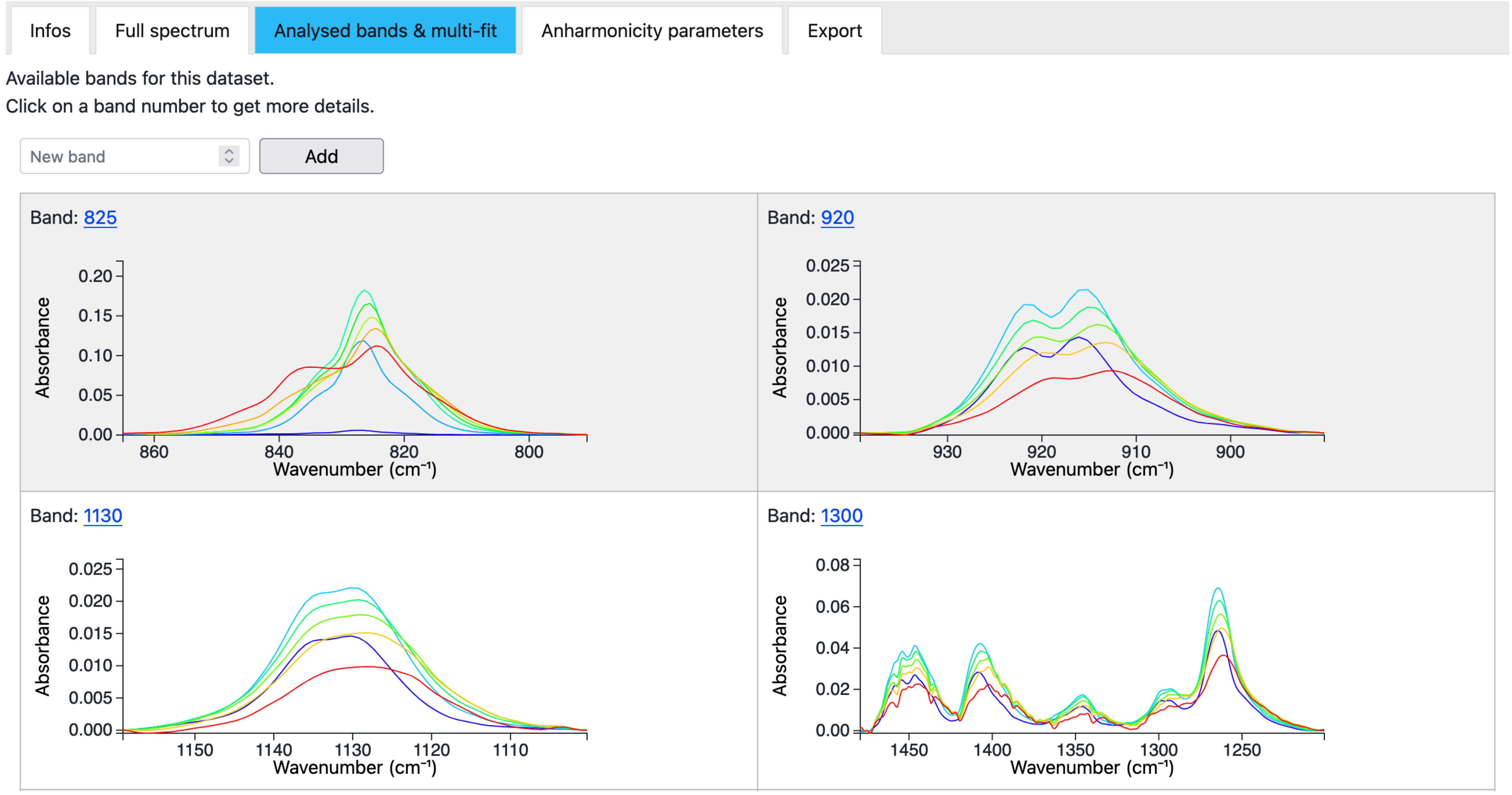
1

Sample name	Structure	Temperature range (K)	Category	Phase	Version	Visibility	Date	Id
Pyrene : $C_{16}H_{10}$		[373-673]	Experimental	Gas	1.1.1	Private	2024-09-02	#1
1-methylpyrene : $C_{17}H_{12}$		[373-623]	Experimental	Gas	1.1.1	Private	2024-09-03	#2
4,5-dihydropyrene : $C_{16}H_{12}$		[373-623]	Experimental	Gas	1.1.1	Private	2024-09-10	#3
4,5,9,10-tetrahydropyrene : $C_{16}H_{14}$		[373-623]	Experimental	Gas	1.1.1	Private	2024-09-04	#4
1,2,36,7,8-hexahydropyrene : $C_{16}H_{16}$		[373-673]	Experimental	Gas	1.1.1	Private	2024-09-04	#5
4,5-dihydropyrene : $C_{16}H_{12}$		[373-623]	Experimental	Gas	1.1.2	Private	2024-10-18	#6
4,5,9,10-tetrahydropyrene : $C_{16}H_{14}$		[373-623]	Experimental	Gas	1.1.2	Private	2024-10-18	#7
Pyrene : $C_{16}H_{10}$		[373-673]	Experimental	Gas	1.1.2	Private	2024-10-22	#8
1,2,36,7,8-hexahydropyrene : $C_{16}H_{16}$		[373-673]	Experimental	Gas	1.1.2	Private	2024-10-25	#9

cosmicPAH-IRDB



Visualisation of spectra over the entire spectral range for each temperature

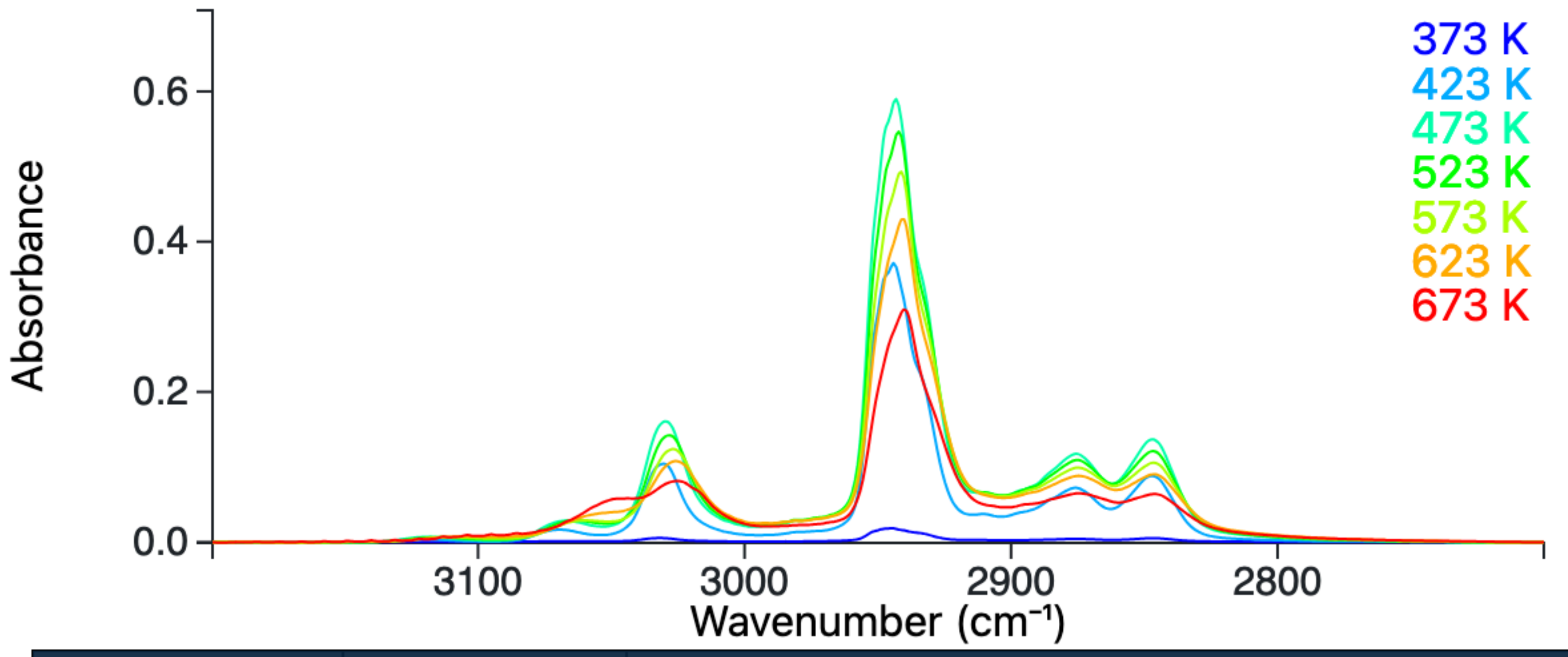


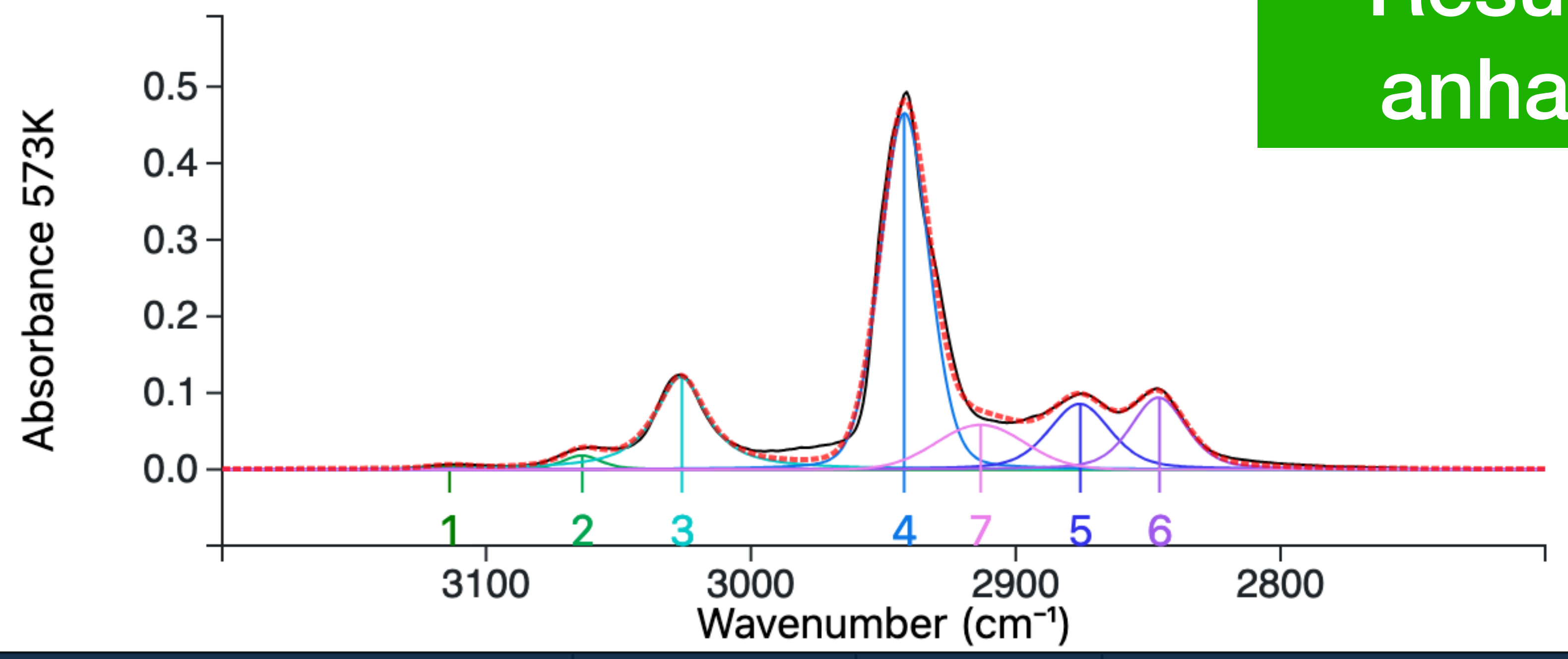
List of specific bands analysed:

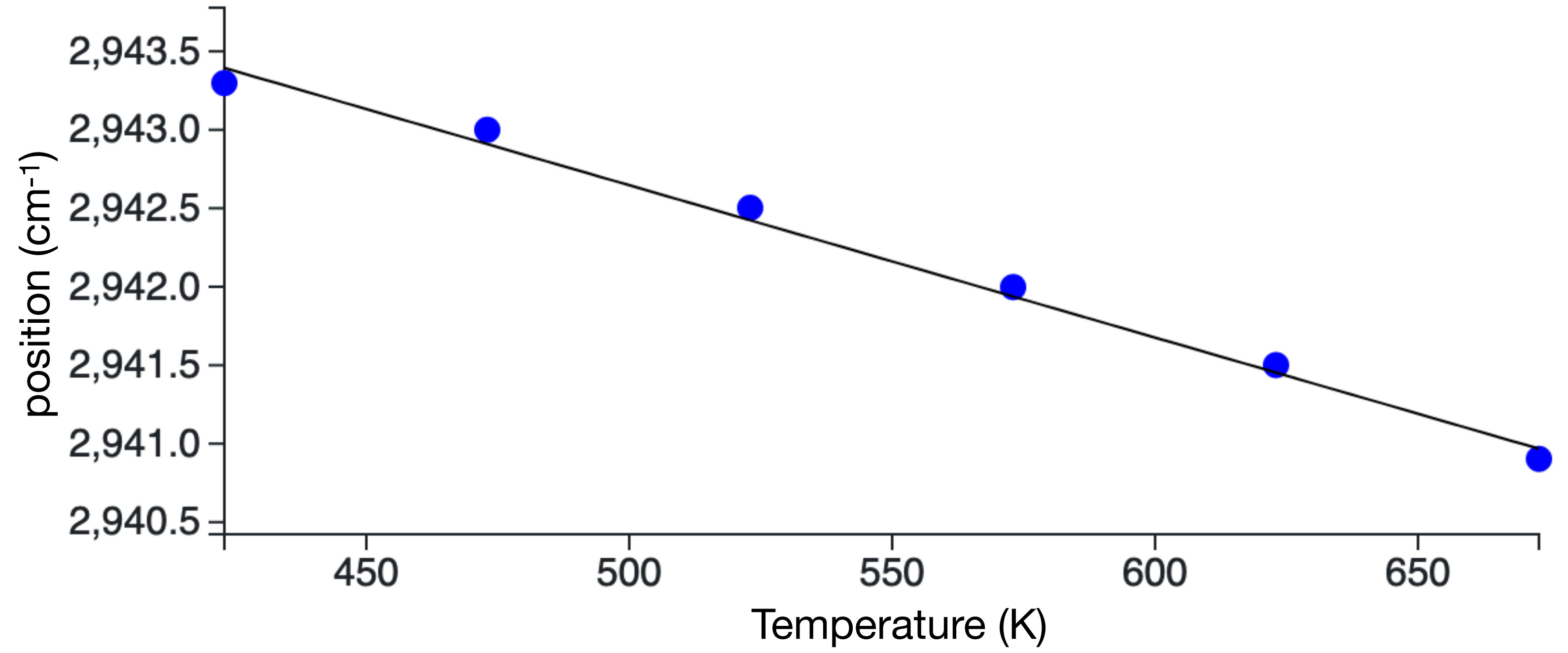
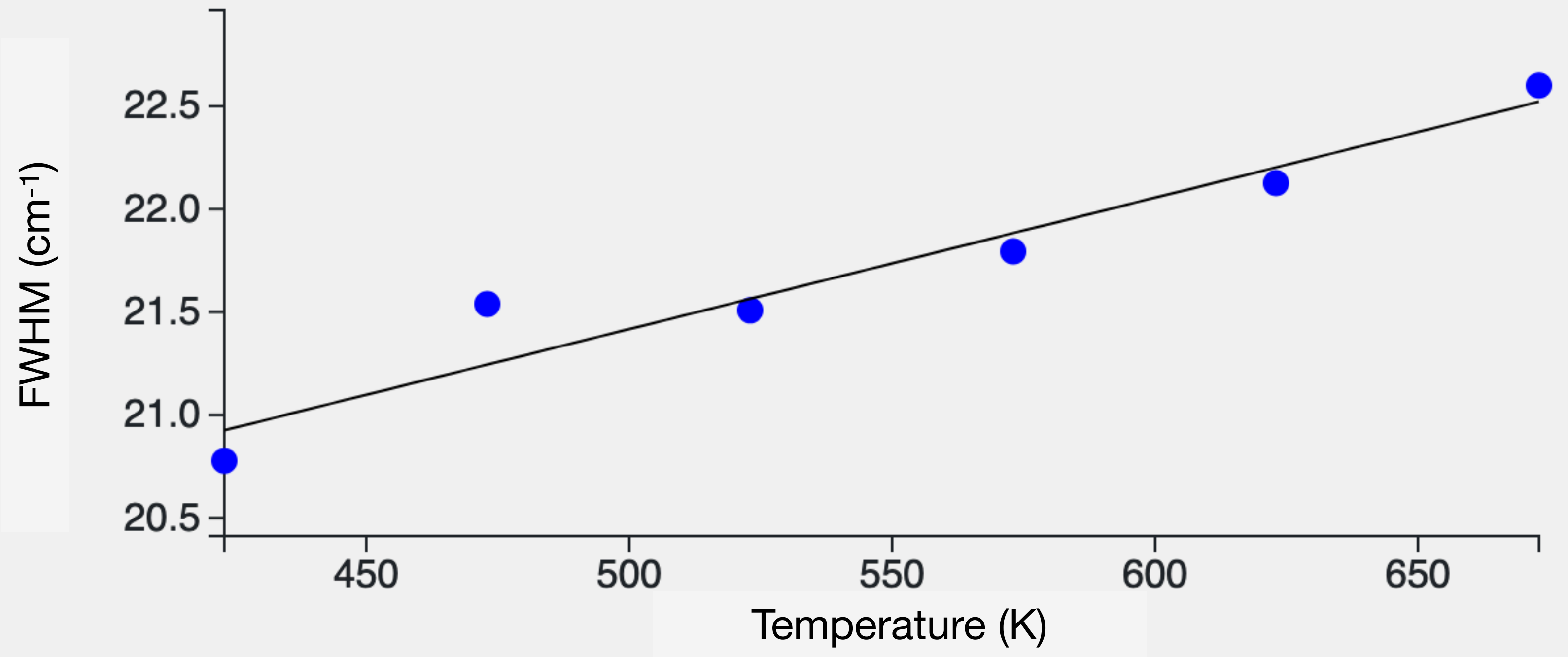
cosmicPAH-IRDB

Results on specific bands : anharmonicity coefficients

Download informations on this band : 1,2,36,7,8-hexahydropyrene $C_{16}H_{16}$ 3030.zip





Components	Parameters	Graph	Fit Range (K)	Origin Y(0)	Anharmonicity factors C1	C2	C3
○ 2 ○ 3 ◉ 4 ○ 5 ○ 6	Profile	Gaussian = 0.85 Lorentzian = 0.15					
	Position		423-673	2947.5	-0.0097066	.	.
	FWHM		423-673	18.226	0.0063819	.	.

cosmicPAH-IRDB

Anharmonicity parameters

Infos | Full spectrum | Analysed bands & multi-fit | Anharmonicity parameters | Export

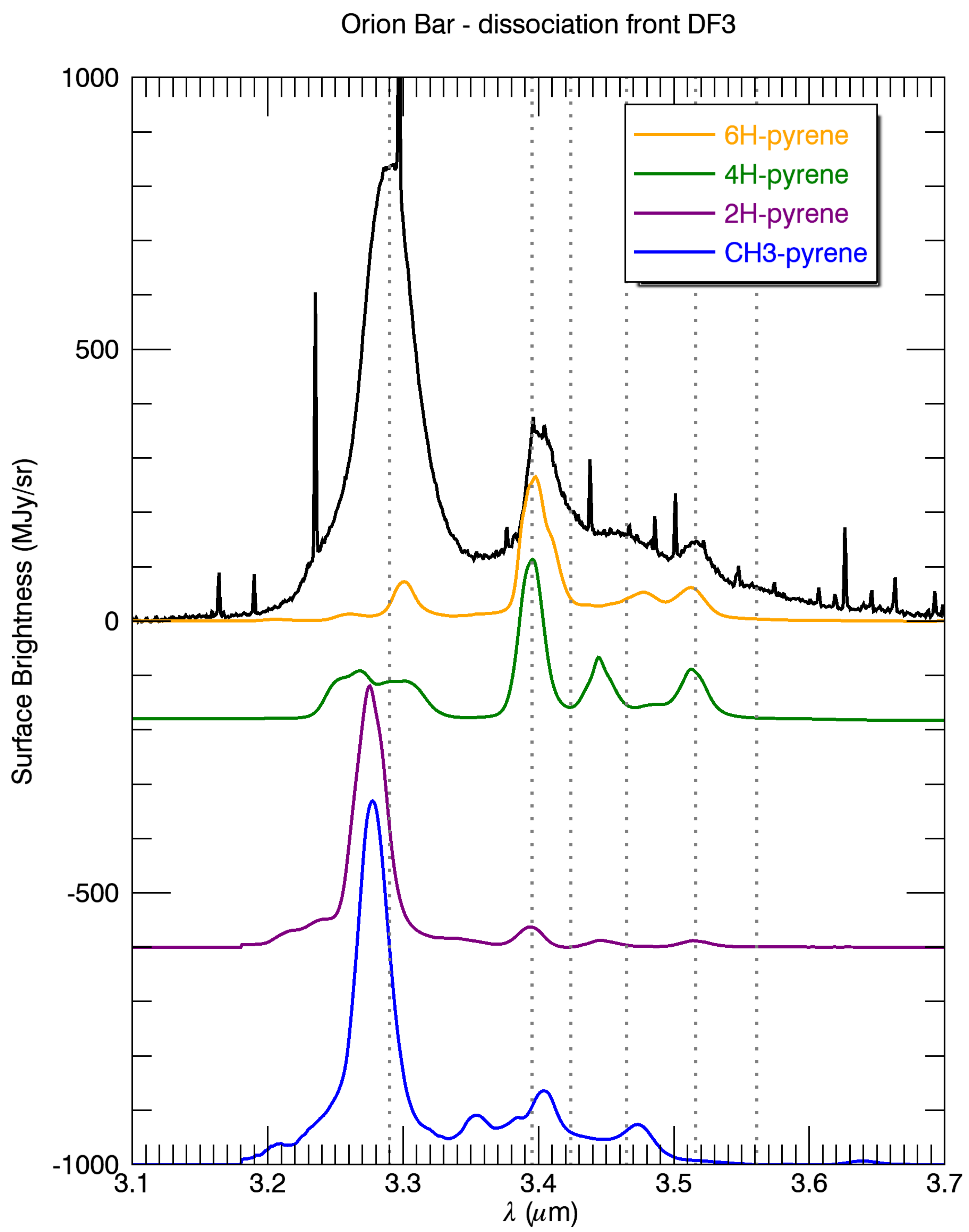
Position

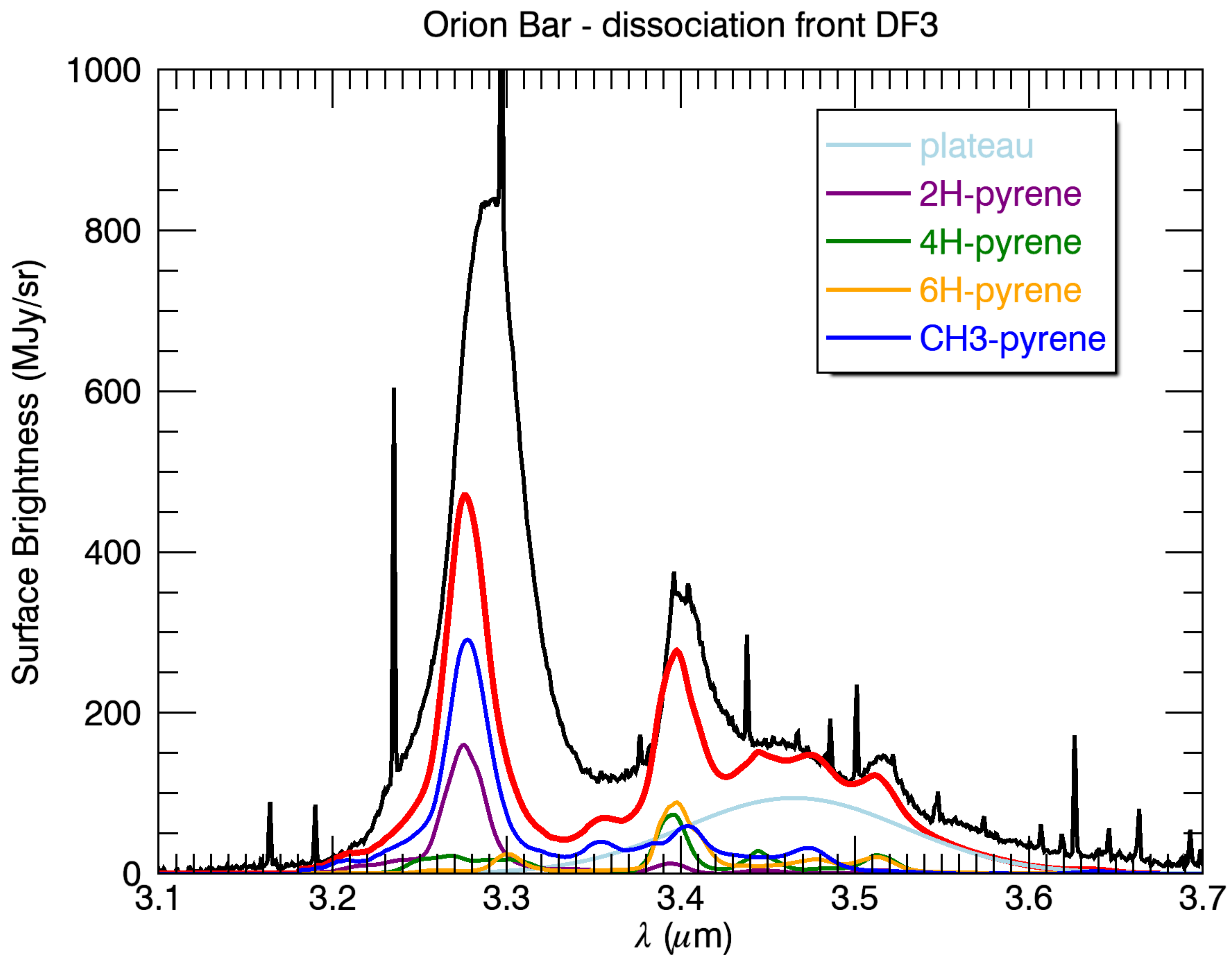
Position		Selected components	Fit range	Origin	Anharmonicity factors		
				Y(0)	c1	c2	c3
µm	cm^{-1}	#	K	cm^{-1}	$cm^{-1}.T^{-1}$	$cm^{-1}.T^{-2}$	$cm^{-1}.T^{-3}$
3.3	3030	2	423 ; 673	3098.9	-0.064346		
		3	423 ; 673	3048.7	-0.054732	2.861e-05	
		6	423 ; 673	2849.8	-0.0065758		
		5	423 ; 673	2877.3	-0.0016084		
		4	423 ; 673	2947.5	-0.0097066		

FWHM

Position		Selected components	Fit range	Origin	Anharmonicity factors		
				Y(0)	c1	c2	c3
µm	cm^{-1}	#	K	cm^{-1}	$cm^{-1}.T^{-1}$	$cm^{-1}.T^{-2}$	$cm^{-1}.T^{-3}$
3.3	3030	2	423 ; 673	-5.873	0.044079		
		3	423 ; 673	30.693	-0.10259	0.00015928	
		6	423 ; 673	-2.628	0.048971		
		5	423 ; 673	17.614	0.018237		
		4	423 ; 673	18.226	0.0063819		

Comparison with JWST observations : spectral match





[Chown+*2023*]
ERS PDRs4All

Linear combination of :

- the experimental spectra
- a plateau as in Pilleri+2015 (aromatic combination and hots bands)

➡ Good spectral match for the aliphatic bands

➡ Aromatic bands not reproduced

Comparison with JWST observations : modelling of the emission

- Emission model from Joblin+02, Mulas+06
- Absorption of 3 and 6 eV photon
- All energy converted to IR bands

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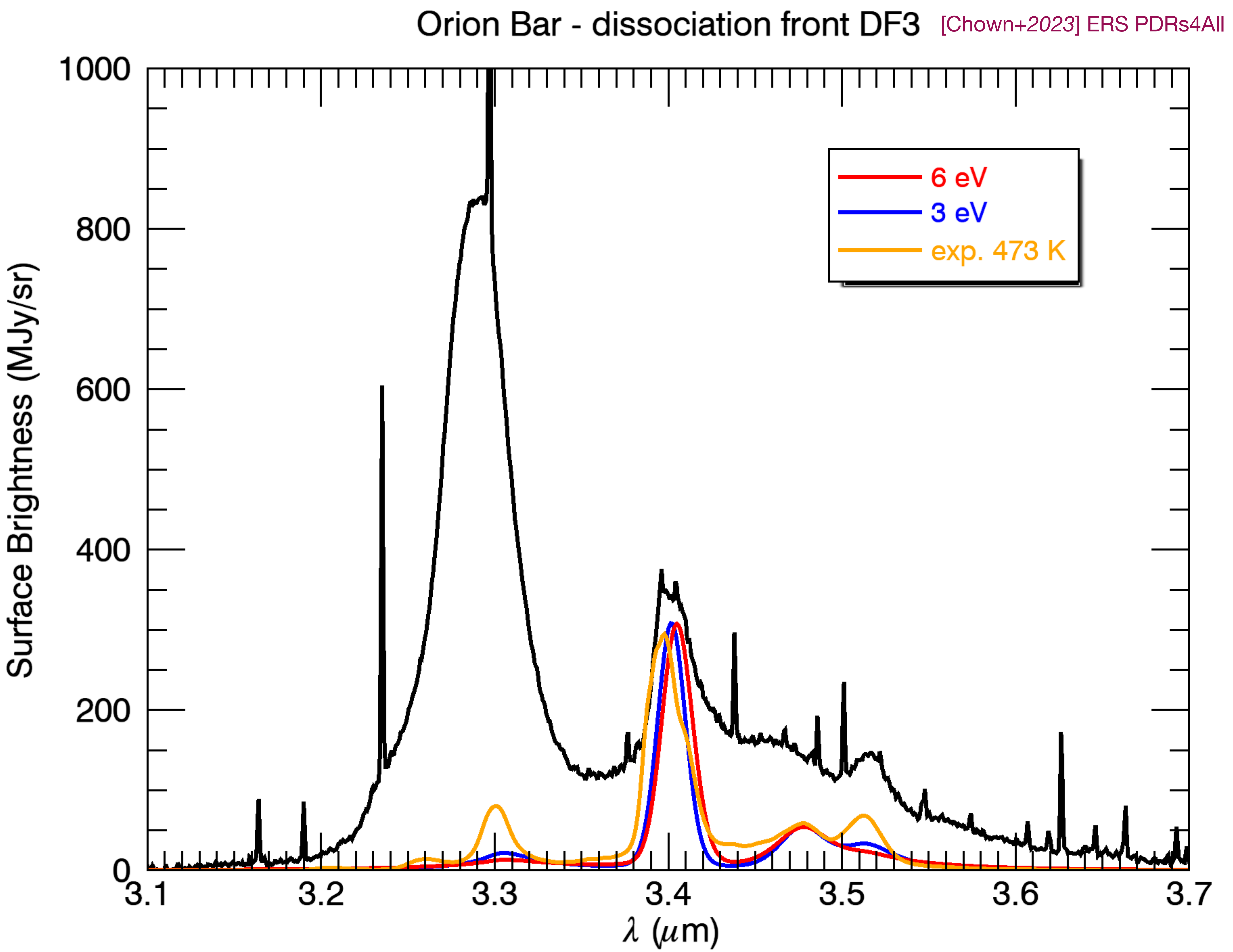
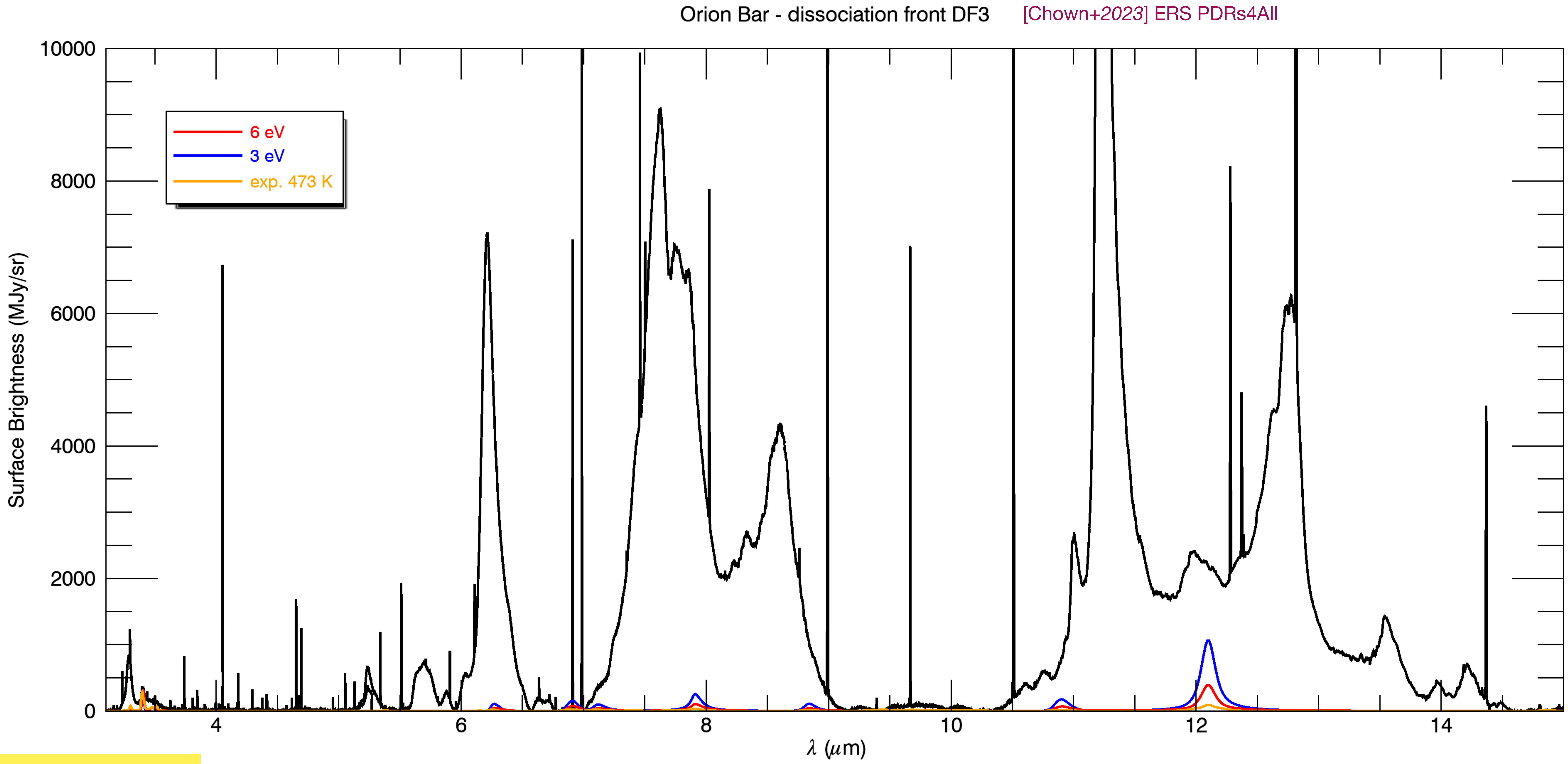


Comparison with JWST observations : modelling of the emission



WORK IN PROGRESS !

➡ No contradiction with others long wavelength bands

Conclusions and perspectives

- Laboratory astrophysics is essential to interpret observations

- New set of optical constants of silicates analogues :
    - see the STOPCODA database
    - use the new THEMIS 2 model
    - continue characterisation beyond 1mm at low temperature

- PAHs MIR spectra as a function of temperature:
    - Data available on the CosmicPAH-IRDB database : https://cosmic-pah.irap.omp.eu (for temporary access of the beta version see de Bentzmann's poster)

    - Hydrogenated and methylated PAH and the 3.3 / 3.4 µm bands :
        - promising candidates : good spectral match with a combination of species + a plateau
        - anharmonicity factor : ⇒ to be coupled with an emission model
        - look for trends : investigate the effect of the size of the PAHs on peak position, anharmonicity factors

    - Analyse set of data of compact PAHs (10 to 48 carbon atoms) & C60
        - combine solid state and gas phase data
        - investigate potential trends of the anharmonicity factors as a function of the size

    - Study 5-member rings PAH