New templates for the analysis of Aromatic Infrared Bands in the JWST era

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1/ Introduction

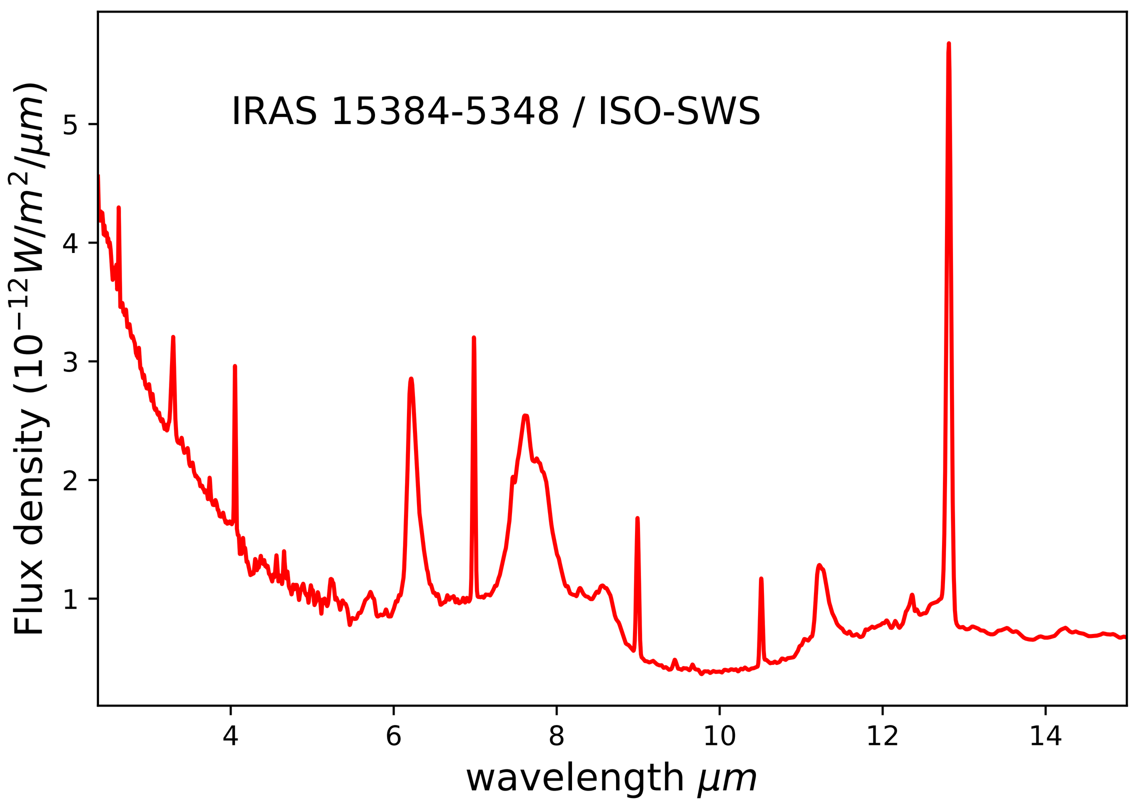

Fig. 1. ISO-SWS Mid-IR spectrum of IRAS 15384-5348 from [4].

Observations of the mid-infrared (mid-IR, 3-15μm, Fig. 1) spectra of photo-dissociation regions (PDRs) reveals ubiquitous and intense emission bands, the Aromatic Infrared Bands (AIBs), attributed to polycyclic aromatic hydrocarbons (PAHs) [1]. In a former study, [2], the authors decomposed Spitzer-IRS spectra presenting AIBs into three different spectra of mean PAHs populations, i.e. neutral, cationic (resp PAH^0 and PAH^+) and evaporating very small grains (eVSG) by the application of a blind signal separation (BSS) method. A fourth component attributed to large, ionized PAH (PAHx) was invoked to better fit the spectra of planetary nebulae (PNe) [3].

In preparation of the launch of the James Webb Space Telescope (JWST), we developed an approach to extract elementary spectra from archival ISO-SWS data [4]. These data have higher spectral resolution ($R >\sim 260$ instead of $R \sim 70$) over a larger spectral range (here 2.3 to 15 μm instead of 5.5 to 14μm), but with no spatial information. We compensate this limitation by using the spectrum from different astrophysical objects. The first step was to extract AIB emission from each spectra and to apply a new BSS method on them. Four new elementary spectra were extracted.

2/ AIB extraction

Fig.1 shows a typical mid-IR observation, i.e. vector s_{obs}. It is composed of four main contributions: gas lines (very narrow features), AIBs (broad features), an underlying continuum and the instrumental noise. The data are considered to be a linear sum of all these contributions. As a first step, we aim at extracting the AIB contribution. We model s_{obs} by s_{mod} as follow:

$$s_{mod} = s_{AIB} + s_{cont} + s_{gas} + s_{inst}.$$

We used independent catalogs of Gaussians to model s_{AIB} and s_{gas} and blackbodies for s_{cont} to estimate s_{mod}. To obtain this estimate, we minimize $||s_{obs} - s_{mod}||^2$. We applied this method to the n observed spectra of our sample of m points. An estimate of s_{AIB} has been isolated for each astrophysical object. A matrix X_{AIB} was constructed whose lines contain these vectors.

3/ MASS-NMF method

BSS is based on the assumption that a signal is a mixture of r elementary sources. Based on the *linear instaneous* model, we can write X_{AIB} as follow:

$$X_{AIB} = A \times S \begin{cases} X_{AIB} : AIB\ matrix,\ (n \times m) \\ A : weight\ matrix,\ (n \times r) \\ S : elementary\ spectra,\ (r \times m) \end{cases}$$

Lin (2007) [5] algorithm of non-negative matrix factorization (NMF) allows us to estimate A and S by respectively $\hat{A}$ and $\hat{S}$.
We initialized $\hat{S}$ with the result of a new geometrical method of BSS, the Maximum Angle Signal Separation (MASS, [6]). MASS gives the r spectra composing the simplicial cone of X_{AIB}. Using MASS allows to avoid the variability induced by a full randomized initialization and the use of a monte carlo method.

References

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4/ Results of the MASS-NMF method

Here, we applied MASS-NMF to X_{AIB} with $n = 31$ spectra of $m = 7949$ points and obtained $r = 4$ elementary spectra using the same methodology proposed in Berné et al. 2007 [2]. Fig. 2 shows the result normalized at the maximum compared to the templates obtained from [2] and [3] by Pilleri et al. (2012) [7].

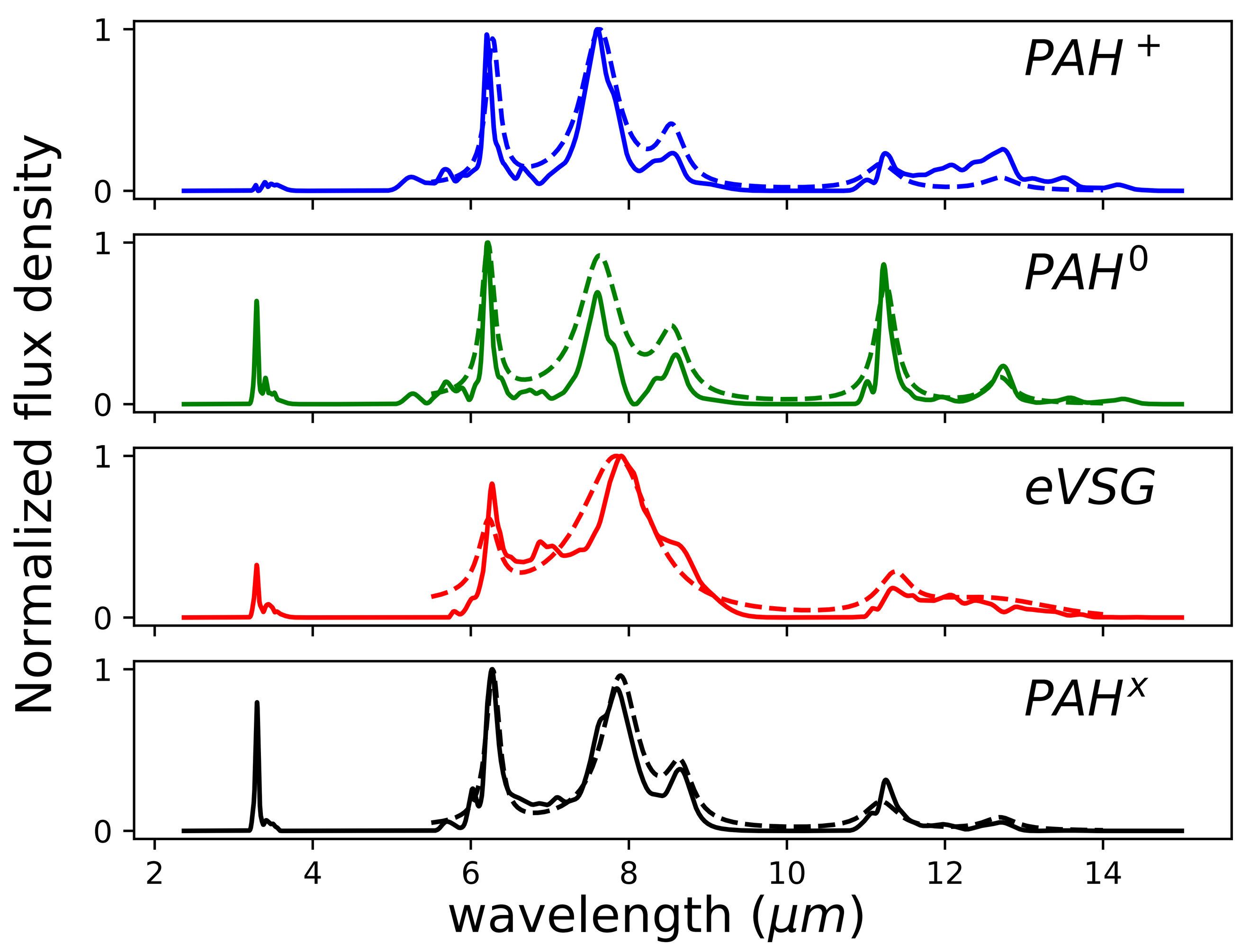

Fig. 2. Elementary spectra, lines of $\hat{S}$ (solid lines) and templates from [7] (dashed lines) normalized.

- 4 elementary spectra were extracted over a larger spectral domain than former studies with a higher spectral resolution of $R \sim 260$.
- Three out of four correspond to the already attributed families cationic and neutral PAHs resp. in blue and green in Fig. 2 and eVSGs in red.
- A fourth elementary spectrum has been extracted which corresponds to large and ionized PAHs, PAH^x in black, fig. 2. It's the first extraction of this spectrum with a BSS method.
- All of them are in good agreement with those of [7] and show more details over a larger spectral domain.

5/ Application

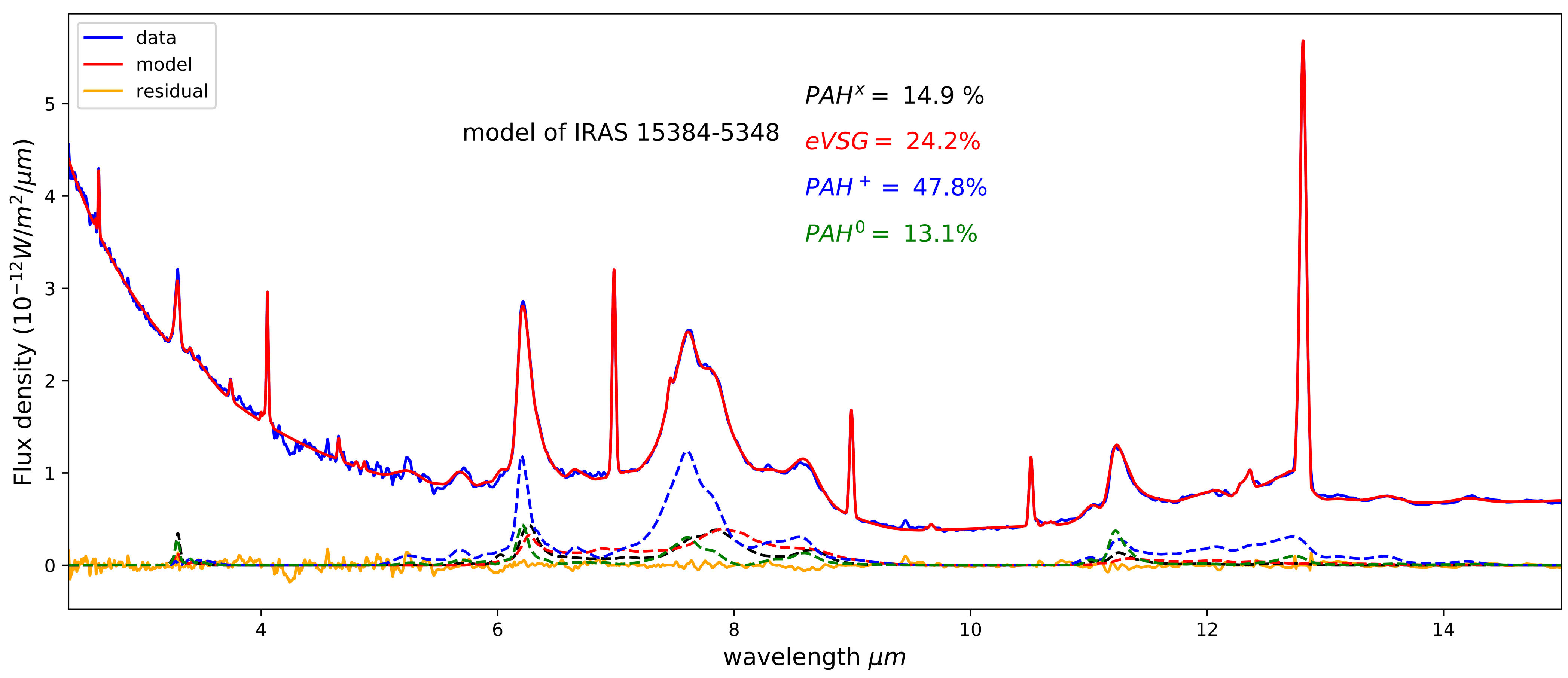

Fig. 3. Reconstruction of s_{obs} from Fig. 1.

Fig. 3 shows an example of spectral fit of a ISO-SWS spectrum using the four elementary spectra (Fig. 2). All the $n = 31$ fit are of good quality.

6/ Conclusion and perspectives

This method will be applied on the JWST data, from NIRSpec and MIRI instruments, provided in the context of the early released science (ERS) program *radiative feedback from massive stars* [8]. The derived elementary spectra will be released to the community as a part of a *science enabling product*.