

The search for PAH bands with Herschel

C. Joblin¹, O. Berne², P. Pilleri¹, G. Mulas³, G. Mallocci³, X. Tielens², T. Bergin⁴, A. Abergel⁵, E. Polehampton⁶, E. Habart⁵, J.-P. Baluteau⁷, J.R. Goicoechea⁸, J. Cernicharo⁸, D. A. Naylor⁹, M. Gerin¹⁰, V. Ossenkopf¹¹, and the HEXOS, SAG 4, WADI, PRISMAS consortia

¹Université de Toulouse [UPS] et CNRS, CESR, France - ²Leiden Observatory, Leiden University, Netherlands - ³INAF Osservatorio Astronomico di Cagliari, Italy - ⁴The University of Michigan, USA - ⁵Université Paris-sud XI et CNRS, IAS, France - ⁶Rutherford Appleton Laboratory, UK - ⁷Université de Provence et CNRS, LAM, France - ⁸Centro de Astrobiología (CSIC/INTA), Spain - ⁹ISIS, University of Lethbridge, Canada - ¹⁰Observatoire de Paris et École Normale Supérieure, CNRS, LERMA, France - ¹¹I. Physikalisches Institut, Universität zu Köln, Germany

Context

PAHs are usually considered as the carriers of the Aromatic Infrared Bands between 3.3 and 12.7 μm , which dominate the mid-IR emission of most galactic and extragalactic objects. These bands are emitted in a vibrational cascade following excitation by absorption of UV photons. PAHs have vibrational bands in the far-IR range and these are more specific of individual species because they involve the whole carbon skeleton of the molecule. They also tend to be preferentially emitted near the end of the cooling cascades and therefore the fine structure of these bands should not be washed out by lifetime broadening, as it happens for mid-IR bands. In this paper, we will discuss the best strategy to detect PAH fingerprints, taking advantage of the three instruments on board Herschel.

Modelling far-IR emission bands of PAHs

Mulas et al. (2006, A&A 460, 93) have reported the detailed photophysics of a vast sample of PAH species in different radiation fields, using a compendium of Monte-Carlo techniques and quantum-chemical calculations (cf. <http://astrochemistry.ca.astro.it/database/>).

We used this model to compute band intensities in the radiation field of the Orion Bar ($G_0=5 \times 10^4$, Figs. 1a-1b). As an example, Fig. 2 shows the sum emission of 24 species including neutrals and cations with N_C between 20 and 48 atoms. The summed spectrum has been normalised to the total number of carbon atoms. This can be compared to the spectrum measured with ISOCAM on the Bar (one of the brightest pixels). From the intensity in the 6-8 μm range, we derive a column density of $N_H=2.3 \cdot 10^{22} \text{ cm}^{-2}$ assuming 20% of the carbon in PAHs, $[C]/[H]=3 \cdot 10^{-4}$ (Joblin et al. 1992, ApJ) and using the model of Pilleri et al. (2010, in prep.) to correct the mid-IR bands for extinction. Using $R_V=5.5$, we derive $A_V=21$, which is a typical expected value for this region.

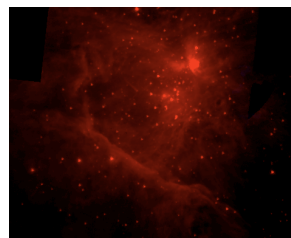


Fig. 1a: Spitzer IRAC 3.6 μm image showing the Orion Bar

Fig. 2: Simulated emission spectrum of 24 PAHs, neutrals and cations ($20 \leq N_C \leq 48$), in the radiation field of the Orion Bar. Model from Mulas et al. 2006 (A&A 460, 93). Note that the spectral range covered by Herschel is well suited for the detection of single PAH bands.

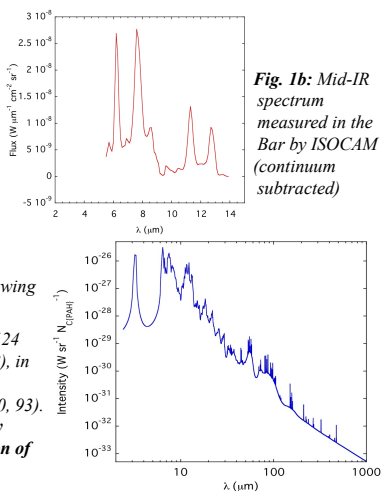


Fig. 1b: Mid-IR spectrum measured in the Orion Bar by ISOCAM (continuum subtracted)

A key aspect in the detection and identification of far-IR bands due to PAHs is related to the exact band profile. For an out-of-plane vibrational band, one can distinguish two main parts in the ro-vibrational band profile: the Q branch in which fine structure is expected due to mode coupling, and the P and R branches that carry the rotational information. The modelling of the band profile requires to know several molecular parameters: the χ matrix of anharmonic parameters and the variations of the rotational constants from the ground to the excited states. These parameters are not easy to access; a first calculation was performed in Mulas et al. (2006, A&A 456, 161) for two small PAHs, $C_{10}H_8$ and $C_{14}H_{10}$, and later by Boersma et al. (2009, ApJ 694, 704).

We present here new calculations performed on two larger molecules, namely neutral hexacene ($C_{26}H_{16}$) and neutral circumvalene ($C_{66}H_{20}$). Realistic χ matrices were built based on the knowledge of the smaller molecules studied by Mulas et al. (2006). A similar educated guess was performed for the variations of the rotational constants. The calculations involve three stages: hot band structure + rotation + convolution at the instrumental resolution.

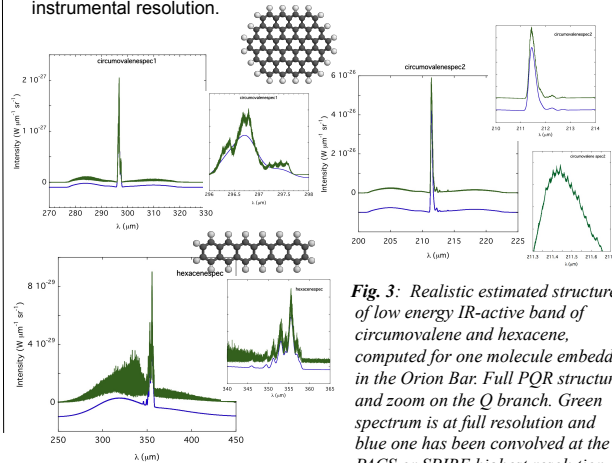


Fig. 3: Realistic estimated structure of low energy IR-active band of circumvalene and hexacene, computed for one molecule embedded in the Orion Bar. Full PQR structure and zoom on the Q branch. Green spectrum is at full resolution and blue one has been convolved at the PACS or SPIRE highest resolution.

Strategy with Herschel and future work

- Deep search for a specific candidate. Which one? Unless we have laboratory data, the precision on the positions given by Density Functional Theory is not high enough for a targeted search with HIFI.
- Spectral survey in the HIFI range [480-1250 GHz] - [1410-1910 GHz] ([625-240 μm]-[212-157 μm])
The Orion Bar survey performed with HIFI in the HEXOS GTKP may reveal some bands due to these molecules. **Work in progress**
- Mixed strategy: search for Q branches with low-resolution spectroscopy with PACS-IFS [57-210 μm] or SPIRE-FTS [194-672 μm] + HIFI follow-up in common spectral ranges. SPIRE-FTS spectra of several PDRs are now taken as part of the SAG4 GTKP, PACS scans are taken on PDRs as part of the WADI and PRISMAS GTKPs. **Work in progress**
- Work is also in progress in different groups to characterize the far-IR spectra of PAHs and PAH-related species both from the theoretical and experimental sides (Ricca et al. 2010, ApJ 709, 42; Simon & Joblin 2010, ApJ 712, 69; Mattioda et al. 2009, AJ, 137, 4054; Pirali et al. 2009, PCCP 11, 3443; Pirali et al. 2006, PCCP 8, 3707; ...)
- Careful choice of the astronomical source: lowest-energy bending modes of PAHs are typically weak, and are emitted (slowly) only when there is no competition by higher energy, more intense bands. Intense illumination cuts the emission cascades before they are emitted, suppressing them (but still enhancing dust emission).
- Search for species with unusually IR-intense lowest-energy bending modes: this happens when a large relative charge is located at the edge of the molecule, due to its particular structure (e.g. corannulene cation) or to the presence of heteroatoms. The lowest energy modes can then have intensities almost 2 orders of magnitude larger than for regular PAHs, enhancing their intensity and reducing the suppression effect mentioned above.