Report on the outcomes of a Short-Term Scientific Mission[1]

Action number: CA21126

Grantee name: Burcu Günay

Details of the STSM

Title: **Bridging Spectral Decomposition and Molecular Interpretation of PAH Emission in PDRs**

Description of the work carried out during the STSM

Description of the activities carried out during the STSM. Any deviations from the initial working plan shall also be described in this section.

The work focused on investigating the carriers of selected infrared emission features through the combined use of observational data (NGC 7023) analysis and theoretical PAH spectral modeling. We select representative features spanning the entire observed PAH characteristics. The analyzed features included the 7.4, 7.7a, 7.7b, 7.7c, and 7.7d and 7.9 (broad) features as subcomponents of the 7.7-μm complex, the 11.0, 11.3a, 11.3b, 11.3c, and 11.3d (broad) features as subcomponents of the 11.3-μm complex as defined by PAHFIT (Van De Putte et al. 2026).

The first stage of the work involved the preparation of continuum-subtracted spectral cubes using PAHFIT. We then prepared observational spectral libraries from the cubes for PAHdb fitting analysis. For this we used the integrated area of each feature subcomponent from the PAHFIT results and obtained subcomponent-to-total of emission complex ratios to select representative extreme (minimum and maximum) spectral samples. We also selected representative spectra from different percentiles (0–10, 10–25, 25–50, 50–75, and 90–100). We repeated this procedure using different total emission ratios by excluding subcomponents exhibiting different characteristics. For each subcomponent, the flux ratio was defined relative to one of four total emission measures. This yielded eight PDR spectra library sets in total, covering both the max/min and percentile ratio analyses.

The custom theoretical PAH spectral libraries were generated from the NASA Ames PAH Infrared Spectroscopic Database (PAHdb) (Ricca et al. 2026). The selection criteria were

[1] This report is submitted by the grantee to the Action MC for approval and for claiming payment of the awarded grant. The Grant Awarding Coordinator coordinates the evaluation of this report on behalf of the Action MC and instructs the Grant Holder Manager to verify the grant documents compliance and proceed with the payment.

designed to include only pure hydrocarbon PAHs, excluding species containing heteroatoms or side groups, and to cover neutral, cationic, and anionic charge states. To investigate the influence of molecular size, the PAHs were used three size groups: small (20–50 carbon atoms), medium (50–70 carbon atoms), and large (>70 carbon atoms).

The PAHdb Ames Suite was then used to fit the PAH spectra to the PDR spectra in order characterize the molecular properties responsible for the observed variations. Comparative analysis of the resulting molecular populations enabled the identification of groups of spectral subcomponents exhibiting similar behavior and allowed the separation of features primarily associated with PAHs from those likely dominated by broader contributions from very large PAHs and/or very small grains (VSGs). Based on these findings, revised PAH-only totals were defined by excluding the broad subcomponent. The complete analysis procedure was subsequently repeated using the revised totals, allowing an investigation of the relationships between spectral subcomponent ratios and the traced PAH properties.

The PAHdb spectral fitting weights obtained from each library were used to investigate relative enrichment trends between PAH charge and size fractions by comparing mean fractions between the high- and low-flux extremes of the subcomponent-to-total flux ratio distributions. We also explored the PAHdb fitting results and examined the similarities between the top PAH species identified in these analyses based on their weights to identify potential biases.

Finally, the continuum-subtracted cubes were fitted using the PAHdb libraries to derive the relative contributions of different PAH molecules. We obtained spatial distributions of PAH charge states (cations, neutrals, and anions) and size classes (small, medium, and large) across the cube. We prepared subcomponent-to-total ratio maps for comparison with the PAH properties derived from the PAHdb fits. We also compared our results with the results of Van De Putte et al. 2026.

Description of the STSM main achievements and planned follow-up activities

Description and assessment of whether the STSM achieved its planned goals and expected outcomes, including specific contribution to Action objective and deliverables, or publications resulting from the STSM. Agreed plans for future follow-up collaborations shall also be described in this section.

We revealed clear trends with charge state, particularly for cationic and neutral PAHs. However, trends with PAH size were more complicated and depended on the classification scheme adopted.

Using subcomponent-to-total emission ratios, we find that elevated flux ratios of the broad 7.9 and 11.3d subcomponents are associated with a relative enrichment of neutral PAH species, whereas elevated ratios of all remaining subcomponents are associated with a relative enrichment of cationic species. This is consistent with the results of Van De Putte et al. (2026), as these broad features are only strong in dissociation front (DF) (Type-I), while all other subcomponents of the 7.7-μm emission complex and the 11.0 and 11.3a subcomponent are strong in atomic regions (Type-III). Their broad nature and spatial distribution suggest that they likely originate from PAH clusters and/or VSGs. Therefore, libraries based on the PAH-only totals were used for the subsequent analysis.

Within the 11.3-μm emission complex, the 11.0 and 11.3a subcomponent ratios were associated with a relative enrichment of cationic (medium-size) PAHs, while the 11.3b and 11.3c

subcomponent ratios were associated with a relative enrichment of neutral (small-size) PAHs. This is also consistent with that, the 11.0 and 11.3a subcomponents were classified as Type-III (strong in atomic region), while the 11.3b band 11.3c subcomponent were of Type-I (suppressed in atomic region).

Additional separation was identified within the 7.7-μm emission complex. Higher 7.7c and 7.7d (redder) subcomponent ratios were associated with a relative enrichment of cationic (medium-size) PAHs, whereas higher 7.4, 7.7a, and 7.7b (bluer) subcomponent ratios were associated with a relative enrichment of neutral (small-size) PAHs. This is also consistent with the expected size dependency of the wavelength of C-C vibration modes. However, since 7.4 and all 7.7 subcomponents are classified as Type-III, we repeated the analysis based on ratios relative to the sum of only the 7.7a–d subcomponents. The results reinforced these trends, more clearly linking the 7.7c and 7.7d ratios to cationic (medium-size) PAHs and the 7.4, 7.7a, and 7.7b ratios to neutral (small-size) PAHs.

We compared subcomponent ratio with charge and size maps and found consistent results with the expected trends in PDRs: large/medium cationic PAHs are enriched in atomic regions, while small neutral PAHs can survive in shielded DF regions. However, additional work is required to clearly identify subcomponent ratios as tracers of PAH nature. Although we did not observe any significant bias arising from the PAHdb decomposition, it remains challenging to simultaneously fit all emission profiles using a fixed FWHM for PAH spectra. More detailed exploration is needed in the future, using different FWHM, improved selections of astro-PAHs and more targeted PAH classifiers (such as “small cation” and “large neutral”).

These preliminary results indicate that subcomponents of the 7.7-μm and 11.3-μm emission complexes have the potential to trace distinct PAH populations characterized by relative enrichments in charge and size distributions. The new tracers identified using the hybrid PAHFIT–PAHdb approach, can provide additional constraints on the photochemical evolution of PAHs through PDRs.