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Spectral modeling of young planetary nebulae in the mid-infrared

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Abstract. Planetary Nebulae (PNe) are important contributors to the chemical enrichment of the interstellar medium, dispersing organic-rich material that affects galactic evolution. This study presents precise spectral modeling aimed at characterizing Polycyclic Aromatic Hydrocarbons (PAHs) in young PNe molecules relevant to prebiotic chemistry and the formation of complex organics. We analyzed 145 PNe using Spitzer/IRS spectra and the Bayesian fitting tool pahfitMCMC, obtaining robust fluxes with quantified uncertainties. Over 50% of the PNe exhibit strong non-standard dust features, requiring additional components that reveal significant mineralogical diversity and are essential for accurate PAH flux determination. Using refined fluxes, we constructed diagnostic diagrams to assess PAH ionization and size distribution. The results show a dispersion extending beyond theoretical PAH model regions, suggesting a diverse population dominated by small, low-ionization molecules, likely reflecting different evolutionary stages and central star properties. These findings provide new insights into PAH processing in evolving nebulae and their contribution to galactic chemical enrichment.

Resumo. As Nebulosas Planetárias (PNe) são importantes contribuintes para o enriquecimento químico do meio interestelar, dispersando material orgânico que influencia a evolução das galáxias. Este estudo apresenta modelagem espectral precisa para caracterizar Hidrocarbonetos Aromáticos Policíclicos (PAHs) em PNe jovens, moléculas relevantes para a química prebiótica e a formação de compostos orgânicos complexos. Analisamos 145 PNe usando espectros Spitzer/IRS e o código Bayesiano pahfitMCMC, obtendo fluxos robustos com incertezas quantificadas. Mais de 50% das fontes exibem feições de poeira não padronizadas, exigindo componentes adicionais que evidenciam grande diversidade mineralógica e são essenciais para determinar corretamente os fluxos de PAHs. Com os fluxos refinados, construímos diagramas diagnósticos para investigar a ionização e a distribuição de tamanhos dos PAHs. Os resultados revelam uma dispersão que ultrapassa as regiões teóricas do modelo, indicando uma população diversa, porém dominada por moléculas pequenas e pouco ionizadas, provavelmente refletindo diferentes estágios evolutivos e propriedades das estrelas centrais. Esses achados oferecem novas perspectivas sobre o processamento de PAHs em nebulosas em evolução e seu papel no enriquecimento químico das galáxias.

Keywords. Astrochemistry – Astrobiology – Planetary nebulae: general

1. Introduction

PNe correspond to the final phase of low to medium mass stars (0.8 – 8 solar masses), when enriched material is ejected into the interstelar medium (ISM), playing a fundamental role in galactic chemical evolution. Among their constituents, PAHs stand out, exhibiting strong emissions in the mid-infrared (MIR) at 3.3, 6.2, 7.7, 8.6, and 11.3μm (Houck et al. 2004). Their intensities are sensitive to the radiation field, size, and molecular ionization state, serving as important diagnostics of nebular conditions (Bauschlicher, Peeters & Allamandola 2008; Li 2004; Ruschel-Dutra et al. 2014; Lebouteiller et al. 2011). However, standard spectral fitting tools do not adequately describe the complex dust mineralogy and the diversity of PAH populations in young PNe, generating uncertainties in fluxes and interpretations.

In this work, we apply Bayesian spectral analysis to 145 young PNe using Spitzer/IRS data, using the pahfitMCMC decomposition tool (Gallimore et al. 2010; Gleisinger et al. 2020). This allowed for the robust decomposition of PAH bands and their uncertainties, as well as the identification of unusual dust components. This enabled the construction of a diagnostic diagram to investigate the evolution of PAHs in extreme environments. These results advance our understanding of PAH formation and processing, providing insights into the origin of complex organic molecules and their contribution to the chemical evolution of the galaxy.

2. Data Selection and Methodology

For the analysis, observational data for 145 galactic PNe were obtained from the Spitzer/IRS (Werner et al. 2004; Houck et al. 2004) data archives, and their data reduction was processed using the CASSIS project (Lebouteiller et al. 2011). The sample used was observed and described by (Stanghellini et al. 2012), with the aim of providing information on the early evolution of post-AGB stars and the impact of dust and metallicity on this process. Therefore, they were selected based on the criterion of diameter <4", which identifies them as young galactic PNe (Villaver, Manchado & García-Segura 2002).

After data selection, spectral modeling was performed with pahfitMCMC, a Bayesian decomposition tool that uses Markov Chain Monte Carlo (MCMC) to fit the spectra. This method precisely quantifies parameters and uncertainties, separating the components of the PAH bands, ionic/molecular emission lines, and dust continuum, allowing the code's features to be adapted to environments such as PNe, as seen in Figure 1. Among the adaptations, the narrowing of the ionic lines, the adaptation of the temperature of the main black body of the continuum to the pattern of a PNe central star and the addition of components designed for dust (still in progress) were essential.

After measuring the fluxes, the PAH ratios were calculated: the ratio of the 11.3 μm complex (neutral PAH tracer) to the 7.7 μm complex (ionized PAH tracer) and the 6.2 μm/7.7 μm

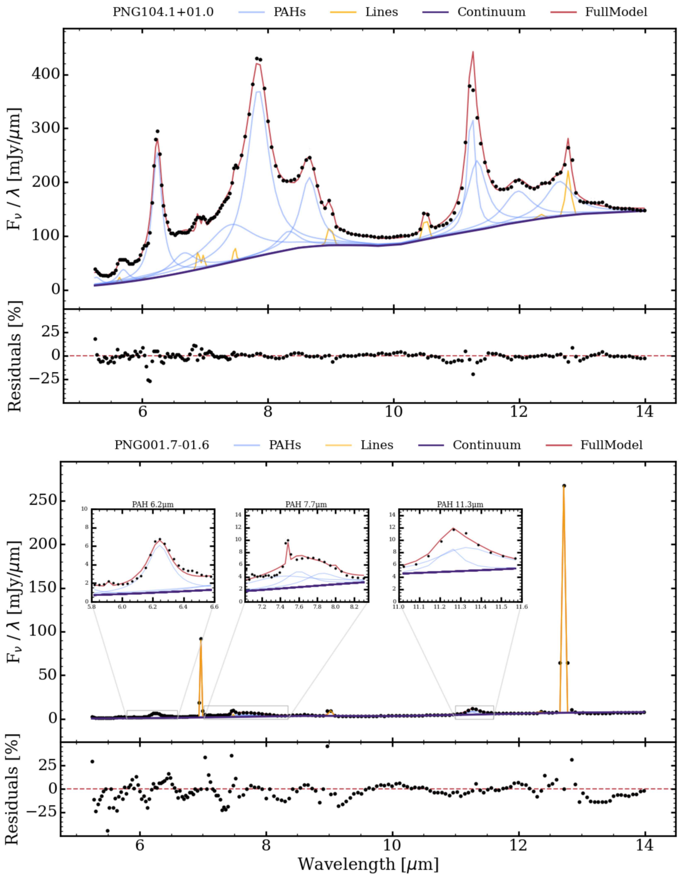

Figure 1. Spectral decomposed by pahfitMCMC.

ratio (PAH size tracer) (Bauschlicher, Peeters & Allamandola 2008; Draine & Li 2001). Using these ratios, it was possible to construct a diagnostic diagram to determine the physicochemical properties of PAHs in these environments.

3. Results

As can be seen in Figure 1, we identified two decompositions performed by the pahfitMCMC code adapted for PNe, one with strong PAH emissions and the other with weak emissions. The code correctly fitted approximately 76% of the objects in the sample, and the remainder had intense emissions that could not be fitted to standard dust profiles and overestimated the PAH bands. Among the unfitted emissions, two main families of features were identified: one possessing a broad continuum at 10-14 μm and 25-35 μm, specifically attributed to amorphous carbons (HACs) and silicon carbide (SiC), and another with prominent features at 8-14 μm and at 23.5, 27.5 and 33.8 μm, associated with crystalline silicates.

From the correctly fitted spectra, reliable flux measurements allowed us to construct the diagnostic PAH diagram, which can be seen in Figure 2, with the ratio of 11.3 μm complex to 7.7 μm complex and the 6.2 μm/7.7 μm complex. The results for PNe show a distribution that exceeds the theoretical regions for the PAH model, confirming a diverse population, but dominated by small, low-ionization molecules. This large scatter remains to be analyzed, but likely reflects different evolutionary stages and properties of the star that gave rise to each PNe.

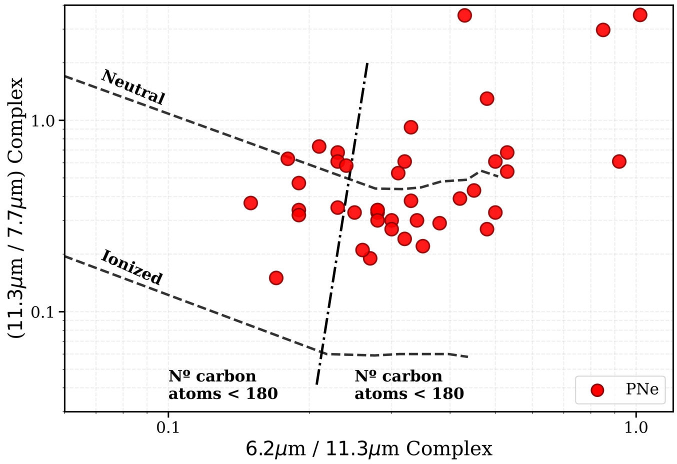

Figure 2. PAH diagnostic diagram 6.2μm/11.3μm vs. 11.3μm/7.7μm.

4. Conclusions and perspectives

Young PNe exhibit a rich and complex spectrum in the MIR that requires sophisticated fitting techniques. The pahfitMCMC code has proven to be a powerful tool for unraveling these complexities and providing statistically rigorous measurements. Silicon carbide or crystalline silicate features were observed in > 50% of the PNe in the sample, confirming mineralogical diversity in these environments and also posing a challenge for spectral modeling and adaptations of the decomposition code. PAH fluxes from 76% of the sample were measured and a diagnostic diagram was constructed, revealing important characteristics of the PAH population in these environments.

To optimize the modeling of these objects, the next step includes creating an average dust component model for the unadjusted region of the PNe and introducing this template into the pahfitMCMC code, adapting to the different nebulae and emissions without suppressing PAH emissions. The work then aims to expand the analysis to include JWST/MIRI data for greater spatial and spectral resolution.

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