Boletim da Sociedade Astronômica Brasileira, **35**, no. 1, 127-128

Computational modeling of polycyclic aromatic hydrocarbons in planetary nebulae

Julia Fischer[1], Dinalva A. Sales[1], Carla Canelo[1], Isabel Aleman[2], Stavros Akras[3] & Juliano Marangoni[1]

[1] Instituto de Matemática, Estatística e Física, Universidade Federal do Rio Grande, 96203-900, RS, Brazil.
e-mail: juh.fischer@gmail.com, dinalvaires@gmail.com, camcanelo@gmail.com, julianomarangoni@furg.br

[2] Instituto de Física e Química, Universidade Federal de Itajubá, 37500-903, MG, Brazil. e-mail: bebel.aleman@gmail.com

[3] Institute for Astronomy, Astrophysics, Space Applications and Remote Sensing, National Observatory of Athens, Penteli GR 15236, Greece. e-mail: stavrosakras@gmail.com

Abstract. We aimed to study objects that contribute to the origin and dispersion of essential elements for the formation of organic compounds and prebiotic material. Planetary Nebulae (PNe), for instance, play a crucial role in enriching the interstellar medium and significantly contribute to the chemical evolution of galaxies. In this work, we investigated certain molecules that are consistently present in these environments, known as Polycyclic Aromatic Hydrocarbons (PAHs), which are linked to the formation of nucleobases, fundamental in the RNA/DNA world. We utilized infrared spectra from 157 PNe obtained by IRS/SPITZER, from which we measured the fluxes of ionic and molecular lines using the PAHFIT code. Out of these fluxes, 145 could be used to calculate ratios of PAH line intensities and various characteristics of the PNe, which underwent multivariate statistical analyses to understand their behavior. With this data, we constructed a correlation matrix using the Spearman method and diagnostic diagrams based on the highest correlation coefficients found. This facilitated the physical and chemical modeling of the molecules present in these environments.A strong correlation was found between the radii of PNe and their degree of ionization. From this, we concluded that larger PNe exhibit a higher potential for molecular ionization, meaning that the received emission consists mostly of ionized molecules. Conversely, smaller PNe tend to have predominantly neutral molecules. Additionally, a significant correlation was observed between radius and infrared (IR) luminosity of the PNe, indicating that smaller nebulae emit more IR light, with this emission primarily originating from smaller PAH molecules (carbon atom count < 180, Fischer et al. in prep.). This study allowed us to model some significant characteristics of PAHs in astrophysical environments like PNe, which may provide insights into the evolutionary trajectory of these molecules and their contribution to their formation.

Resumo. Nosso objetivo foi estudar objetos que contribuem para a origem e dispersão de elementos essenciais para a formação de compostos orgânicos e material prebiótico. As Nebulosas Planetárias (PNe), por exemplo, desempenham um papel crucial no enriquecimento do meio interestelar e contribuem significativamente para a evolução química das galáxias. Nesse trabalho, investigamos certas moléculas que estão consistentemente presentes nesses ambientes, conhecidas como Hidrocarbonetos Aromáticos Policíclicos (PAHs), que estão ligadas à formação de nucleobases, fundamentais no mundo RNA/DNA. Utilizamos espectros infravermelhos de 157 PNe obtidos por IRS/SPITZER, a partir do qual medimos os fluxos de linhas iônicas e moleculares usando o código PAHFIT. Desses fluxos, 145 puderam ser usados para calcular proporções de intensidades de linhas de PAHs e diversas características do PNe, que passaram por análises estatísticas multivariadas para entender seu comportamento. Com esses dados, construímos uma matriz de correlação utilizando o método de Spearman e diagramas diagnósticos baseados nos maiores coeficientes de correlação encontrados. Isso facilitou a modelagem física e química das moléculas presentes nesses ambientes. Foi encontrada uma forte correlação entre os raios das PNe e seu grau de ionização. A partir disso, concluímos que PNe maiores apresentam maior potencial de ionização molecular, o que significa que a emissão recebida consiste principalmente em moléculas ionizadas. Por outro lado, PNe menores tendem a ter moléculas predominantemente neutras. Além disso, foi observada uma correlação significativa entre o raio e a luminosidade infravermelha (IR) das PNe, indicando que nebulosas menores emitem mais luz infravermelha, com esta emissão originada principalmente de moléculas menores de PAH (contagem de átomos de carbono <180, Fischer et al. na preparação). Este estudo nos permitiu modelar algumas características significativas dos PAHs em ambientes astrofísicos como PNe, o que pode fornecer insights sobre a trajetória evolutiva dessas moléculas e sua contribuição para sua formação.

Keywords. Astrochemistry – Astrobiology – Planetary nebulae: general

1. Introduction

When low and medium-mass stars (0.8 to 8 solar masses) reach their final stages of evolution, they expel their outermost layers, leaving behind only a hot and compact stellar core that ionizes the ejected material, forming a plasma envelope. This stage is referred to as a Planetary Nebula (PNe) and is of great significance as it enriches the interstellar medium with elements produced during the star's nucleosynthesis processes. As this material cools and mixes with the surrounding medium, it plays a crucial role in the chemical evolution of stars and consequently in their host galaxies.

This circumstellar gas cloud contains ionized material but also a substantial amount of neutral and molecular material. For instance, it generates intense emission lines detected in the mid-infrared at wavelengths of 3.3, 6.2, 7.7, 8.6, and 11.2 μm (Li 2004; Sales, Pastoriza & Riffel 2010; Sales et al. 2013; Ruschel-Dutra et al. 2014). These lines can account for up to 50% of the luminosity in this spectral range and have been the subject of intense investigation since their first observation in PNe in the 1970s. These bands have been attributed to Polycyclic Aromatic Hydrocarbon molecules (PAHs) and hold great importance in the fields of Astrochemistry and Astrobiology due to their potential to form prebiotic molecules (Canelo et al. 2018).

The present work investigates the behavior of PAHs and correlates it with the properties of the environment in which they are found. In order to do it we used correlation matrix of the ten properties of PNe's sample. We therefore aimed to understand the contribution of PNe and how they may be responsible for an evolutionary cycle of these aromatics (Shannon & Boersma 2019).

2. Observation and data reduction

For the analysis, observational data from 157 galactic PNe were taken from Spitzer (Werner et al. 2004) IRS (Houck et al. 2004) data archive and their data reduction were processed using CASSIS (Lebouteiller et al. 2011) project. Our sample was selected with the aim of providing information about the early evolution of post-AGB stars and the impact of dust and metallicity on this process. To achieve this, they are chosen with the criterion of having a diameter < 4", which identifies them as young PNe. Some properties of the selected sample published in (Stanghellini et al. 2012) were also utilized. The properties employed include: total infrared luminosity (LIR), distance to the galactic center (RGal), nebula radius (R), dust temperature (Tdust), electron density (N), excitation class (EC), and central star temperature (T*).

The PAH line ratios used here were 11.3μm/7.7μm, to determine PAH's ionization potential, and 6.2μm/7.7μm, which indicates the size of emitting molecules (Bauschlicher, Peeters & Allamandola 2008). We also calculated the ratio of [NeIII]/[NeII] ionic lines, which points out the hardness of the local radiation field (Thornley et al. 2000).

3. Results

Figure 1 shows the correlation matrix derived where we can observe several high correlation coefficients, both positive and negative, which may indicate significant correlations. In this work, we will focus on correlation coefficients equal to or greater than 0.5, suggesting that the data exhibit a correlation of approximately 50%.

The highest positive coefficient of interest is 0.66, between the variable representing the central star temperature of the nebula (T*) and the excitation class (EC). This correlation is well-known since excitation classes are defined using lines that depend on the temperature of the central star of such objects.

Next, the coefficient of 0.63 between the 11.3μm/7.7μm and 6.2μm/7.7μm band ratios has been found, indicating a high positive correlation between these variables. This suggests that the degree of ionization of molecules decreases when smaller PAH molecules dominate this emission, as it also has been found in a sample of the active galaxies (Sales, Pastoriza & Riffel 2010).

The following coefficient is 0.53, indicating a correlation between infrared luminosity (LIR) and the ratio 6.2μm/7.7μm. This correlation may suggest a relationship between the predominance of emission from smaller molecules and high infrared luminosity.

There are two negative correlation of -0.5, indicating inverse correlations between variables. The first one is the nebula radius (R) and the 11.3μm/7.7μm band ratio, implying that larger-radius nebulae in the sample tend to have a higher potential for ionization of PAH molecules. In other words, the emitted radiation is primarily from ionized molecules in larger nebulae, while smaller nebulae exhibit a predominance of neutral molecules. The second correlation shows -0.5 value between the radius (R) and the emitted LIR, suggesting that the radius is also inversely correlated with the infrared luminosity emitted by the nebulae. In this case, smaller nebulae emit more in the infrared, while larger nebulae emit less.

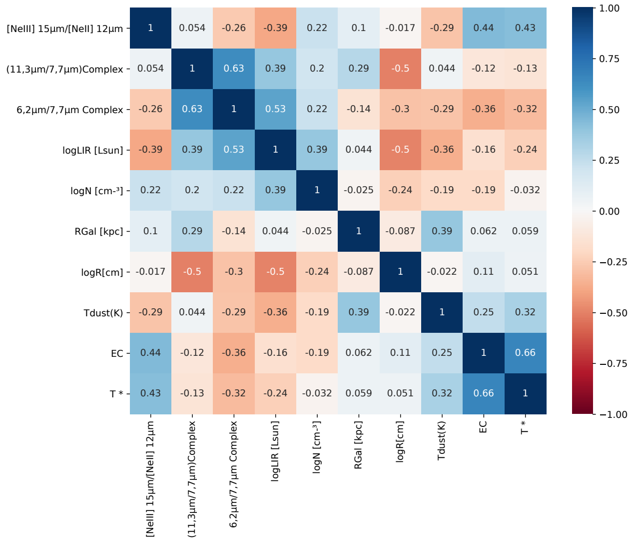

Figure 1. Correlation Matrix

4. Conclusions and perspectives

Our statistical data analysis of ten physical properties of the PNe sample is important to derive the ionization and size the PAH molecular emission these class of stars. Through the analyses conducted here, it is possible to characterize and identify significant correlation values among certain properties of PNe and their PAH emission bands.

Our analysis reveals a tendency for values of the excitation class, central star temperature, and nebula radius to positively correlate, as well as for the ratios of PAH molecules and certain data such as nebula radius and luminosity to exhibit inverse relationships, suggesting an exponential connection.

This work has enabled the interpretation of some initial data study, but further investigation using more robust statistical method is in progress to address PAH dusty molecular material evolution in PNe environments. Therefore, additional indices observed here will also be assessed and explored, incorporating data on the chemical characteristics of dust and nebula morphologies, enhancing this analysis.

Acknowledgements. JFischer is grateful to the Brazilian National Council for Scientific and Technological Development (CNPq), and to the Research Support Foundation of the State of Rio Grande do Sul (FAPERGS), for the funding support. DASales also thanks to CNPq and FAPERGS to financial support.

References

Bauschlicher Jr, C. W., Peeters, E., & Allamandola, L. J. 2008, ApJ, 678, 316.
Canelo, C. M., Friaça, A. C., Sales, D. A., Pastoriza, M. G., & Ruschel-Dutra, D. 2018, MNRAS, 475, 3746.
Houck J. R., et al. 2004, ApJS, 154, 18.
Lebouteiller, V., et al. 2011, ApJS, 196, 8.
Li A. 2004, In: Astrophysics of Dust. [S.l.: s.n.], 309, 417.
Ruschel-Dutra, D., Pastoriza, M., Riffel, R., Sales, D. A., & Winge, C. 2014, MNRAS, 438, 3434.
Sales, D. A., Pastoriza, M. G., & Riffel, R. 2010, ApJ, 725, 605.
Sales, D. A., Pastoriza, M. G., Riffel, R., & Winge, C. 2013, MNRAS, 429, 2634.
Shannon, M. J., & Boersma, C. 2019, ApJ, 871, 124.
Smith, J. D. T., et al. 2007, ApJ, 656, 770.
Stanghellini, L., et al. 2012, ApJ, 753, 172.
Thornley, M. D., Schreiber, N. M. F., Lutz, D., Genzel, R., Spoon, H. W., Kunze, D., & Sternberg, A. 2000, ApJ, 539, 641.
Werner, M. W., et al. 2004, ApJS, 154, 1.