Hydrogenated amorphous carbon grains as an alternative carrier of the 9–13 μm plateau feature in the fullerene planetary nebula Tc 1

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ABSTRACT

Fullerenes have been observed in several astronomical objects since the discovery of C_60 in the mid-infrared (mid-IR) spectrum of the planetary nebula (PN) Tc 1. It has been suggested that the carriers of the broad unidentified infrared (UIR) plateau features, such as the 9–13 μm emission feature (12 μm hereafter), may be related to the formation of fullerenes. In particular, their carriers have been suggested to be mixed aromatic or aliphatic hydrocarbons such as hydrogenated amorphous carbon (HAC-like hereafter) grains. For this study, we modeled the mid-IR emission of the C_60-PN Tc 1 with a photoionization code, including for the first time the laboratory optical constants (n and k indices) of HAC-like dust at 300 K. Interestingly, we find that the broad 12 μm plateau feature in Tc 1 is well reproduced by using a distribution of canonical HAC grains, while at the same time they provide an important fraction of the IR dust continuum emission and are consistent with the other UIR features observed (e.g., the broad 6–9 μm plateau feature). This finding suggests that HAC-like grains may be possible carriers of the 12 μm plateau feature, being likely related to the fullerene formation mechanism in PNe. More laboratory experiments, to obtain the optical constants of HAC-like dust with several structures or a composition at different physical conditions, are strongly encouraged – that is, in order to extend this pilot study to more fullerene PNe, and to unveil the details of fullerene formation and of the potential carriers of the elusive UIR plateau features.

Key words. astrochemistry – stars: AGB and post-AGB – planetary nebulae: individual: PN Tc 1

1. Introduction

Planetary nebulae (PNe) represent the late stages in the evolution of low- and intermediate-mass stars (LIM; \( \sim 1–8 M_\odot \)), the majority of stars in the Universe. On their way to the PN phase, LIM stars experience a strong mass loss during the preceding asymptotic giant branch (AGB; see e.g., Herwig 2005 for a review) phase and they chemically enrich the surrounding interstellar medium (ISM). The AGB stars are also major suppliers of dust grains and molecular species that are routinely seen in the local Universe (e.g., Ferrarotti & Gail 2006), which makes them (and their subsequent evolutionary stages) very important for our fundamental understanding of the enrichment and chemical composition of the ISM.

Fullerenes, among the most resistant and stable three-dimensional molecules that are only formed by C atoms, such as C_60 (first discovered in the laboratory by Kroto et al. 1985), were supposed to be widely spread in space for decades. The presence of fullerenes in astrophysical environments was under debate until the infrared (IR) signatures of the C_60 and C_70 fullerenes were unambiguously detected in the Spitzer mid-IR spectrum of the young PN Tc 1 (Cami et al. 2010). After the first detection of fullerenes in a PN, the presence of C_60 was found in several other astrophysical objects such as reflection nebulae (Sellgren et al. 2010), additional PNe (García-Hernández et al. 2010, 2011a, 2012; Otsuka et al. 2014), peculiar R Coronae Borealis (RCB) stars (García-Hernández et al. 2011b), post-AGB stars (Zhang & Kwok 2011; Gielen et al. 2011), and Herbig Ae/Be stars (Arun et al. 2023), among others, by its four strongest mid-IR emission features at \( \sim 7.0, 8.5, 17.4, \) and 18.9 μm. However, the formation route of fullerenes in such H-rich objects, similar to the majority of PNe, is not well understood. Nowadays, the most suitable routes for the formation of fullerenes are: i) the photochemical processing of hydrogenated amorphous carbon (HAC) grains or similar mixed aromatic or aliphatic hydrocarbons (i.e., same chemical composition but a different internal structure; hereafter HAC-like; García-Hernández et al. 2010) and ii) the photochemical processing of large polycyclic aromatic hydrocarbons (PAHs; Berné & Tielens 2012; Murga et al. 2022).

The C_60 fullerenes are mainly detected toward PNe, and fullerene PNe are very young low-excitation (\( T_{\text{eff}} \sim 30 000–45 000 \) K) C-rich objects, which evolved from low-mass (\( \sim 1–3 M_\odot \)) progenitors (García-Hernández et al. 2012; Otsuka et al. 2014). Remarkably, the IR Spitzer spectra (\( \sim 5–38 \mu m \)) of the

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1 We note that, more recently, Bernal et al. (2019) proposed the shock heating and ion bombardment induced processing of SiC grains as an alternative route toward fullerenes in the ISM, but such a strong energetic process seems to be unlikely to happen in the circumstellar environments of fullerene PNe where the atomic nebular emission lines can be well explained by photoionization and shocks seem to be unimportant for fullerene formation (see e.g., García-Hernández et al. 2012).
fullerene-rich PNe are dominated by aliphatic hydrocarbon-rich dust emission features (superimposed on the underlying and featureless dust continuum emission), showing several broad unidentified IR (UIR) plateau emission features at 6–9 (hereafter 7 μm), 9–13 (hereafter 12 μm), 15–20, and 25–35 μm (e.g., García-Hernández et al. 2012). Characteristic aliphatic discrete features are located at 3.4 and 6.9 μm, arising from symmetric and asymmetric C-H stretching and bending modes of methyl and methylene groups attached to aromatic rings, respectively (see e.g., Kwok & Zhang 2011). The identification of the carrier(s) of the broad (and discrete) UIR emission features widely observed in space (toward Solar System bodies, circumstellar envelopes of PNe, diffuse ISM, and remote galaxies, among others) is a long-standing problem in astrophysics (see e.g., Kwok 2016 for a review). Thus, the potential identification of the carrier(s) of any of the broad UIR plateau emission features in fullerene PNe would impact very different astronomical fields.

Nano- and micro-sized particles in the ISM and circumstellar environment play an important role in astrophysical processes that lead to the formation of such exotic UIR emissions seen in the spectra of C-rich PNe and other astrophysical objects. The optical constants, which are the complex refractive indices or the complex dielectric function, of different materials (e.g., graphite, silicates, SiC, MgS, and HAC) are commonly used, in conjunction with radiative transfer codes, to explain the origin of the IR emission in astronomical spectra (e.g., HACs, soots, SiC, and other hydrocarbon materials; Bernard-Salas et al. 2012; Gavilan et al. 2016; Gómez-Llanos et al. 2018; Dubosq et al. 2023 see respectively). Fortunately, the latter can be done thanks to the databases2 dedicated to compile optical properties of analog materials of cosmic dust in the wavelength range from the UV to the far-IR.

In particular, the broad UIR plateau emission feature at 12 μm was first observed in the low resolution spectrometer of the IR astronomical satellite (LRS IRAS) spectra by Cohen et al. (1985), and its carrier’s identification has been a long outstanding problem. Cohen et al. (1985) attributed the carrier to PAHs, while Blanco et al. (1988) and Buss et al. (1990) attributed both the 7 and 12 μm plateau features to a mixture of large PAHs and HAC grains. Later, Kwok et al. (2001) specifically suggested that the 7 and 12 μm plateaus are superpositions of in-plane and out-of-plane bending modes of aliphatic side groups. Despite these earlier suggestions, the broad UIR emission at 12 μm has been generally attributed, in the literature, to SiC (α-SiC; e.g., Speck et al. 2009; Jones et al. 2023). García-Hernández (2012) argued against the SiC identification of this feature in fullerene PNe because the spectral characteristics (position and shape) (see Table 4 in García-Hernández et al. 2012) of the 9–13 μm emission in C₆₀-PNe significantly differ from those of the SiC 11.5 μm feature seen in the preceding AGB phase. This may suggest that the carrier could be different in AGBs and in fullerene PNe or even that the identification of SiC in AGB stars could be revisited.

The PN Tc 1 is the prototypical fullerene-rich PN (e.g., Cami et al. 2010; Aleman et al. 2019), being one of the best objects to study because of its simple round-elliptical morphology, the available high-quality and high-resolution IR Spitzer spectra, and the lack of PAH emission at 6.2, 7.7, 8.6, and 11.3 μm (Cami et al. 2010), which could strongly contribute to the fullerene and broad (and discrete) UIR emission features.

In this Letter, we present an analysis of the high-quality Spitzer spectrum of PN Tc 1 in comparison with a photoionization model that includes, for the first time, the emission of HAC-like dust grains as measured in laboratory, showing that HAC-like grains are a possible explanation, different from the often assumed SiC, for the broad 12 μm plateau emission feature.

2. Infrared spectrum of the C₆₀-PN Tc 1

We downloaded all the available mid-IR spectra from the Spitzer IR Spectrograph (IRS) (Werner et al. 2004; Houck et al. 2004) Heritage archive of the PN Tc 1 for which high-quality – a signal-to-noise ratio ($S/N$) > 50 – short-low (SL; 5.2–14.5 μm), short-high (SH; 9.9–19.6 μm), and long-high (LH; 18.7–37.2 μm) spectra were available (Program Identifier 3633) (see below and Perea-Calderón et al. 2009 for more data reduction details). We used the package SMART3 (v8.2.9; Higdon et al. 2004) to process the extracted wavelength and flux calibrated 1D spectra for each nod position, that is, to clean for bad data points, spurious jumps, and glitches and to combine and merge into one single spectrum per module (SL, SH, and LH). In order to get the final merged spectrum, we scaled the flux density of the SH spectra to match the overlapping wavelength region in the LH. Then, we scaled the SL spectra to match the overlapping wavelength region to the SH spectra. Finally, we scaled the flux density of the resulted combined spectra to that of the Wide-field IR Survey Explorer (WISE) band 4 ($λ_c = 22$ μm) photometric value (similarly to what was done in Otsuka et al. 2014). The resulting final Tc 1 Spitzer IR spectrum is shown in Fig. 1, where the emission features such as the C₆₀ and C₇₀ IR bands, and the broad 7 and 12 μm plateau emission features are indicated.

3. Cloudy simulations

To the best of our knowledge, the only previous attempt to model the 7 and 12 μm plateau emission features seen in the Spitzer spectrum of the C₆₀-PN Tc 1 (Fig. 1) was made by Bernard-Salas et al. (2012). They used the Jones (2012) theoretical absorption coefficients ($Q_{abs}$) of 3 nm HAC particles with a different H content (H/C = 0.23, 0.29, and 0.35) in conjunction with a 200 K blackbody (see Fig. 7 in Bernard-Salas et al. 2012). They could reproduce the 7 μm plateau emission feature as– seen in the Tc 1 continuum-subtracted Spitzer spectrum – with some degree of success, depending on the atom hydrogen fractions of the HAC particles. However, they could not reproduce the Tc 1 12 μm plateau emission feature. In particular, a too strong 11.3 μm feature was theoretically predicted for all H/C ratios, and they did not study or analyze the HAC contribution to the IR dust continuum emission. Bernard-Salas et al. (2012) concluded that their approximate reproduction of the 7 μm plateau emission feature may imply that fullerenes are formed by photochemical processing of HACs. Below we explain how we used, for the first time, a detailed photoionization model of Tc 1 together with the laboratory optical constants of HAC-like dust in order to model the 7 and 12 μm plateau features and the underlying dust continuum emission.

3.1. Modeling the 12 μm plateau emission

We used the stellar parameters and nebular abundances predicted in the detailed photoionization model developed by

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2 For example, the Jena database (https://www2.mpia-hd.mpg.de/HJPPDOC/index.php) and the refractive index database (https://refractiveindex.info/).

3 SMART was developed by the IRS Team at Cornell University and is available through the Spitzer Science Center at Caltech.

Aleman et al. (2019)\textsuperscript{4} (without graphite as the IR dust continuum source; see below) as input in CLOUDY (v22.02; Ferland et al. 2017) to model the mid-IR emission of the C\textsubscript{60}–PN Tc 1 by using, for the first time, the laboratory optical constants of HAC-like dust. We note that a change in the dust composition does not significantly change the emission line and H\textsubscript{2} fluxes predicted in the Aleman et al. model (a maximum flux difference of \textasciitilde5\% is obtained), and so the stellar and nebular parameters and chemical abundances are unaffected. The laboratory optical constants, that is, the complex refractive indices \(n\) and \(k\) of HAC-like particles were obtained from Prof. W. Duley (priv. comm.; see Duley 1984 for a detailed description of the laboratory measurements), covering a spectral range from 0.1 to 17 \(\mu\text{m}\) with a gap between 0.65 to 2.5 \(\mu\text{m}\) due to a limitation of the laboratory instrumentation to measure over this wavelength range (Fig. 2). The former are the only available laboratory optical constants, prepared under simulated interstellar conditions, covering a sufficient range from the UV to the mid-IR. The laboratory \(n\) and \(k\) values were measured in HAC thin films, \textasciitilde50–200 nm thickness, deposited at 300 K and with slightly different hydrogen concentrations (H/C \textasciitilde0.3–0.4; Duley et al. 1998; Duley & Hu 2012). However, it should be noted that it is mostly the \(k\) index that is sensitive to the H content; this is because the concentration of CH and CH\(_2\) in the HAC samples determines the IR \(k\). For simplicity, we adopted the mean \(n\) and \(k\) values (presumably with H/C \textasciitilde0.35), which are shown in Fig. 2. Because CLOUDY needs a minimum wavelength mesh (\textasciitilde0.001–96 \(\mu\text{m}\)), an extension of the \(n\) and \(k\) values to lower and upper wavelengths was carried out in a similar way as in Gómez-Llanos et al. (2018); that is, we extrapolated the \(n\) value to lower wavelengths on the basis of the BE1 amorphous carbon included in CLOUDY (Rouleau & Martin 1991), and for \(k\) we extrapolated using a power law of slope 2, whereas for higher wavelengths we extrapolated \(n\) as a constant value and \(k\) using a power law of slope \textasciitilde1. For the gap between 0.65 to 2.5 \(\mu\text{m}\), a linear extrapolation was used.

For the model, we compiled the HAC optical constants with the grains command inside CLOUDY, using a canonical ISM grain distribution (\(a_{\text{min}} = 0.001\) \(\mu\text{m}\) to \(a_{\text{max}} = 0.25\) \(\mu\text{m}\); 1–250 \(\text{nm}\)), distributed in ten grain size logarithmic steps following a power of \textasciitilde3.5), and generated the opacities (with the integrated Mie code for spherical grains; see van Hoof et al. 2004) needed for the CLOUDY simulations. We note that CLOUDY takes into account the molar mass of the HAC (12.36 g mol\(^{-1}\)), the band gap energy (\(E_{\text{gap}} = 1.27\) eV; Duley & Hu 2012), and the density of the material (1.5 g \text{cm}\(^{-3}\)) (see Duley et al. 1998; Duley & Hu 2012). A reduced \(\chi^2\) minimization was carried out for a grid of CLOUDY models – by varying the HAC grains’ relative content – to find a convergence between the model and the observed spectrum of Tc 1 between 10 and 14 \(\mu\text{m}\) (485 spectral points), yielding a \(\chi^2_{\text{red}} = 1.6\) assuming a 10\% error in the observations. This resulted in a C abundance (in units of log(C/H)) of \textasciitilde4.60 for the HAC-like grains, which is \textasciitilde3\% of the total C abundance (gas + dust phase abundance; C = \textasciitilde3.08), a mean dust

\textsuperscript{4} Aleman et al. (2019) developed a detailed photoionization model to obtain accurate stellar and physical parameters of the star and the nebula, respectively, and in which they assumed graphite in order to model the IR dust continuum emission. It is available at https://github.com/Morisset/Tc1

\textsuperscript{5} We note that equally good fits were obtained for different grain size distributions such as very small grains (VSG) or nanograins (1–15 nm), only big grains (15–250 nm), or the selected canonical ISM grain distribution (1–250 nm).
temperature across the nebula of \( \sim 215 \) K, and a dust-to-gas (D/G) ratio of \( 2.1 \times 10^{-4} \).

Figure 1 also shows the best CLOUDY model (green line) obtained from the \( \chi^2_{\text{red}} \) analysis applied to the observed spectrum of Tc 1. As it can be seen, the HAC-like grains at 300 K provide a very good fit to the broad 12 \( \mu \)m plateau feature in Tc 1, while at the same time they fully reproduce the IR dust continuum emission from 9 to 14 \( \mu \)m. For comparison, \( \alpha \)-SiC dust grains were also used to similarly model the mid-IR spectrum of Tc 1, which resulted in a worst fit to the 12 \( \mu \)m feature (see Appendix A). Interestingly, it turns out that HAC-like grains may be an alternative explanation of the broad 12 \( \mu \)m feature because it is very well reproduced with a simple spherical grain size distribution using the laboratory HAC optical constants at a deposition temperature close to the fullerene-dust temperature in Tc 1.

In addition, there is a small contribution to the observed 7 \( \mu \)m plateau feature, which is also clearly seen in the model spectrum. However, we still would need to include other emitters and/or an additional dust component to reproduce the 7 \( \mu \)m plateau feature (see below) in addition to the shape and rise of the underlying dust continuum emission at 5–9 and 14–17 \( \mu \)m, respectively.

### 3.2. Modeling the 12 \( \mu \)m plateau emission and dust continuum

Thus, in conjunction with the HAC-like grains as above, we added graphite dust grains separately as a possible additional dust continuum component (as assumed by Aleman et al. (2019)) and we again applied a \( \chi^2_{\text{red}} \) analysis to a grid of CLOUDY models in order to find the best fit by varying the HAC grains and graphite relative contents in the 9–16 \( \mu \)m range, yielding a value of \( \chi^2_{\text{red}} = 1.3 \). This resulted in C abundances of \(-3.74\) and \(-4.90\), which correspond to \( \sim 18.7\% \) and \( \sim 1.3\% \) of the total C abundance (gas + dust phase) as well as D/G of \( 1.5 \times 10^{-3} \) and \( 1.1 \times 10^{-4} \) for graphite and HAC grains, respectively.

We note that other carbon materials such as amorphous carbon (AC), generally used in the literature to model the IR dust continuum emission, provide worst fits because AC marginally contribute below 14 \( \mu \)m. Figure 3 displays the best photoionization model spectra for HAC-like grains and graphite, overplotted on the Tc 1 Spitzer spectrum; the HAC-like and graphite IR emission contributions are also shown separately for comparison. This way, we can reproduce the Tc 1 IR spectrum well from \( 5 \) to 17 \( \mu \)m (both the 12 \( \mu \)m plateau feature and the dust continuum) with the HAC-like grains providing an important fraction (\( \sim 20\% \)–\( 40\% \)) of the dust continuum emission, as evaluated from the integrated IR fluxes due to only graphite and HACs with respect to the total integrated IR continuum flux at three different wavelengths (5.6, 9.6, and 15.2 \( \mu \)m) representative of the dust continuum emission. Again, for comparison, \( \alpha \)-SiC dust grains in conjunction with graphite dust grains were also used to similarly model the mid-IR spectrum of Tc 1, resulting in a worst fit of the red wing of the broad 12 \( \mu \)m feature (see the Appendix A). Finally, we stress that preliminary photoionization models with HAC-like grains deposited at 300 K also provide acceptable good fits to the 12 \( \mu \)m plateau feature (and dust continuum) in another fullerene PN such as IC 418 and SMC 16, when playing with the model parameters (e.g., grain size and shape distribution; Gómez-Muñoz et al., in prep.).

### 4. Astrophysical implications

To the best of our knowledge, this is the first time that HAC grains convincingly reproduce the 12 \( \mu \)m plateau emission feature in a fullerene PN (Tc 1), posing doubts on the generally accepted SiC identification in the literature as the main carrier of this feature. Remarkably, the HAC grains naturally provide an important fraction of the IR dust continuum emission and are consistent with the other UV features observed such as the 7 \( \mu \)m plateau feature (see below). From our CLOUDY models, we determined that \( \sim 1.3\% \)–\( 3.0\% \) (with and without graphite, respectively) of the C in Tc 1 is in the form of HAC-like dust. These values are comparable to the amount of C that is estimated to be in the form of fullerenes, such as \( C_{60} \), in Tc 1 (\( \sim 1.5\% \); see Cami et al. 2010).

The laboratory HAC-like grains (\( H/C \sim 0.35 \)) used in our models (Duley & Hu 2012) mainly contain aliphatic carbon chains (sp\(^3\) content), which represent 72\% (i.e., aromatic/aliphatic ratio of 0.4) of the chemical composition, but also polyyne (-C≡C-)\(_n\) and cumulenic (-C≡C-)\(_n\) chains. According to Duley & Hu (2012), these HAC-like grains can have more aromatic rings than aromatic chains. In fact, they suggest that above 10 \( \mu \)m, the features can be caused by a variety...
of vibrational modes associated with ring deformation and with CH₂ groups (i.e., out-of-plane CH vibrations). In particular, the spectral range of the broad 12\,\mu\text{m} plateau emission may contain the features produced by small aromatic rings (pentagons and hexagons) with side chains such as dimethylnapthalene or dimethylphenanthrene, but also those produced by solo, duo CH, and CH₂ groups as components of the hydrocarbon matrix (Duley & Hu 2012). Clearly, the broadening of the 12\,\mu\text{m} plateau emission is the result of this coexistence of small aromatic rings and hydrocarbon chains; that is, the mixed aromatic and aliphatic hydrocarbon composition inside the HAC-like material is the key behind the broadening of the 12\,\mu\text{m} feature. We remark that the only other laboratory optical constants available to us correspond to those measured in HAC films deposited at a lower temperature of 77\,K (Prof. W. Duley, priv. comm.) and with slightly higher H concentrations (H/C ∼ 0.5–0.6), which have fewer aromatic rings in its composition (Duley et al. 1998). The 12\,\mu\text{m} plateau feature in Tc 1 cannot be reproduced with the 77\,K HAC-like sample (i.e., it is absent; Gómez-Muñoz et al., in prep.), suggesting that the aromatic ring/chain ratio, rather than the aromatic/aliphatic ratio, is a key parameter for the formation of the 12\,\mu\text{m} plateau feature.

The presence of HAC-like grains in conjunction with fullerenes have been previously proposed in the literature as proof of the photochemical processing of HAC-like grains for fullerene formation (see e.g., García-Hernández et al. 2010, 2011a,b, 2012; Bernard-Salas et al. 2012). Naturally, our finding in Tc 1 suggests that the formation of fullerenes in PNe circumstellar environments may be related to the photochemical processing of HAC-like grains. However, the only experimental data on the formation of HAC-like grains are those from Scott et al. (1997), where they performed laser ablation (UV radiation-induced decomposition) of HAC films and found PAHs and fullerenes, among other species, but the chemical reactions are presently unknown. The lower aromatic content compared to more dehydrogenated hydrocarbons in our HAC sample suggest that the main process to generate the precursors to form C₆₀, for example, the dehydrogenation of the HAC, is through radiative processing as aliphatic hydrocarbons have been proven to be efficiently dehydrogenated in the ISM by UV radiation (e.g., Muñoz Caro et al. 2001). We speculate that the presence of some small aromatic rings in our 300\,K HAC-like sample might act as templates or catalysts for the formation of more complex C₆₀ structures when the material is subjected to photochemical processing. More sophisticated laboratory experiments on the photochemical transformation of HAC-like grains at circumstellar conditions would be needed to unveil the details of fullerene formation via chemical reaction routes.

Another obvious implication of our work involves the carriers of the 7\,\mu\text{m} plateau emission feature seen in the fullerene PN Tc 1. Our findings also suggest that HAC-like grains, with H/C = 0.35 and mainly composed by aliphatic carbon chains (72%; see above) with some small aromatic rings, are not a main contributor to such a 7\,\mu\text{m} emission complex and that other still unidentified species should be the carriers. Fullerenes-based species are natural candidate species as potential additional emitters at these wavelengths in fullerene PNe. Very recent quantum-chemistry simulations of metallofullerenes (neutral and charged endohedral and exohedral species) do indeed demonstrate that they strongly emit at 6–9\,\mu\text{m} (Barzaga et al. 2023a,b; Hou et al. 2023) with no significant contribution in the 9–13\,\mu\text{m} spectral region.

5. Concluding remarks

This pilot work leads us to conclude that HAC-like grains are a convincing alternative explanation (i.e., different from the often assumed SiC) for the broad 12\,\mu\text{m} plateau emission feature seen in the fullerene PN Tc 1. In addition, our work suggests that HAC-like grains may be possible carriers of the 12\,\mu\text{m} plateau feature, being likely related to the fullerene formation process (possibly as fullerenene precursors) in the circumstellar environment of PNe.

Interestingly, HAC-like grains can also reproduce the far-ultraviolet (FUV) rise seen in the extinction curve (Gavilan et al. 2016, 2017) and very recently detected also in the International Ultraviolet Explorer (IUE) UV spectrum of Tc 1 (Gómez-Muñoz et al. 2024). In this particular case, Gómez-Muñoz et al. (2024) could reproduce the FUV rise toward Tc 1 very well by using HAC-like nanograins (1–15\,nm). Although other carbonaceous materials such as hydrogenated carbon clusters and large PAHs, possibly among others, may also explain the FUV rise in extinction curves (see e.g., Dubosq et al. 2023; Lin et al. 2023); such an independent finding would be consistent with the results presented here.

Yet, we do not fully understand the exact chemical pathways from large HAC-like dust grains toward the most stable fullerene molecules as well as the origin of the other broad plateau emission features seen in fullerene PNe, such as 6–9, 15–20, and 25–35\,\mu\text{m}. The James Webb Space Telescope offers the opportunity to observe these broad features in fullerene PNe at a much higher sensitivity and spectral resolution than Spitzer, permitting the variations in their positions and shapes to be studied precisely (even resolving a possible substructure) and providing new additional constraints for future modeling studies. Undoubtedly, more laboratory efforts are needed in order to definitively reveal the details of fullerene formation in PNe circumstellar environments as well as the carriers of the elusive UIR plateau features. Our work strongly encourages more laboratory experiments to obtain the refractive indices n and k (over a large wavelength range, from the UV to the far-IR) of HAC-like dust grains with several structures and a composition (e.g., H/C ratios) as well as at different physical conditions (e.g., temperatures or aromatic ring/chain ratios). Such laboratory measurements (not presently available) would be used to expand the pilot novel work presented here for Tc 1 to a larger sample of fullerene PNe.

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References


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Appendix A: Modeling the Tc 1 mid-IR spectrum using α-SiC grains

For comparison, Fig. A.1 shows the mid-IR spectrum of Tc 1 together with the best CLOUDY model spectrum obtained using α-SiC grains (as in Gómez-Llanos et al. 2018, for the case of the PN IC 418) with the same shape (spherical) and grain size distribution as when using HAC-like grains. As can be seen from the figure, when using only α-SiC (top panel), the best model spectrum only fits the weak 11.3 μm feature seen in Tc 1 and not the entire broad 12 μm feature. On the other hand, when using α-SiC+graphite (bottom panel), the dust continuum is very well fitted but the red wing of the broad 12 μm emission is poorly reproduced.

We remark that it is already well known that much better fits with α-SiC can be obtained when playing with very different extreme shapes and grain size distributions (e.g., the case of PN IC 418: Gómez-Llanos et al. 2018) but here we are exploring if there is any other contribution to or explanation for the broad 12 μm plateau feature in PNe with fullerene-dominated IR spectra such as Tc 1, that is, different from the often assumed SiC.

It is important to mention that the 12 μm feature in IC 418 has different characteristics (position, width, and emission strength) than in Tc 1 (Otsuka et al. 2014). Gómez-Llanos et al. (2018) needed to use very different shapes (spheres and five extreme ellipsoid types) and grain size distributions along the nebula in order to fit the red wing of the 12 μm feature with α-SiC. Also, the IR spectrum of IC 418 is contaminated by other species (e.g., PAHs), displaying weaker C₆₀ bands and a different fullerene and dust temperature than Tc 1.