AstroPAH

A Newsletter on Astronomical PAHs

Issue 129 • June 2026

Exposed Cranium Dusty Nebula

Editorial

Dear Colleagues,

Welcome to the 128^{th} edition of AstroPAH!

This month, our cover showcases a dual view of the Exposed Cranium Nebula captured by JWST, showing how JWST's infrared instruments reveal different features. NIRCam highlights intricate dust structures along with numerous background stars and galaxies, while MIRI emphasizes the glowing cosmic dust and heated gas, providing the sharpest view of this late-stage stellar nebula to date.

Our In Focus section comes from Dr. Marie van de Sande, Dr. Miguel Montarges, Dr. Taissa Danilovic, and Dr. Jacco van Loon who together comprise the editorial board of the new Cool Evolved Stars Newsletter (CESN). The In Focus highlights the history and recent revival of the AGB Newsletter under the new umbrella CESN which is welcoming new submissions via https://cesn.obspm.fr.

In the Abstracts section, we highlight the detection of C_{60} combination bands within NIRSpec observations of the planetary nebula Tc 1, an exciting new outcome of the JWST era. Other new insights on carbonaceous grains throughout the universe include observations of grain and PAH destruction in a galactic nucleus and a discussion of the evolution of the 3.3 µm band and its neighboring vibrational features. Additional spectroscopic contributions feature new evidence that the 11.3 µm band is not expected to be polarized, as well as a new spectral prediction tool for PAHs that more accurately predicts the dominant spectral features of charged PAHs. Other exciting work on the chemical modeling side examines the astrochemical processes that could occur on carbon nitride graphene analogs and the inclination of the cationic pyrene dimer to undergo complexation with water. Finally, experiment and theory investigations of the reactivity of long-lived isomers of the methylnaphthalene cation uncovered links to acenaphthalene chemistry in interstellar environs such as TMC-1.

AstroPAH can help you promote your research. Please send your contributions to our email address.

Thank you all for your contributions!

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Next issue: 16 July 2026.
Submission deadline: 3 July 2026.

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PAH Picture of the Month

JWST's NIRCam (left) and mid-infrared MIRI (right) observations provide the most detailed view yet of the Exposed Cranium Nebula (PMR 1), revealing intricate dust structures, glowing gas in the environment surrounding a puzzling late-stage star.

Credits: NASA, ESA, CSA, STScI; Image Processing: Joseph DePasquale (STScI). The image is available here.

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From AGB Newsletter to Cool Evolved Stars Newsletter (CESN) – an Evolutionary Tale

by Jacco van Loon[1], Taïssa Danilovich[2], Miguel Montargès[3] & Marie Van de Sande[4]

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Following the example of Bo Reipurth's hugely popular Star Formation Newsletter, Thierry Forveille and Claudine Kahane took the initiative to launch the **AGB Newsletter**. That was in 1994, at the dawn of the electronic era. One of us was only just about to start their PhD and remembers vividly and fondly the time spent in libraries reading and photo-copying paper copies of journals and preprints, observing IUE microfiches under a microscope and spending cloudy nights in the La Silla library getting blissfully lost in maps. The internet was a revelation, the world wide web just spun.

After a brief hiatus in 2004-2006 and taking the opportunity of a long observing run at Parkes to self-learn php scripting and MySQL database management, the AGB Newsletter continued to be hosted by Jacco van Loon at Keele University from 2006 until the start of 2023. After the COVID-19 pandemic, IT safety restrictions made it impossible, first to send automatic e-mails and then to accept submissions into a database, so the newsletter had no choice but to shut down.

Meanwhile, the importance of the AGB Newsletter became apparent to Taïssa Danilovich, shortly after she started her PhD. There was a clear benefit to having most of the papers in the field collected in a monthly newsletter, not to mention the time saved in scouring the daily arXiv uploads. When the AGB Newsletter shut down, enquiries were made and options considered. Finally, Taïssa teamed up with Miguel Montargès to take the bull by the horns and, with help of a wonderful team of people at Paris Observatory set up a modern electronic platform to host the Cool Evolved Stars Newsletter (CESN). Together with Jacco van Loon and Marie Van de Sande, they make up the CESN editorial team.

You can access CESN by visiting our new home page (https://cesn.obspm.fr) to subscribe or read the latest newsletter. It is even possible to submit a paper to the newsletter using only the DOI, which reduces the friction in filling out the form.

Thierry and Claudine's vision was for the AGB Newsletter "to cover stellar evolution from the early AGB to dispersal of the planetary nebulae, with an emphasis on mass loss and circumstellar matter [..] More massive objects such as Wolf Rayet stars and supernovae are excluded since the two communities have relatively little overlap."This changed from 2006 onwards, and more explicitly when the AGB Newsletter became the official communiqué of the renamed IAU Working Group on Red Giants and Supergiants, to include all types of red giant, from (first ascent) RGB to red supergiant, and all related phenomena. CESN continues this path, and enjoys the IAU Working Group's blessings.

There has always been overlap with other fields of astrophysics, and much is learnt from looking over the fence (and talking to one's neighbour). The same is true for the PAH community: there are more than a few astronomers who study both cool evolved stars and the interstellar medium, and this is no surprise since both environments are the sites of enigmatic and ill understood gas and solid-state chemistry that are key in the lifecycle of matter and the seeding of life.

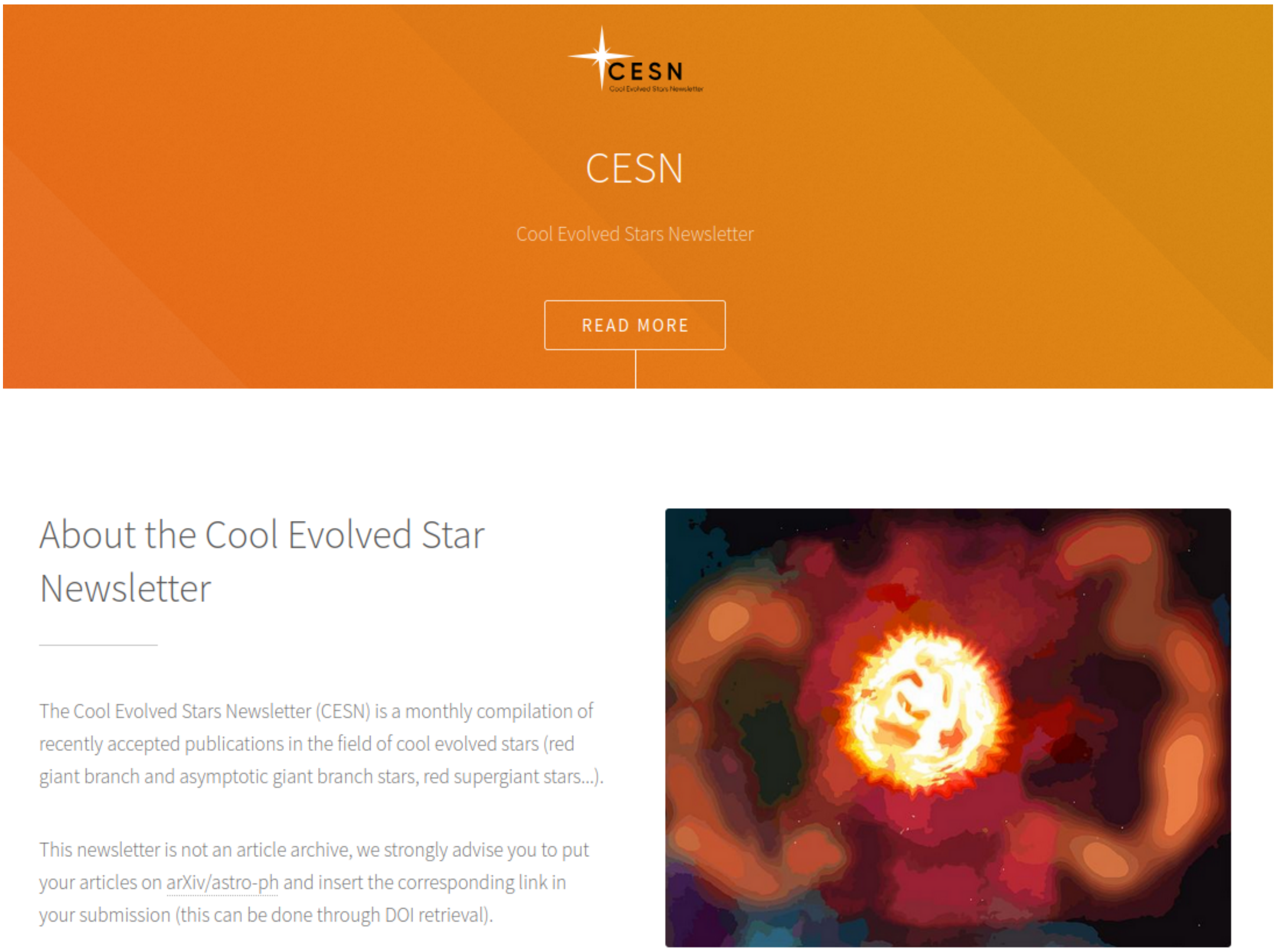
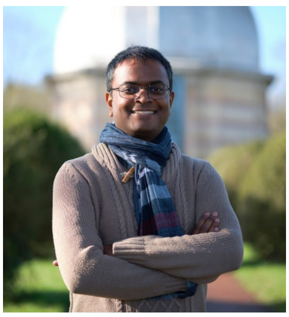


Figure 1 *– CESN webpage screenshot.*

Dr. Marie Van de Sande is an astrochemist specialised in the chemistry of AGB outflows. She develops chemical kinetics models and uses them to interpret observations of these complex environments. She obtained her PhD in 2018 at KU Leuven and will move to University College Dublin this August as an assistant professor, starting her ERC Starting Grant ASHES.



Dr. Miguel Montargès is assistant astronomer at Paris Observatory – PSL in the Laboratory for Instrumentation and Research in Astrophysics (LIRA), since 2024. He characterizes the environment of cool evolved stars (asymptotic giant branch stars and red supergiants) through high angular resolution observations. He also uses 3D radiative transfer code to reproduce continuum observations (dust).

Dr. Taïssa Danilovich specialises in observational astrochemistry and radiative transfer modelling of cool evolved stars. Her favourite active telescope is ALMA and her favourite decommissioned telescope is the Herschel Space Observatory.

Dr. Jacco van Loon studies complex systems such as mass-losing stars, the interstellar medium, galaxies and life. They are based at Keele University and care about equity and inclusion.

Abstracts

Detection of C_{60} Combination Bands in the Near-IR Spectrum of Tc 1

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We report the detection of a set of new near-infrared emission features between 3.5 and 5.2 μm in JWST/NIRSpec observations of Tc 1, the planetary nebula known for displaying the cleanest and most prominent mid-infrared cosmic fullerene spectrum. These broad features share the same spatial distribution as the well-known C_{60} and C_{70} mid-infrared

emission bands, peaking in an asymmetric ring approximately 5–6" from the central star. Through comparison with new anharmonic quantum chemical calculations, we demonstrate that these features arise from C_{60} combination bands, marking their first detection in an astrophysical environment. The total energy radiated in the combination bands amounts to $\sim$17% of the total energy emitted from all C_{60} modes, with direct implications for fullerene cooling models. These near-infrared combination bands offer a promising new window for identifying and studying the molecular astrophysics of C_{60} in sources where mid-infrared spectra are more complex.

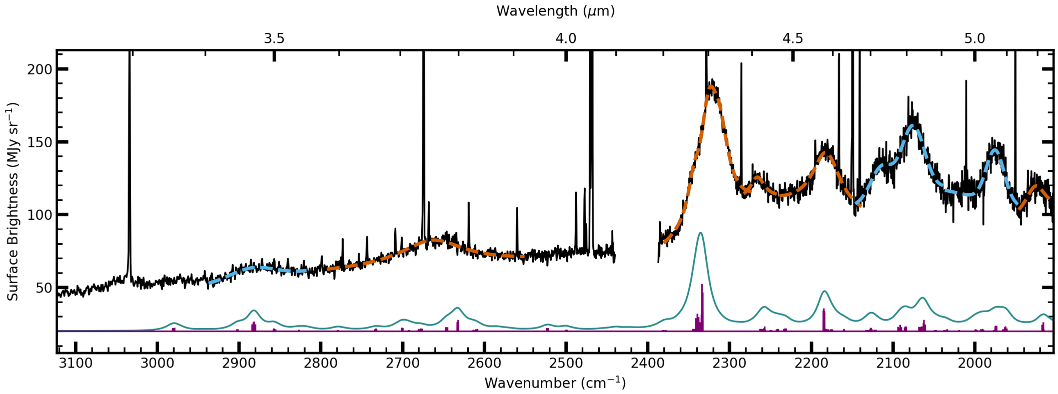

Figure 2 *– JWST/NIRSpec Segment 3 spectrum of Tc 1 (black) corresponding to a pixel within the fullerene ring; its location is denoted by a black circle in Figure 1. Gaussian (light blue, dashed) and Lorentzian (orange, dashed) fits are shown on top of the spectrum. Anharmonic calculations of C_60 combination bands are shown scaled to an arbitrary absolute intensity (teal, solid), with the stick spectrum (purple) convolved with Lorentzian profiles with line width 20 cm^{-1} and shifted by -45 cm^{-1} to match the observations.*

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The Astrophysical Journal Letters, **1004**, L32 (2026)

https://iopscience.iop.org/article/10.3847/2041-8213/ae76d5

Abundant hydrocarbons in a buried galactic nucleus with signs of carbonaceous grain and polycyclic aromatic hydrocarbon processing

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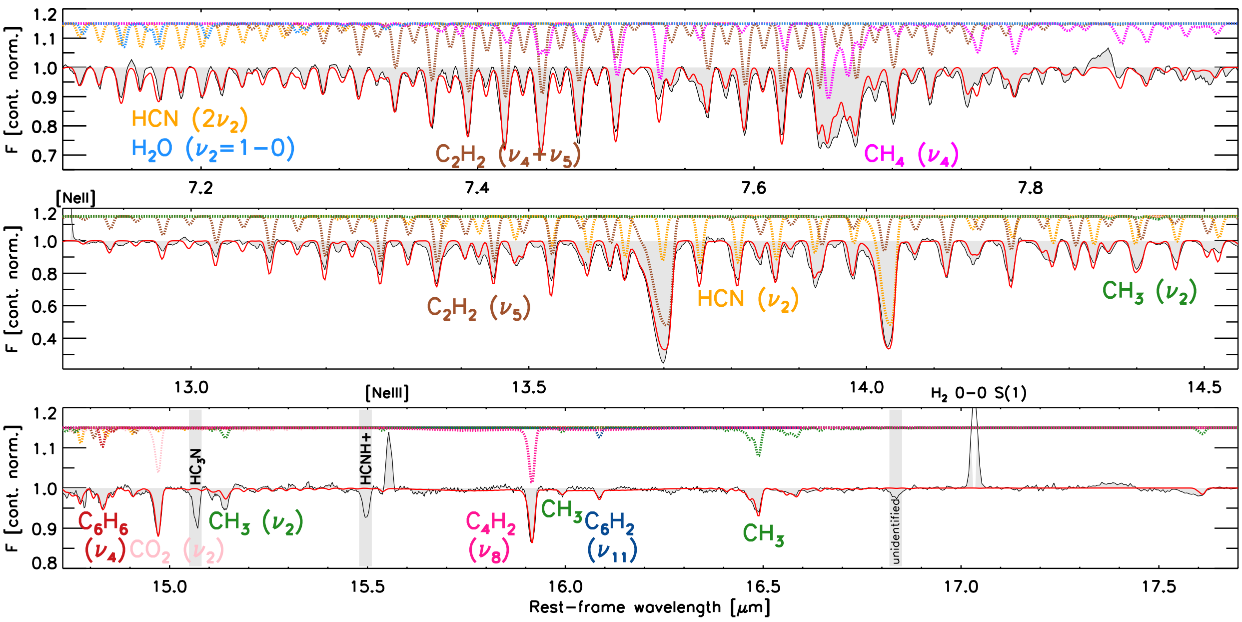

Figure 3 *– Main mid-IR gas-phase molecular rovibrational bands in IRAS 07251−0248. The top panel shows the ∼7-8 μm molecular bands and the middle and bottom panels the ∼13-18 μm bands. Each panel shows the JWST/MIRI-MRS rest-frame continuum-normalized spectra (Extended data Fig. 1; black solid line filled in gray) together with the total best-fit model (red solid line). The contribution of the fit by the different species are shown with an offset (+0.15) to improve clarity: C_6H_6 (dark red), C_6H_2 (blue), C_4H_2 (deep pink), CH_4 (magenta), CH_3 (green), C_2H_2 (brown), CO_2 (light pink) and HCN (orange).*

Hydrocarbons play a key role in shaping the chemistry of the interstellar medium (ISM), but their enrichment and relationship with carbonaceous grains and polycyclic aromatic hydrocarbons (PAHs) still lack clear observational constraints. We report JWST NIRSpec+MIRI/MRS infrared (IR; ∼3-28 μm) observations of the local ultra-luminous IR galaxy (ULIRG) IRAS 07251−0248, revealing the extragalactic detection of small gas-phase hydrocarbons such as benzene (C_6H_6), triacetylene (C_6H_2), diacetylene (C_4H_2), acetylene (C_2H_2), methane (CH_4), and methyl radical (CH_3) as well as deep amorphous C–H absorptions in the solid phase. The unexpectedly high abundance of these molecules indicates an extremely rich hydrocarbon chemistry, not explained by high-temperature gas-phase chemistry, ice desorption or oxygen depletion. Instead, the most plausible explanation is the erosion and fragmentation of carbonaceous grains and PAHs. This scenario is

supported by the correlation between the abundance of one of their main fragmentation products, C_2H_2, and cosmic ray (CR) ionization rate for a sample of local ULIRGs. These hydrocarbons are outflowing at ∼160 km/s, which may represent a potential formation pathway for hydrogenated amorphous grains. Our results suggest that IRAS 07251−0248 might not be unique but represents an extreme example of the commonly rich hydrocarbon chemistry prevalent in deeply obscured galactic nuclei.

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Nature Astronomy, **10**, 420 (2026)

https://doi.org/10.1038/s41550-025-02750-0
Link to the paper: https://www.nature.com/articles/s41550-025-02750-0
Link to the research briefing: https://www.nature.com/articles/s41550-025-02768-4

The nature and evolution of a-C(:H) nanoparticle substructures and speculations on the origin of the 3-4 micron emission bands

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The nature and evolution of hydrocarbonaceous grains within interstellar and circumstellar media is still far from resolved, perhaps owing to the complex nature of their seemingly simple binary atomic compositions. This work explores the fine details of the composition of amorphous hydrocarbon nanoparticles, a-C(:H), as well as the evolution of their inherent substructures under extreme conditions, focusing on the characteristic CHn bands in the 3-4 micron wavelength region. Particular attention is paid to the role of dehydrogenation and its effects on the sp^3 and sp^2 hybridisations that can lead to an extensive conjugated domain functionalisation of the contiguous structural network within a-C(:H) nanoparticles. Qualitatively, this approach is able to explain the origin and evolution, including the appearance and disappearance, of emission bands observed in the 3-4 micron wavelength regime without a significant aromatic moiety content within the structures. A diatomic a-C(:H) phase is likely at the heart of the dust evolution in the interstellar medium and circumstellar and photodissociation regions observed at short wavelengths. It appears that we have some way to go in fully understanding these complex materials. Much laboratory work is required to elucidate their chemical and structural evolution at nanoparticle sizes under extreme conditions.

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Astronomy & Astrophysics, **703**, A29 (2025)

https://doi.org/10.1051/0004-6361/202556756

No Evidence of Polarization in the 11.3 μm Polycyclic Aromatic Hydrocarbon Emission Line by Independent Analyses

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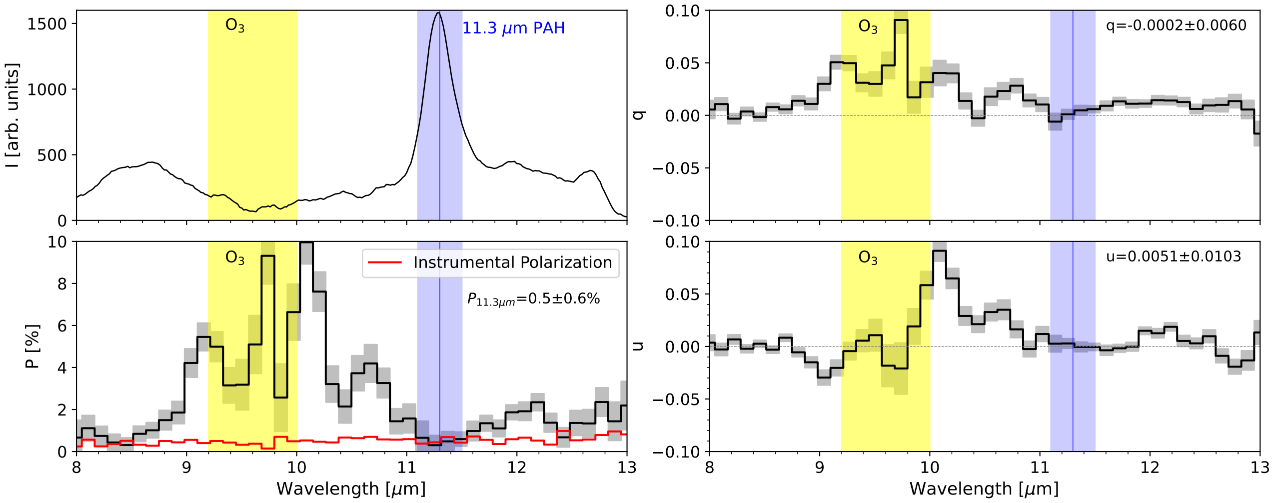

***Figure 4** – Spectro-polarimetric observations of MWC 1080 NW. The Stokes I (top-left), q (top-right), and u (bottom-right), the polarization fraction (bottom-left) spectra (black line), and their 1σ uncertainties (gray region) are shown. The instrumental polarization (red line) is displayed in the same panel as the polarization fraction spectrum. The Stokes I has been smoothed using a 0.06 μm boxcar, while the Stokes q and u are downsampled to 0.12 μm and then smoothed with a 0.36 μm boxcar. The 11.3 μm PAH emission (blue solid line), the aperture width of 0.4 μm (blue region), and the approximated extent of the telluric 0_3 band (yellow region) are shown. The values of the Stokes q and u and the polarization fraction and their uncertainties, within the 11.3 $\pm$ 0.2 μm wavelength range (blue region), are displayed.*

Polycyclic aromatic hydrocarbons (PAHs) are commonly used as proxies for star formation, molecular gas content, and other interstellar medium (ISM) properties in our Galaxy and other galaxies. Given their abundance and brightness, polarization measurements of PAH features could, in principle, provide a probe of the ISM magnetic field and intrinsic PAH properties; however, the diagnostic power of PAH polarization remains to be established. Previous studies reported that the 11.3 μm PAH emission line in the northwestern nebula of the Herbig Be star MWC1080 was polarized at 1.9 $\pm$ 0.2%. This level of polarization was explained via the paramagnetic relaxation process, which may allow the characterization of magnetic fields in the ISM. Using the same observations, here, we reanalyzed the 8-13 μm spectropolarimetric observations taken with CanariCam on the 10.4m Gran Telescopio CANARIAS (GTC), and we measure a polarization of 0.5 $\pm$ 0.6% within 11.3 $\pm$ 0.2 μm, consistent with an unpolarized source, 0.6 $\pm$ 0.2% (instrumental polarization). We reproduce the previously reported polarized PAH emission line if the polarization fraction spectrum is oversubtracted by a constant instrumental polarization and the polarization uncertainties, which is inconsistent with the fundamentals of polarimetric data analysis. Thus, the published 8-13 μm spectropolarimetric data taken with CanariCam/GTC provide no statistical evidence for a polarized 11.3 μm PAH emission line, in agreement with current dust models.

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The Astrophysical Journal, **1001**, 147 (2026)

https://ui.adsabs.harvard.edu/abs/2026ApJ..1001..147L/abstract
https://iopscience.iop.org/article/10.3847/1538-4357/ae5654/pdf

AstroSpec-LLM: A chemical language model for fast, charge-aware PAH infrared spectra

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The JWST observations of aromatic infrared bands (AIBs) calls for reference spectra of polycyclic aromatic hydrocarbons (PAHs) that go beyond the usual neutral, small-to-medium sized species. Traditional quantum chemical calculations, however, scale as $\mathrm{O}(N_\mathrm{C}^4)$ with the number of carbon atoms, making large ($N_\mathrm{C} \gtrsim 100$) PAHs prohibitively expensive. In a recent paper (Liu et al., 2026), the authors present `AstroSpec-LLM`, a deep-learning framework that adapts a large language model (LLM) architecture to read molecular strings as "chemical sentences" and predict their infrared spectra (see Figure 5). Fine-tuned on a data set of 24 146 PAH spectra spanning four charge states (-1, 0, $+1$, $+2$), the model captures continuous ionization trends rather than treating each charge state as an isolated category.

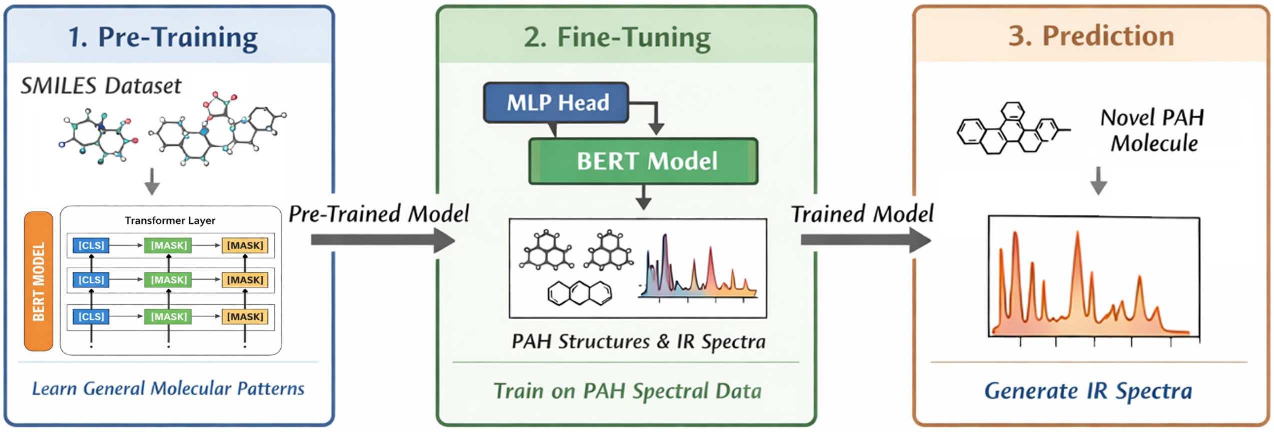

Figure 5 *– Three-phase AstroSpec-LLM workflow for PAH IR spectral prediction.*

The result is a six-order-of-magnitude speedup compared to density functional theory (DFT), with stable extrapolation performance to species with $N_\mathrm{C} \geq 100$. Importantly, the model's attention maps reveal physically meaningful band preferences: charged PAHs direct focus to the 6.2 and 8.6 micron C-C modes, whereas neutrals prioritise the 3.3 and 11.2 micron features, consistent with established interstellar ionization tracers. AstroSpec-LLM thus offers a practical, high-throughput tool for building massive, charge-aware spectral libraries for large PAHs, helping to decode the aromatic universe seen by JWST. The code, data, and trained models are publicly available at the Git repository: AstroSpec-LLM.

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Monthly Notices of the Royal Astronomical Society, **549**, stag893 (2026)

https://doi.org/10.1093/mnras/stag893

Carbon nitride monolayer nanosheets: astrochemical insights into the fate of interstellar hydrogen

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Ubiquitously found in the Universe, atomic hydrogen represents up to 70% of the neutral gas composition of the Milky Way. As an adatom, hydrogen can physisorb or chemisorb onto interstellar dust grains and icy mantles, thereby contributing to the formation of H_2 and, potentially, to the synthesis of more complex hydrogenated species. In addition, structures with relatively large specific surface areas – such as silicates, amorphous carbon, graphene sheets, or water ice – host heterogeneous chemistry that is thought to facilitate the emergence of complex organic matter in astrophysical environments. Although the fundamental physical and chemical processes occurring at dust/gas interfaces are well characterized, current understanding of dust properties governing the formation of H_2 and complex molecules remains incomplete. In this context, we introduce graphitic-like two-dimensional carbon nitride monolayer structures (2D-CN) as a putative molecular family of potential relevance to astrochemistry. The physicochemical and electronic properties of these materials have been extensively examined in recent years for industrial and technological applications. Here, we propose that their importance may likewise extend to interstellar and circumstellar environments. To explore this possibility, we employed density functional theory (DFT) calculations to investigate the characteristics and extent of H adsorption onto C_2N_1, C_3N_1, C_3N_2, C_3N_4, C_4N_3, C_6N_6, C_6N_8, C_9N_4, and C_9N_7 monolayer nanosheets. We identify multiple adsorption sites over C–C bonds, above C and N atoms, and hollow (macropore) locations at which energetically favorable binding of atomic hydrogen could occur in the interstellar medium (ISM). From an astrochemical perspective, these 2D-CN structures, if formed, could therefore contribute to the physicochemical processing and evolution of hydrogen in the ISM. As such, given their structural similarities to prebiotic nitrogen-bearing frameworks (many found in meteoritic samples and organic aerosols), 2D-CN molecules may emerge as promising candidates for exploring the complex interstellar chemistry of astrophysically relevant molecules.

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Physical Chemistry Chemical Physics, **28**, 11292 (2026)

https://doi.org/10.1039/D6CP00221H
https://arxiv.org/abs/2603.22443

Microsolvation of charged PAH clusters: modeling interaction of water aggregates with cationic pyrene dimer

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The interaction of polycyclic aromatic hydrocarbons (PAHs) aggregates with water plays a key role in both atmospheric and interstellar chemistry. However, its characterization at the molecular level represents experimental and theoretical challenges. In this work, we propose a detailed characterization of the potential energy surfaces (PES) of cationic pyrene dimer interacting with water molecules and clusters, $Py_2^+(H_2O)_n$ (n=1–10). A dedicated PES global exploration algorithm parallel tempering Monte Carlo, combined with the density functional tight binding configuration interaction potential, was employed with further refinement at the density functional theory level. Structural patterns were identified and their relative stabilities were determined. For small clusters, side isomers are found the most stable, while face isomers become competitive for larger sizes. Analysis of cohesive energies, relative stabilities and evaporation energies highlights the subtle effects of non-covalent interactions and reveals size-dependent patterns. Infrared spectral signatures are predicted in the spectral region corresponding to interstellar aromatic infrared bands (AIBs), including modifications of the C-H stretch band with a new red-shifted component, and the appearance of new features in the 10–20 μm region, while the 6–10 μm range remains quite unaffected. These results provide molecular-level insight into microhydrated PAH cationic clusters that are experimentally out-of-reach. The obtained data are relevant for astrochemical models and the interpretation of astronomical observations, particularly in the context of James Webb Space Telescope observations.

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ACS Earth and Space Chemistry **online** (2026)

https://pubs.acs.org/doi/full/10.1021/acsearthspacechem.6c00099

Acenaphthene Derivatives as Signatures of $C_{11}H_{19}^+$ Reactivity with Methylated Naphthalenes

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$C_{11}H_9^+$ ion is the dominant fragment cation formed from methyl-naphthalene (MeNp) and dimethyl-naphthalene (diMeNp). Using the multiplex capabilities of PIRENEA, a setup dedicated to laboratory astrophysics, we studied the reactivity of the benzylium-like isomers of $C_{11}H_9^+$ with diMeNp under isolated conditions relevant to radiative association. Two reaction products are observed, $C_{12}H_{11}^+$ – also formed in the reaction with MeNp – and $C_{13}H_{13}^+$, with branching ratios that depend on the specific diMeNp isomer. The reaction products were subsequently exposed to UV–visible irradiation to gain insight into their structures. The acenaphthylene radical cation, $\cdot C_{12}H_8^+$, was identified as the most stable photofragment. We show that this experimental approach, supported by density functional theory calculations and molecular dynamics simulations, provides new constraints on the chemistry of benzylium-type species. We highlight the role that long-lived ion–molecule complexes can have in promoting C–C coupling and the formation of a pentagonal cycle. Moreover, the chemistry uncovered here highlights new pathways for the formation of pentagonal rings during PAH growth under low-pressure and cold conditions. In particular, it can lead to efficient formation of acenaphthylene-like species, recently detected in the TMC-1 cold cloud.

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ACS Earth and Space Chemistry, **10**, 5, 1254 (2026)

https://doi.org/10.1021/acsearthspacechem.5c00386
https://doi.org/10.48550/arXiv.2606.03575
https://cnrs.hal.science/hal-05447383

AstroPAH Newsletter

http://astropah-news.strw.leidenuniv.nl — Next issue: 16 July 2026

astropah@strw.leidenuniv.nl — Submission deadline: 3 July 2026