AstroPAH

A Newsletter on Astronomical PAHs

Issue 115 • February 2025

NGC 1333: A Nearby Star-Forming Cluster

Editorial

Dear Colleagues,

Welcome to our 115th issue! We are back for a new orbit with our first publication of the year!

For a fresh start, we are excited to share a total of **15** of your contributions! They cover a wide range of topics, from O-bearing PAHs to the idea of PAHs as extraterrestrial technosignatures!

We would like to draw your attention to a couple of things. First, we congratulate Prof. J. Tennyson for being awarded the Royal Astronomical Society's Gold Medal for 2025. This amazing prize serves as a recognition of the large contributions of laboratory data to support astronomical searches in support of cutting-edge astronomical research, notably through the ExoMol database. Congratulations for this well-deserved prize!.

Second, we are happy to share with you announcements for the COST NanoSpace joint meeting which will take place in Kaunas, Lithuania, May 2025, and a special Astrochemistry symposium at the International Symposium on Molecular Spectroscopy (ISMS) in June. Don't miss the deadlines!

Finally, a Postdoc position in molecular physics/laboratory astrophysics is open at the Berlin Institute of Technology, Germany. Check out the announcements for more details!

Thank you all for all your contributions and keep them coming in 2025!

The Editorial Team

Next issue: 20 March 2025.
Submission deadline: 7 March 2025.

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PAH Picture of the Month

This month's featured image highlights NGC 1333, a nearby star-forming cluster located within the Perseus molecular cloud, approximately 960 light-years from Earth. The image was captured by the NASA/ESA/CSA James Webb Space Telescope (Langeveld et al. 2024). PAHs have been previously detected in this object (e.g. Knight et al. 2022 and references therein).

Credits: ESA/Webb, NASA CSA, A. Scholz, K. Muzic, A. Langeveld, R. Jayawardhana. The image is available here.

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Theoretical Rotational and Vibrational Investigation of Oxygen-Functionalized Interstellar PAHs

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Oxygen-functionalized polycyclic aromatic hydrocarbons (OPAHs) with OH, CHO, and CO side groups can form in the interstellar medium (ISM) mainly through the UV irradiation of PAHs in water ice. Inspired by the detection of nitrogen-containing PAHs in the ISM, this study uses highly accurate computational techniques to investigate the rotational and vibrational spectra of oxygen-functionalized pyrene derivatives (Py-OH, Py-CHO, Py-HO, and Py-O_2) for comparison with experiments that could aid in their future detection. All four OPAHs exhibit strong dipole moments and rotational lines, observable in denser ISM regions near 12 GHz, 10.2 GHz, 12.6 GHz, and 9.6 GHz, respectively. The strongest IR absorption features are identified at 1179.9 cm^{-1} (8.47 μm) and 1385.0 cm^{-1} (7.22 μm) for Py-OH, 1733.4 cm^{-1} (5.77 μm) for Py-CHO, 1747.7 cm^{-1} (5.72 μm) for Py-HO, and 1613.0 cm^{-1} (6.20 μm) for Py-O_2. The IR features of Py-OH and Py-O_2 exhibit peaks in the CO stretching region around 6.0 μm, while those of Py-CHO and Py-HO are blue-shifted due to anharmonicity from the additional CH bond. This suggests PAHs with CO group and no additional peripheral CH bond better explain the observed 6.0 μm PAH emission. However, to explain the observed PAH emission bands with the OPAHs, a fully emission-cascade treatment is required in the anharmonic IR spectra. The accurate spectral data presented here are crucial for experimental classification and potential interstellar observations.

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https://academic.oup.com/mnras/article/536/4/3357/7919729

The First JWST View of a 30-Myr-old Protoplanetary Disk Reveals a Late-stage Carbon-rich Phase

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We present a JWST MIRI/MRS spectrum of the inner disk of WISE J044634.16−262756.1B (hereafter J0446B), an old (∼34 Myr) M4.5 star but with hints of ongoing accretion. The spectrum is molecule-rich and dominated by hydrocarbons. We detect 14 molecular species (H_2, CH_3, CH_4, C_2H_2, $^{13}CCH_2$, C_2H_4, C_2H_6, C_3H_4, C_4H_2, C_6H_6, HCN, HC_3N, CO_2 and $^{13}CO_2$) and 2 atomic lines ([Ne II] and [Ar II]), all observed for the first time in a disk at this age. The detection of spatially unresolved H_2 and Ne gas strongly supports that J0446B hosts a long-lived primordial disk, rather than a debris disk. The marginal H_2O detection and the high C_2H_2/CO_2 column density ratio indicate that the inner disk of J0446B has a very carbon-rich chemistry, with a gas-phase C/O ratio $\gtrsim$2, consistent with what have been found in most primordial disks around similarly low-mass stars. In the absence of significant outer disk dust substructures, inner disks are expected to first become water-rich due to the rapid inward drift of icy pebbles, and evolve into carbon-rich as outer disk gas flows inward on longer timescales. The faint millimeter emission in such low-mass star disks implies that they may have depleted their outer icy pebble reservoir early and already passed the water-rich phase. Models with pebble drift and volatile transport suggest that maintaining a carbon-rich chemistry for tens of Myr likely requires a slowly evolving disk with $\alpha-$viscosity $\lesssim 10^{-4}$. This study represents the first detailed characterization of disk gas at ∼30 Myr, strongly motivating further studies into the final stages of disk evolution.

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The Astrophysical Journal Letters, in press

https://arxiv.org/abs/2412.05535

Mutual neutralization of C_{60}^{+} and C_{60}^{-} ions: Excitation energies and state-selective rate coefficients

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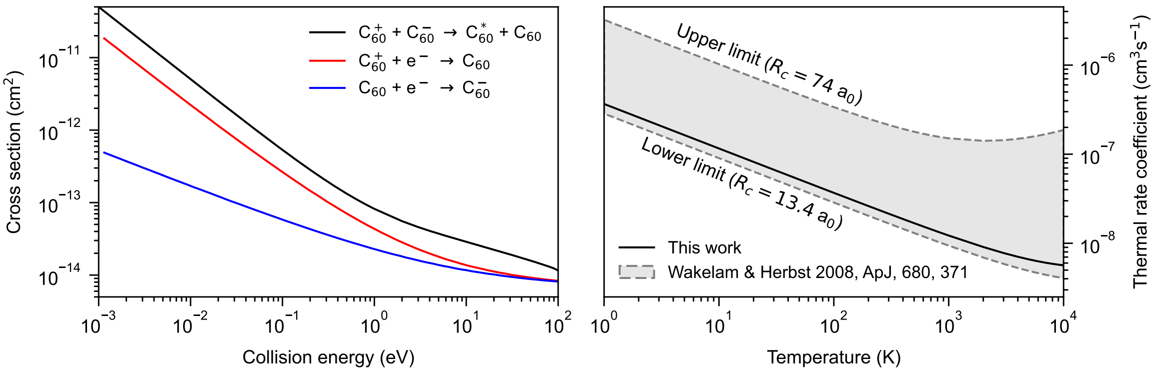
Mutual neutralization (MN) between cations and anions plays an important role in determining the charge balance in certain astrophysical environments. However, empirical data for such reactions involving complex molecular species have been lacking due to challenges in performing experimental studies, leaving the astronomical community to rely on decades-old models with large uncertainties for describing these processes in the interstellar medium. Our aim is to investigate the MN reaction $C_{60}^{+} + C_{60}^{-} \rightarrow C_{60}^{*} + C_{60}$ for collisions at interstellar-like conditions. We studied the MN reaction between C_{60}^{+} and C_{60}^{-} at collision energies of 100 meV using the Double ElectroStatic Ion Ring ExpEriment (DESIREE) and its merged beam capabilities. To aid in the interpretation of the experimental results, semiclassical modeling based on the Landau-Zener approach was performed for the studied reaction. We experimentally identified a narrow range of kinetic energies for the neutral reaction products. Modeling was used to calculate the quantum state-selective reaction probabilities, absolute cross sections, and rate coefficients of these MN reactions, using the experimental results as a benchmark. We compared the MN cross sections with model results for electron attachment to C_{60} and electron recombination with C_{60}^{+}. Our results show that it is crucial to take mutual polarization effects, the finite sizes, and the final quantum states of both molecular ions into account in order to obtain reliable predictions of MN rates expected to strongly influence the charge balance and chemistry in environments such as dense molecular clouds.



Semi-empirical MN cross section (left) and thermal rate coefficient (right) as functions of center-of-mass collision energy and temperature, respectively.

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CO-to-H_2 conversion factor and grain size distribution through the analysis of α_{CO}–q_{PAH} relation

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The CO-to-H_2 conversion factor (α_{CO}) is expected to vary with dust abundance and grain size distribution through the efficiency of shielding gas from CO-dissociation radiation. We present a comprehensive analysis of α_{CO} and grain size distribution for nearby galaxies, using the PAH fraction (q_{PAH}) as an observable proxy of grain size distribution. We adopt the resolved observations at 2 kpc resolution in 42 nearby galaxies, where α_{CO} is derived from measured metallicity and surface densities of dust and H I assuming a fixed dust-to-metals ratio. We use an analytical model for the evolution of H_2 and CO, in which the evolution of grain size distribution is controlled by the dense gas fraction (η). We find that the observed level of q_{PAH} is consistent with the diffuse-gas-dominated model ($\eta = 0.2$) where dust shattering is more efficient. Meanwhile, the slight decreasing trend of observed q_{PAH} with metallicity is more consistent with high-η predictions, likely due to the more efficient loss of PAHs by coagulation. We discuss how grain size distribution (indicated by q_{PAH}) and metallicity impact α_{CO}; we however did not obtain conclusive evidence that the grain size distribution affects α_{CO}. Observations and model predictions show similar anti-correlation between α_{CO} and 12+log(O/H). Meanwhile, there is a considerable difference in how resolved α_{CO} behaves with q_{PAH}. The observed α_{CO} has a positive correlation with q_{PAH}, while the model-predicted α_{CO} does not have a definite correlation with q_{PAH}. This difference is likely due to the limitation of one-zone treatment in the model.

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Pinpointing the CN stretch frequency of neutral cyano-polycyclic aromatic hydrocarbons: a laboratory and quantum chemical spectroscopic study of 9-cyanoanthracene

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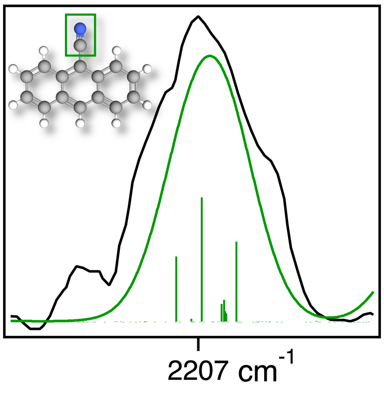
The CN stretch frequency of neutral, gas-phase 9-cyanoanthracene is 2207 cm^{-1} (4.531 µm) based on high-resolution infrared absorption experiments coupled with a new hybrid anharmonic quantum chemical methodology. A broad band (full-width at half-maximum of 47 cm^{-1}) is observed and assigned to multiple transitions, including the CN stretch fundamental and various combination bands that gather intensity from strong anharmonic coupling with the bright CN stretch. The new hybrid computational approach utilizes the harmonic force constants from the double-hybrid rev-DSDPBEP86 functional that includes MP2 electron correlation, and the cubic and quartic force constants from the B3LYP density functional. In combination, this method computes a band center of 2207 cm^{-1} for 9-cyanoanthracene, a direct match with experiment. Further, the hybrid method produces a difference of less than 1 cm^{-1} for both isomers of cyanonaphthalene and cyanobenzene. As shown from comparison with CCSD(T)-F12b anharmonic frequency computations of cyanobenzene, inclusion of electron correlation is required to properly characterize the electronic structure of the highly electron withdrawing CN group on polycyclic aromatic hydrocarbons. In agreement with earlier studies, computation of the CN stretch of 14 small CN-PAHs produces a narrow (∼20 cm^{-1}) band from 2207 - 2229 cm^{-1} (4.53 - 4.48 µm). The remainder of the spectrum below 2000 cm^{-1} and from 3000 - 3120 cm^{-1} shows good agreement between experiment and the hybrid theory with a mean absolute error of 16 and 14 cm^{-1}, respectively.



Experimental (black) and rev-DSDPBEP86/jun-cc-pVTZ + B3LYP/N07D hybrid (green) anharmonic absorption spectra of the CN stretch feature in 9-cyanoanthracene.

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The EDIBLES survey IX: Simulations of the λ6614 DIB profile variations: a surprising connection with CH$^+$

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The profiles of several diffuse interstellar bands (DIBs) show substructures that resemble unresolved rotational bands of electronic transitions of large molecules. Their profiles show clear variations along lines of sight probing different physical conditions. Analysis of variations in such profiles can constrain the sizes and geometries of the DIB carriers and the physical conditions of the interstellar environments in which they reside. We investigate the properties of rotational band contours for perpendicular transitions in planar, oblate symmetric top molecules and compare such contours to the observed profile of the λ6614 DIB. We examine the shapes of the profiles as a function of the model parameters: the rotational constant B in the ground state, the relative change in the rotational constant of the excited state ΔB, the Coriolis coupling constant ζ, the rotational excitation temperature T$_{\rm rot}$ and line width σ. We determine which parameters can reproduce the overall triple-peak profile of the λ6614 DIB as well as the variations across different lines of sight. We find that the substructures in the λ6614 DIB can be reproduced with an oblate top with rotational constant $B = (2.2 \pm 1.8) \times 10^{-3}$ cm^{-1}, $\Delta B = (-7.2 \pm 0.4) \times 10^{-2}$%, and Coriolis coupling constant $\zeta = (2.9 \pm 0.1) \times 10^{-1}$ cm^{-1}. Thus, if the λ6614 DIB carrier conforms to an oblate symmetric top geometry, it is most likely to be a $\sim$54 C atom molecule. The profile variations correspond to changes in the rotational temperature from 81 to 92 K. We furthermore find that the intrinsic line width is a key parameter for each sightline, and requires a range from 0.14 to 0.21cm^{-1} (or 2.8 to 4.2 kms^{-1}) across our sample to reproduce the observations. The intrinsic line width of the λ6614 DIB correlates with the width of the CH$^+$ lines, suggesting an origin in the same environment. We conclude that the λ6614 DIB carrier resides in the same hot gas at low density that is probed by CH$^+$.

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Dust-extinction-curve Variation in the Translucent Interstellar Medium Is Driven by Polycyclic Aromatic Hydrocarbon Growth

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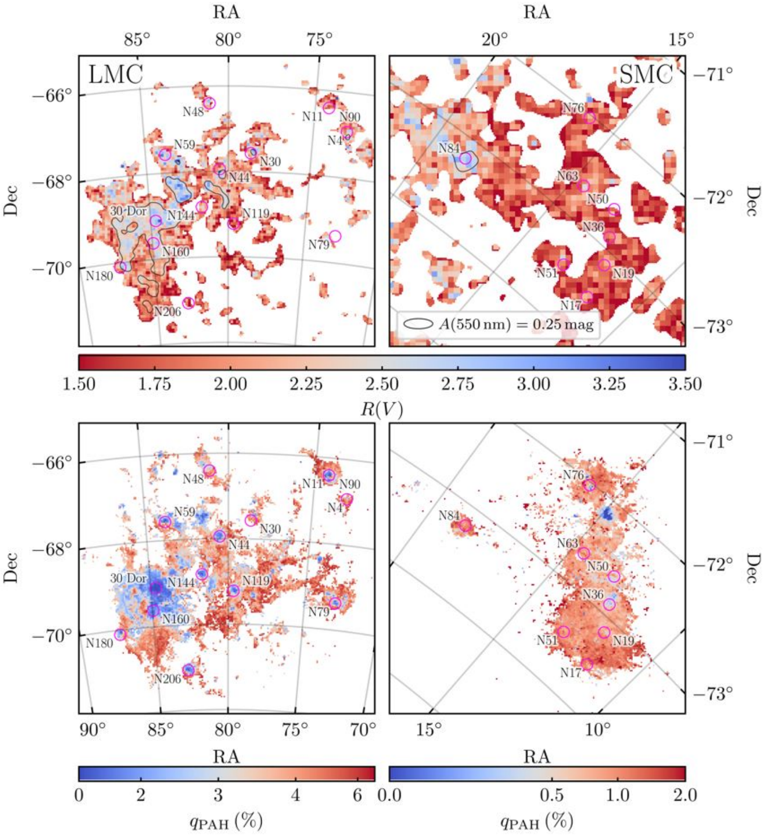
The first all-sky, high-resolution, 3D map of the optical extinction curve of the Milky Way (Zhang & Green 2024) revealed an unexpected steepening of the extinction curve in the moderate-density, "translucent" interstellar medium (ISM). We argue that this trend is driven by growth of the total mass of polycyclic aromatic hydrocarbons (PAHs) through gas-phase accretion. We find a strong anti-correlation between the slope of the optical extinction curve – parameterized by $R(V)$ – and maps of the PAH mass fraction (relative to the total dust mass) – parameterized by $q_{\rm PAH}$ – derived from infrared emission. The range of observed $q_{\rm PAH}$ indicates PAH growth by a factor of $\sim$2 between $A_V \simeq 1$ and 3. This implies a factor-of-two stronger 2175 Å feature, which is sufficient to lower $R(V)$ by the observed amount. This level of PAH growth is possible given rapid accretion timescales and the depletion of carbon in the translucent ISM. Spectral observations by JWST would provide a definitive test of this proposed explanation of $R(V)$ variation.



2D $R(V)$ distribution of LMC and SMC is shown in the top panels. PAH mass fraction ($q_{\rm PAH}$) distribution (Chastenet et al. 2019) is in the bottom panels. $R(V)$ is generally higher when PAH mass fraction is lower. Dense dust clouds are labeled in magenta circles indicated by H II (Lopez et al. 2014).

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https://iopscience.iop.org/article/10.3847/2041-8213/ada28f

PAH Feature Ratios Around Stellar Clusters and Associations in 19 Nearby Galaxies

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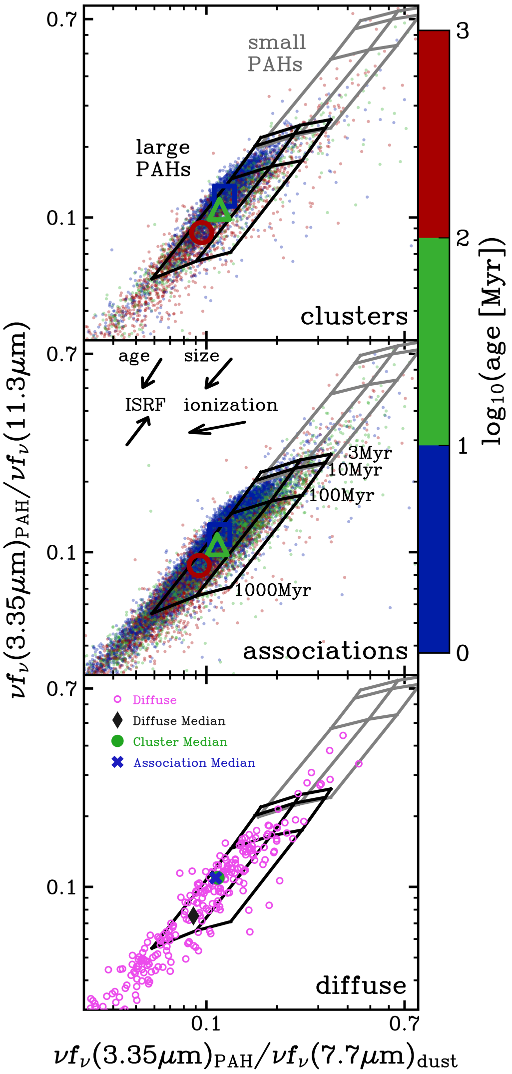
We present a comparison of observed polycyclic aromatic hydrocarbon (PAH) feature ratios in 19 nearby galaxies with a grid of theoretical expectations for near- and mid-infrared dust emission. The PAH feature ratios are drawn from Cycle 1 JWST observations and are measured for 7 224 stellar clusters and 29 176 stellar associations for which we have robust ages and mass estimates from HST five-band photometry. Though there are galaxy-to-galaxy variations, the observed PAH feature ratios largely agree with the theoretical models, particularly those that are skewed toward more ionized and larger PAH size distributions. For each galaxy we also extract PAH feature ratios for 200 pc-wide circular regions in the diffuse interstellar medium, which serve as a non-cluster/association control sample. Compared to what we find for stellar clusters and associations, the 3.3μm/7.7μm and 3.3μm/11.3μm ratios from the diffuse interstellar medium are $\sim 0.10 - 0.15$ dex smaller. When the observed PAH

feature ratios are compared to the radiation field hardness as probed by the [OIII]/Hβ ratio, we find anti-correlations for nearly all galaxies in the sample. These results together suggest that the PAH feature ratios are driven by the shape and intensity of the radiation field, and that the smallest PAHs—observed via JWST F335M imaging—are increasingly ‘processed’ or destroyed in regions with the most intense and hard radiation fields.



Continuum-subtracted flux ratios for stellar clusters in all 19 PHANGS-JWST Cycle 1 galaxies. The small data points are colored according to their ages as quantified in the color bar. The large open symbols indicate the median values for each age bin. Overlaid tracks are included for select subsets of the synthetic ratios extracted from the dust emission models of Draine et al. (2021), and the general trends for these tracks are indicated with the inset arrows/descriptions. The grey and black tracks are for small ($a_{01} = 3$ Å) and large ($a_{01} = 5$ Å) modeled PAH distributions, respectively, with both assuming `logU=0`, `ion=0,1,2`, and `age=3,10,100,1000` Myr. Middle: Using stellar associations instead of compact clusters. Bottom: Individual diffuse regions along with the median values for clusters, associations, and diffuse regions.

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https://iopscience.iop.org/article/10.3847/1538-3881/ada89f

PHANGS-ML: the universal relation between PAH band and optical line ratios across nearby star-forming galaxies

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The structure and chemistry of the dusty interstellar medium (ISM) are shaped by complex processes that depend on the local radiation field, gas composition, and dust grain properties. Of particular importance are Polycyclic Aromatic Hydrocarbons (PAHs), which emit strong vibrational bands in the mid-infrared, and play a key role in the ISM energy balance. We recently identified global correlations between PAH band and optical line ratios across three nearby galaxies, suggesting a connection between PAH heating and gas ionization throughout the ISM. In this work, we perform a census of the PAH heating – gas ionization connection using $\sim$700,000 independent pixels that probe scales of 40–150 pc in nineteen nearby star-forming galaxies from the PHANGS survey. We find a universal relation between $\log$PAH(11.3 μm/7.7 μm) and $\log$([SII]/Hα) with a slope of ~0.2 and a scatter of ~0.025 dex. The only exception is a group of anomalous pixels that show unusually high (11.3 μm/7.7 μm) PAH ratios in regions with old stellar populations and high starlight-to-dust emission ratios. Their mid-infrared spectra resemble those of elliptical galaxies. AGN hosts show modestly steeper slopes, with a ~10% increase in PAH(11.3 μm/7.7 μm) in the diffuse gas on kpc scales. This universal relation implies an emerging simplicity in the complex ISM, with a sequence that is driven by a single varying property: the spectral shape of the interstellar radiation field. This suggests that other properties, such as gas-phase abundances, gas ionization parameter, and grain charge distribution, are relatively uniform in all but specific cases.

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Polycyclic Aromatic Hydrocarbons as an Extraterrestrial Atmospheric Technosignature

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Polycyclic aromatic hydrocarbons (PAHs) are prevalent in the Universe and interstellar medium but are primarily attributed to anthropogenic sources on Earth, such as fossil fuel combustion and firewood burning. Drawing upon the idea of PAHs being suitable candidates for technosignatures, we investigate the detectability of those PAHs that have available absorption cross sections in the atmospheres of Earth-like exoplanets (orbiting G-type stars at a distance of 10 pc) with an 8 m mirror of the Habitable Worlds Observatory (HWO). Specifically, we focus on Naphthalene, Anthracene, Phenanthrene, and Pyrene. Our simulations indicate that under current-Earth-like conditions, detecting PAH signatures between 0.2 and 0.515 µm is infeasible. To account for the historical decline in PAH production post the industrial revolution, we explore varying PAH concentrations to assess instrumental capabilities of detecting civilizations resembling modern Earth. We also evaluate telescope architectures (6 m, 8 m, and 10 m mirror diameters) to put our results into the context of the future HWO mission. With these four molecules, PAH detection remains infeasible, even at concentrations 10 times higher than current levels. While larger mirrors provide some advantages, they fail to resolve the spectral signatures of these molecules with significant signal-to-noise ratios. The UV absorption features of PAHs—caused by π-orbital $\rightarrow$ π*-orbital electronic transitions—serve as valuable markers, due to their distinct and detectable nature, preserved by the aromatic stability of PAHs. Additional lab measurements are necessary to gather absorption cross-sectional data beyond UV for more abundant PAHs. This may help further in improving the detectability of these molecules.

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Polycyclic aromatic hydrocarbons in exoplanet atmospheres I. Thermochemical equilibrium models

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Context. Polycyclic aromatic hydrocarbons, largely known as PAHs, are widespread in the Universe and have been identified in a vast array of astronomical observations, from the interstellar medium to protoplanetary disks. They are likely to be associated with the chemical history of the Universe and the emergence of life on Earth. However, their abundance on exoplanets remains unknown.

Aims. We aim to investigate the feasibility of PAH formation in the thermalized atmospheres of irradiated and non-irradiated hot Jupiters around Sun-like stars.

Methods. To this aim, we introduced PAHs in the 1D, self-consistent forward modeling code petitCODE. We simulated a large number of planet atmospheres with different parameters (e.g., carbon to oxygen ratio, metallicity, and effective planetary temperature) to study PAH formation. By coupling the thermochemical equilibrium solution from petitCODE with the 1D radiative transfer code, petitRADTRANS, we calculated the synthetic transmission and emission spectra for irradiated and non-irradiated planets, respectively, and explored the role of PAHs in planet spectra.

Results. Our models show strong correlations between PAH abundance and the aforementioned parameters. In thermochemical equilibrium scenarios, an optimal temperature, elevated carbon to oxygen ratio, and increased metallicity values are conducive to the formation of PAHs, with the carbon to oxygen ratio having the largest effect.

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Polycyclic Aromatic Hydrocarbon and the Ultraviolet Extinction Bump at the Cosmic Dawn

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First detected in 1965, the mysterious ultraviolet (UV) extinction bump at 2175 Å is the most prominent spectroscopic feature superimposed on the interstellar extinction curve. Its carrier remains unidentified over the past six decades ever since its first detection, although many candidate materials have been proposed. Widely seen in the interstellar medium (ISM) of the Milky Way as well as several nearby galaxies, this bump was recently also detected by the James Webb Space Telescope (JWST) at the cosmic dawn in JADES-GS-z6-0, a distant galaxy at redshift $z \approx 6.71$, corresponding to a cosmic age of just 800 million years after the Big Bang. Differing from that of the known Galactic and extragalactic interstellar sightlines which always peak at $\sim$2175 Å, the bump seen at $z \approx 6.71$ in JADES-GS-z6-0 peaks at an appreciably longer wavelength of $\sim$2263 Å and is the narrowest among all known Galactic and extragalactic extinction bumps. Here we show that the combined electronic absorption spectra quantum-chemically computed for a number of polycyclic aromatic hydrocarbon (PAH) molecules closely reproduce the bump detected by JWST in JADES-GS-z6-0. This suggests that PAH molecules have already been pervasive in the Universe at an epoch when asymptotic giant branch stars have not yet evolved to make dust.

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http://arxiv.org/abs/2502.08113
https://www.aanda.org/articles/aa/abs/2025/02/aa52372-24/aa52372-24.html

What causes the ultraviolet extinction bump at the cosmic dawn?

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The enigmatic ultraviolet (UV) extinction bump at 2175 Å, the strongest spectroscopic absorption feature superimposed on the interstellar extinction curve, has recently been detected at the cosmic dawn by the James Webb Space Telescope (JWST) in JADES-GS-z6-0, a distant galaxy at redshift $z \approx 6.71$, corresponding to a cosmic age of just 800 million years after the Big Bang. Although small graphite grains have historically long been suggested as the carrier of the 2175 Å extinction bump and graphite grains are expected to have already been pervasive in the early Universe, in this work we demonstrate that small graphite grains are not responsible for the UV extinction bump seen at the cosmic dawn in JADES-GS-z6-0, as the extinction bump arising from small graphite grains is too broad and peaks at wavelengths that are too short to be consistent with what is seen in JADES-GS-z6-0.

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Monthly Notice of Royal Astronomical Society Letters, **535**, L58-L62 (2024)

http://arxiv.org/abs/2502.08112
https://academic.oup.com/mnrasl/article/535/1/L58/7815911

Molecular gas stratification and disturbed kinematics in the Seyfert galaxy MCG-05-23-16 revealed by JWST and ALMA

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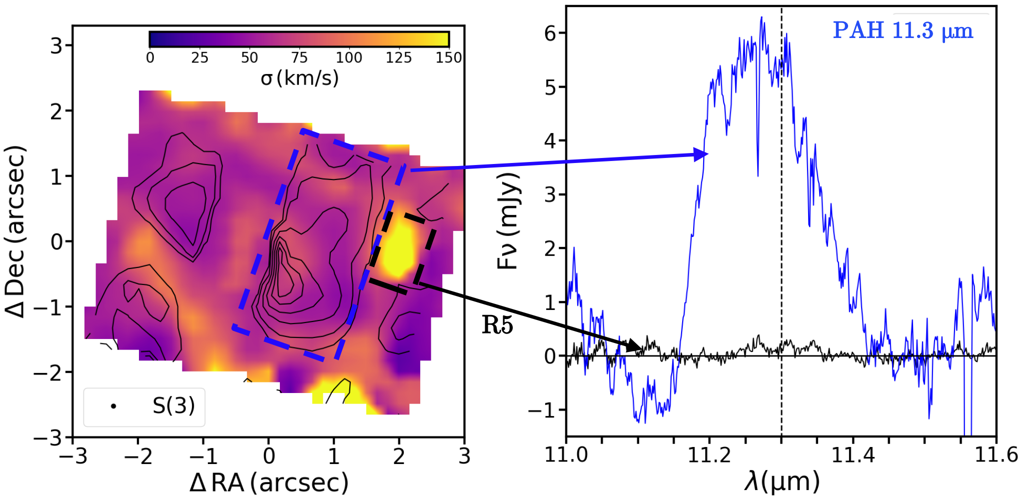
Understanding the processes that drive the morphology and kinematics of molecular gas in galaxies is crucial for comprehending star formation and, ultimately, galaxy evolution. Using data from the Galactic Activity, Torus and Outflow Survey (GATOS) obtained with the *James Webb* Space Telescope (JWST) and the archival data from the Atacama Large Millimeter/submillimeter Array (ALMA), we study the behavior of the warm molecular gas at temperatures of hundreds of Kelvin and the cold molecular gas at tens of Kelvin in the galaxy MCG$-$05$-$23$-$16, which hosts an active galactic nucleus (AGN). *Hubble* Space Telescope (HST) images of this spheroidal galaxy, classified in the optical as S0, show a dust lane resembling a nuclear spiral and a surrounding ring. These features are also detected in CO(2$-$1) and H_2, and their morphologies and kinematics are consistent with rotation plus local inward gas motions along the kinematic minor axis in the presence of a nuclear bar. The H_2 transitions 0-0 S(3), 0-0 S(4), and 0-0 S(5), which trace warmer and more excited gas, show more disrupted kinematics than 0-0 S(1) and 0-0 S(2), including clumps of high velocity dispersion (of up to $\sim$160 km s^{-1}), in regions devoid of CO(2$-$1). The kinematics of one of these clumps, located $\sim$350 pc westward of the nucleus, are consistent with outflowing gas, possibly driven by localized star formation traced by polycyclic aromatic hydrocarbon emission at 11.3 μm. Overall, we observe a stratification of the molecular gas, with the colder gas located in the nuclear spiral, ring, and connecting arms, and most of the warmer gas with a higher velocity dispersion filling the inter-arm space.



Comparison of H_2 0-0 S(3) velocity dispersion map and 11.3 μm PAH feature. The left panel shows the H_2 0-0 S(3) velocity dispersion map with contours of the 11.3 μm PAH feature overlaid in black. The right panel shows the profiles of the 11.3 μm PAH feature extracted from the regions indicated in the left panel.

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https://ui.adsabs.harvard.edu/link_gateway/2025A&A...693A.174E/arxiv:2411.12398

Perturbing Pentalene: Aromaticity and Antiaromaticity in a Non-alternant Polycyclic Aromatic Hydrocarbon and BN-heteroanalogues

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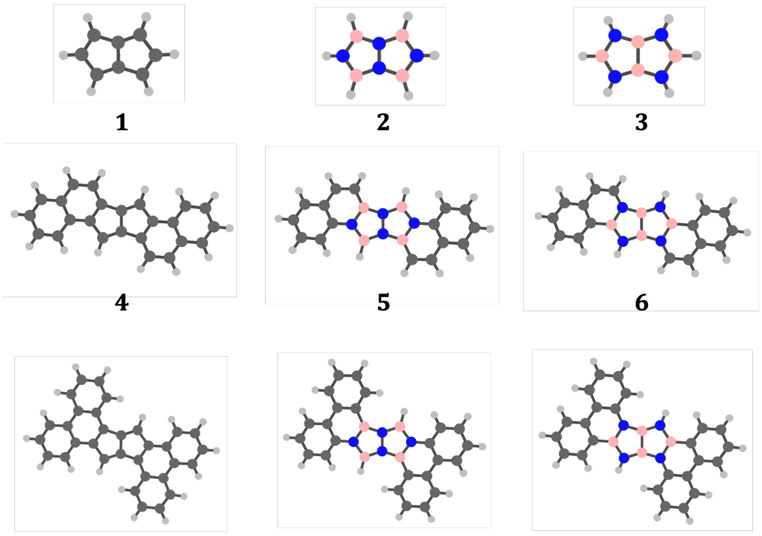
Pentalene (C_8H_6) and NN- and BB-bridged heterocyclic analogues $(BN)_4H_6$, derived by replacement of perimeter CC pairs with BN, are taken as paradigms for tuning of ring-current (anti)aromaticity by variation of π charge, electronegativity and substitution pattern. *Ab initio* calculation of maps for the π current density induced in these model systems by a perpendicular external magnetic field exhibits the full range of tropicity, from diatropic aromatic to nonaromatic to paratropic antiaromatic, with a ready rationalisation in terms of an orbital model. Further calculations on systems of varying charge in which these motifs are embedded in extended PAH systems with naphthalene and phenanthrene 'clamps' show promise for switching between current patterns and related opto-electronic properties. Particular sensitivity to charge is found for the experimentally accessible NN-bridged heteropentalene hybrids.



1 **2** **3**

4 **5** **6**

7 **8** **9**

*Molecular graphs of the systems studied; pentalene (**1**) and the two $B_4N_4H_6$-isosteres with minimum edge frustration, NN-frustrated **2** and BB-frustrated **3** (top row). Extended π frameworks that incorporate (hetero)pentalenes are shown in the middle and bottom row. In the colour scheme for atoms, H is grey, C is charcoal, N is blue, and B is pink.*

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3rd COST NanoSpace Joint Scientific Meeting 1st Announcement

Kaunas, Lithuania
13 - 15 May, 2025

https://nanospace.ktu.edu/

General Action Scope:

The main aim and objective of the COST Action NanoSpace (”Carbon molecular nanostructures in space”; CA21126) is to advance the fundamental understanding of the physics and chemistry of cosmic carbon nanomaterials (nanocarbons; nC) and their relevance in non-terrestrial environments by promoting the interdisciplinary combination of state-of-the-art astronomical, laboratory, and theoretical studies, among others.

The main scientific challenges are the following:

* What nanocarbon species are present in space and how can we identify them? * What are the chemical pathways that lead to their formation and destruction? * What is the role of nanocarbon species in non-terrestrial environments? This is in cosmic and in prebiotic chemistry (astrobiology) and in astrophysics.

In order to attack the scientific challenge, NanoSpace proposes an interdisciplinary approach, combining the expertise from a wide range of disciplines like observational astronomy, laboratory astrophysics, astrobiology, theoretical chemistry, synthetic chemistry, molecular reaction dynamics, material science, spectroscopy, graph theory, and data science (AI, big data). The ambitious interdisciplinary nature of NanoSpace has the advantage that nanocarbons have potential applications in nanotechnology. Researchers and innovators from all these fields are thus welcome to participate both in the meeting and in the Action (see below).

NanoSpace takes advantage of the recent successful operation of the James Webb Space Telescope (JWST), the new facilities that can better mimic the interstellar medium (ISM) on the ground as well as the recent developments in the computational facilities and in laboratory techniques.

The Action is organized in four interdisciplinary Working Groups (WG):

- WG 1: ”The Cosmic Inventory of nanocarbons”.
- WG 2: ”Processing, reactivity and relaxation pathways of nC”.

- WG 3: ”Role and Importance of nC in Non-Terrestrial Environments”.
- WG 4: ”Impact, Inclusiveness and Outreach”.

Specific 3rd Action Meeting Scope:

The 3rd Action Joint Meeting will be focussed on the fundamental and applied research of diverse carbon molecular nanostructures (fullerenes, graphene, carbon nanotubes, and their derivatives) in the context of space science and exploration. The meeting will attack key questions on the formation, properties, and potential applications of these nanocarbon materials under space conditions. Another key nanocarbon topics for discussion will include: i) Formation and Characterization; ii) Space Radiation and Stability; iii) Astrobiology and Planetary Science; iv) Applications in Space Technology; and v) Laboratory Studies.

This is the third NanoSpace Joint Scientific Meeting (in person), which will consolidate the interaction and collaboration among the diversity of disciplines (laboratory astrophysics, theoretical chemistry and physics, astronomy, among others) and researchers present in the Action. The program will be composed by scientific sessions separated by topic, with special attention to the Action progress and scientific results.

Deadline for registration (free) and abstract submission: 5th April 2025

Organizing committee (LOC/SOC):

Dr. Rasa Kandrotaitė Janutienė
Dr. Laura Gegeckienė
Dr. Ingrida Venytė
Dr. Darius Mažeika
Dr. Domingo Anibal García Hernández, Instituto de Astrofísica de Canarias, Spain
Prof. Eleanor Campbell, University of Edinburgh, Scotland
Dr. Chris Ewels, CNRS – Institut des Materiaux Jean Rouxell, France
Dr. Polona Umek, Jozef Stefan Institute, Slovenia
Dr. Dogan Erbahar, Dogus University, Turkey
Dr. Alicja Domaracka, CNRS – CIMAP, France
Dr. Ko-Ju Chuang, Leiden University, Netherlands

The Action NanoSpace in the internet:
https://research.iac.es/proyecto/nanospace/

The Action NanoSpace in the COST website:
https://www.cost.eu/actions/CA21126/

Apply to join the COST Action NanoSpace:
https://www.cost.eu/actions/CA21126/#tabs+Name:Working%20Groups%20and%20Membership

Final note: Please check the meeting website for news and updates about the final list of invited speakers, hotel registration links, etc. More detailed information will be given in a second announcement.

E-mail for contact: nanospace@ktu.edu

Mini-Symposium on Astrochemistry

Laboratory, Computations, and Observations

at the International Symposium on Molecular Spectroscopy (ISMS)
Champaign-Urbana, Illinois

23 - 27 June, 2025

https://isms.illinois.edu

Organized by: Brett McGuire (MIT), Laurent Margulés (Université de Lille), Marie-Aline Martin-Drumel (Université Paris Saclay, CNRS), Arielle Moullet (NRAO)

We want to draw your attention to this year's International Symposium on Molecular Spectroscopy (ISMS) where we have organized a mini-symposium entitled:

"Astrochemistry - Laboratory, Computations, and Observations."

With the forthcoming explosion in observational data driven by the bandwidth upgrades from the ALMA Wideband Sensitivity Upgrade (WSU) and ngVLA in particular, it is more important than ever that the laboratory, computational, and observational communities come together. This mini-symposium aims to get all areas of astrochemistry talking to best understand the landscape of needs so we can coordinate our limited resources to maximum effect in the face of this new era. All areas of astrochemical research are welcomed, across all wavelength ranges, including laboratory, observational, and computational work.

Whether you have never been to ISMS before, haven't been in a while, or are a regular attendee, we highly encourage you to join us. ISMS is known as an extremely collegial and relaxed environment with a strong emphasis on informal discussion and collaboration as well as being a welcoming and accessible environment for students to give their first (and second, and third, and ...) talks. Registration and housing costs for students in particular are extremely economical, and the meeting is known to be one of the most accessible and affordable in general.

Abstract submission is open now and closes March 1st.

More information is available on the ISMS website: isms.illinois.edu

We hope to see you there!

Announcements

Postdoc position in Molecular Physics / Physical Chemistry / Laboratory Astrophysics

Advertised by Otto Dopfer

A postdoctoral position for up to five years is available in the laser molecular spectroscopy group of Otto Dopfer at the Berlin Institute of Technology (TU Berlin), Germany.

The predominantly experimental research of our group involves the laser spectroscopic, mass spectrometric, and quantum chemical investigation of molecules, radicals, ions, clusters, and nanostructures in the gas phase, with strong relevance to a broad range of interdisciplinary topics ranging from materials science to biophysics, catalysis, astrochemistry, environmental chemistry, and plasma physics.

Available equipment includes a variety of pulsed and tuneable IR and UV lasers, several ion sources and cryogenic rf-traps, as well as several types of tandem mass spectrometers. The group is also strongly involved in international collaborations with groups in Japan, France, USA, Taiwan, and has been a regular user of the IR free electron laser facilities CLIO (France), FELIX (Netherlands), and more recently the FHI-FEL (Berlin).

Qualified candidates for the postdoc position hold a PhD in Physics, Physical Chemistry, or related fields with a strong publication record and ideally already some initial postdoctoral experience (all in experimental science) which is not substantially longer than 5 years.

The successful candidate will be involved in supervising PhD and undergraduate students, will take high responsibility for several existing research projects, and will be strongly involved in developing new research directions (i.e. writing proposals). The position is ideal for candidates who are pursuing an academic career (with possibility for Habilitation) by developing also their own research interests. The position is funded by TU Berlin and involves also teaching duties in the area of Experimental (mostly Molecular) Physics (either in German or in English).

Experience in several of the following fields is mandatory:

1. laser spectroscopy, mass spectrometry, ion sources and traps, cluster science
2. vacuum, optics, data acquisition, construction of apparatus
3. writing of publications, reports, and proposals
4. strong communication and presentation skills

Interested and highly qualified candidates are encouraged to send their application (in a single pdf file) to Prof. Otto Dopfer (dopfer@physik.tu-berlin.de), including a cover letter, a CV (including a list of publications), a statement of qualifications relevant for the position (max. 1 page), a statement of research interests (max. 1 page) as well as names and complete addresses of two referees.

Evaluation of the applications will begin at April 13 (2025) and will continue until the position is filled. The desired starting date is as soon as possible but is negotiable to some extent.

Berlin is an international city and offers an exciting scientific and cultural environment.

Deadline: April 13, 2025

E-mail for contact: dopfer@physik.tu-berlin.de

Webpage: https://www.tu.berlin/en/lmsu

AstroPAH Newsletter

http://astropah-news.strw.leidenuniv.nl
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astropah@strw.leidenuniv.nl
Submission deadline: 7 March 2025