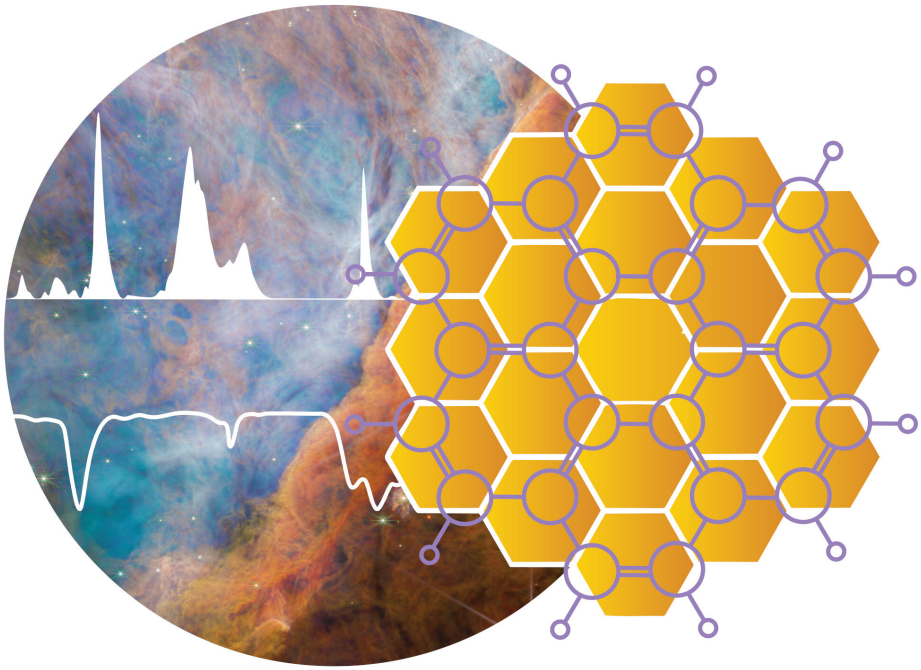
Exploring the Aromatic Universe in the JWST era

July 6–10, 2026

Western University
London, Ontario, Canada



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Abstract Book

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1 Talks

1.1 Illuminating the Aromatic Universe **[I]**

***Alessandra Candian**, University of Amsterdam*

We are living in exciting times for the study of aromatic molecules in space. The launch of the James Webb Space Telescope in 2021 has opened an unprecedented window into the infrared universe, enabling observations of the emission from polycyclic aromatic hydrocarbons (PAHs), fullerenes, and related species with remarkable sensitivity and spatial resolution.

Together with state-of-the-art theoretical and laboratory models, these observations now allow us to characterize aromatic molecules across a wide range of spatial scales—from star-forming regions in galaxies to nearby protoplanetary disks—and to investigate their lifecycle in diverse astrophysical environments. At the same time, small aromatic molecules have been identified through radioastronomical observations in cold molecular clouds, effectively settling the long-standing question of whether PAHs can exist in such environments.

Yet this wealth of new data has also revealed how much remains to be understood about the aromatic universe. In this talk, I will provide a high-level overview of our current knowledge of aromatic molecules in space and highlight key interdisciplinary questions that must be addressed by the community to understand the lifecycle of PAHs and their broader role in the Universe.

1.2 Spectroscopic Signatures of PAHs in Astrophysical Environments **[I]**

***Alexandros Maragkoudakis**, NASA Ames Research Center*

Spectroscopic signatures of polycyclic aromatic hydrocarbons (PAHs) provide much of our understanding of the carbon cycle in space and the physical and chemical conditions of the interstellar medium. As dominant carriers of the ubiquitous aromatic infrared bands, PAHs trace energy balance, local ionization conditions, and molecular evolution across a wide range of astrophysical environments. This talk surveys how infrared spectroscopy—now transformed by JWST's sensitivity and resolution—sheds light on the vibrational, structural, and environmental diversity of PAHs. I will outline our current understanding of the major aromatic and aliphatic bands, the assignment of key vibrational modes, and the spectral distinctions between pure PAHs, functionalized and heteroatom-substituted species, deuterated analogs, and the population of very small grains that bridges the molecular–solid-state boundary. I will examine how these signatures vary within individual objects and across environments, from diffuse clouds and PDRs to disks, evolved stars, and external galaxies, and what these variations imply about PAH size, charge, structure, and processing history.

1.3 PDRs4All: Decoding PAH and Very Small Grain signatures in the Orion Bar

***Baria Khan** (1); Ben Abbott (2); Samuel Alejandro Daza Rodríguez (1); Els Peeters (1); Alexander Tielens (3); Takashi Onaka (4); Jan Cami (1); Bethany Schefter (1); PDRs4All team*
(1) Western University, (2) Durham University, (3) University of Maryland, (4) University of Tokyo

Polycyclic aromatic hydrocarbons (PAHs) dominate the IR emission of many cosmic environments through aromatic infrared bands (AIBs) and play an important role in the energy balance and chemistry of the interstellar medium. Owing to the superb capability of JWST, we can now trace, for the first time, the PAH molecular properties in exquisite detail across the full transition from ionized to molecular gas.

We present MIRI MRS observations of the photodissociation region (PDR) the Orion Bar from the PDRs4All program. Analysis of the 6.2, 7.7, 8.6, and 11.0 μm AIBs reveals two groups tracing distinct PAH populations. The 6.2 and 7.7 μm AIBs trace medium-sized PAH cations, while the 8.6 and 11.0 μm AIBs arise from larger, compact PAH cations. These relations establish the 6.2/8.6

and 7.7/8.6 ratios as new diagnostics of PAH size, while the 6.2/11.2 ratio robustly traces the PAH ionization fraction.

The 10–15 μm AIBs probe molecular edge structures through the CH out-of-plane bending modes. PAHs in the Orion Bar are dominated by solo and trio CH groups, while the abundance of duo and quartet CH groups decreases toward the PDR surface, consistent with photolysis of fragile hydrogens. Profile variations in the 11.2 and 12.0 μm AIBs reveal contributions from PAH clusters and very small grains (VSGs), which can be separated from the PAH emission. These fragile carriers undergo photolysis as they are advected toward the PDR surface and exposed to a stronger radiation field.

These results demonstrate how JWST's transformative capabilities unlock a comprehensive picture of PAH photochemical processing in strongly irradiated PDRs — simultaneously revealing charge state, size distribution, molecular structure, and the distinct contribution of very small grains to specific AIBs.

1.4 JWST and ALMA Views of the Orion Bar PDR: Results from the PDRs4All Program **[I]**

Javier Goicoechea *(1); PDRs4All team*
(1) IFF-CSIC

The interaction between UV radiation and interstellar clouds occurs in photodissociation regions (PDRs), where UV photons regulate gas heating, ionization, and chemistry. Aromatic infrared band (AIB) emission—which mainly results from IR fluorescence of UV-pumped PAHs—together with enhanced abundances of simple hydrocarbon radicals, is a robust tracer of this interaction. AIB emission is a distinctive tracer of PDR environments and dominates the IR spectra of many Galactic sources and star-forming galaxies. In this talk, I will summarize the most relevant results from the PDRs4All JWST program on the Orion Bar, the prototypical strongly irradiated PDR and an excellent template and laboratory for spatially resolving the chemical stratification of key carbon carriers as a function of UV radiation attenuation. The observed changes in PAH emission in the Bar suggest that the species responsible for this emission undergo photochemical modifications. In particular, near the strongly irradiated PDR edge, small PAHs are readily destroyed and the aliphatic content of the AIB carriers is reduced. Overall, both bottom-up and top-down processes appear to link simple hydrocarbon radicals with PAHs; however, the exact chemical pathways and their relative contributions remain to be quantified.

1.5 Aromatics and Aliphatics in the JWST-Era **[I]**

Xuejuan Yang *(1,2); Aigen Li (2)*
(1) Xiangtan University, (2) University of Missouri

The so-called "unidentified" infrared emission (UIE) features at 3.3, 6.2, 7.7, 8.6, 11.3 and 12.7 μm, commonly attributed to the stretching and bending vibrations of polycyclic aromatic hydrocarbon (PAH) molecules, are ubiquitously seen in a wide variety of astrophysical regions in the Milky Way and nearby galaxies as well as distant galaxies at redshifts $z \geq 4$. The aliphatic features have been used to explore the chemical structure, and therefore then the properties of the environment of the UIE carriers. While these PAH emission bands are frequently seen in Galactic sources, their detections in extragalactic sources are rare and limited to only several nearby galaxies. I will present the theoretical effort of the PAH modelling, especially regarding the aliphatic features, and report the recent detections of the aliphatic features in our Galaxy and galaxies at redshift $z > 0.2$ by JWST. Finally, I will review the current state and key open questions.

1.6 Spectroscopy of PAHs and Fullerenes: Insights from Laboratory Astrophysics **[I]**

***Christine Joblin**, IRAP, Université de Toulouse, CNRS, CNES*

In the PAH model, gas-phase polycyclic aromatic hydrocarbons (PAHs) are proposed as the smallest interstellar dust particles, absorbing stellar UV radiation and emitting the aromatic infrared bands (AIBs). Despite their central role, no individual PAH has yet been identified through its contribution to the AIBs, UV extinction curve, or diffuse interstellar bands (DIBs).

The PAH model persists due to the photophysical and spectroscopic properties of PAHs, consistent with observations. Support also comes from the detection of C_{60}/C_{60}^+ (a related species) via its AIB and DIB contributions, and the identification of rotational emission from relatively small, substituted PAHs in the cold molecular cloud TMC-1. However, these findings still do not allow the identification of specific PAHs through their AIB or DIB contributions.

This presentation highlights how advances in this field are intrinsically linked to laboratory astrophysics activities, both experimental and theoretical. Spectroscopic techniques have been optimized to span the full range of astrophysically relevant temperatures, from $\sim$10 K (for DIBs) to over 1000 K (for AIBs). Most of them, however, specifically target either neutral or ionized PAHs. Moreover, they can realistically investigate only a limited number of species, while the PAH family is vast and encompasses a very large number of isomeric structures.

To address this challenge, theoretical simulations provide spectral information, though less precise than experimental data, for a wide variety of species. In addition, complementarily, experiments that simulate astrophysical conditions, including PAH formation and evolution upon UV irradiation, can guide these studies by revealing new structures of interest and their unique spectral fingerprints.

1.7 IR spectroscopy of aromatic molecules as predicted by quantum chemistry **[I]**

***Vincent Esposito**, Chapman University*

Through the ability to produce comprehensive vibrational spectra and understand the specific molecular motions that lead to the individual IR emissions bands seen in space, deep insights into the chemical and physical properties of observed environments are now emerging in ways unimaginable a decade ago. In recent years, increased computational power and novel approaches have allowed the inclusion of anharmonicity in PAH IR spectroscopy. The inclusion of these higher-order terms in the vibrational potential has pushed computational accuracy to within 0.5% of experiment for neutral PAHs without the need for empirical scaling factors. This departure from the harmonic framework has also revealed the incredible complexity that exists in the vibrational spectroscopic structure of PAHs due to strong couplings, many concurrent vibrational resonances (Fermi, Darling-Dennison, etc.), and the presence of intense combination band and overtone transitions. Additionally, anharmonicity has proven vital in the accurate vibrational characterization of cyano- and ethynyl-substituted PAHs and has only recently been introduced into the spectral calculations of fullerenes. In this talk, we will take a deep dive into anharmonic quantum chemical computations of PAH IR spectroscopy, detailing what we have learned and what has yet to be uncovered.

1.8 ALPAHCAS: Computing Anharmonic Spectra of Polycyclic Aromatic Hydrocarbons (PAHs) from Absorption to Emission

Lars Reems *(1); Alessandra Candian (1); Evert Rol (1); Vincent Esposito (2); Inga Kamp (3); Wybren Jan Buma (1); Alexander Tielens (4)*
(1) University of Amsterdam, (2) Chapman University, (3) University of Groningen, (4) University of Maryland

With the exquisite spectral resolution of the James Webb Space Telescope (JWST), more sophisticated emission models are required to model PAHs and characterize their astronomical environments, especially models considering important properties such as anharmonicity and resonant interactions. ALPAHCAS (Anharmonic Level calculations of PAH Cascade emission and Absorption Spectra), an open-source package which builds upon code developed by Mackie et al. (2018), can calculate detailed absorption and emission spectra of PAHs based on second-order vibrational perturbation theory applied to Density Functional Theory (DFT) Quartic Force Fields. To assess the quality of our DFT calculations, we performed a benchmark of different model chemistries against the experimental absorption spectrum of cold pyrene cation obtained at the HFML-FELIX (Panchagnula et al., 2020). We find that our optimal model chemistry B3LYP/N07D shows a very good agreement with the experiment, with an absolute average deviation of 3.3 cm^{-1} (relative deviation of 0.047%) and a maximum deviation of 13.8 cm^{-1} (relative deviation of 1.1%). ALPAHCAS is then used to compute the emission spectrum of a sample of PAH cations to look for trends that can help decode their spectral signatures and provide tracers for different properties like PAH size.

This Project is financially supported by the Dutch Astrochemistry Network of the Dutch Research Council (NWO) under grant no. ASTRO.JWST.001.

1.9 PAHs in Galaxies Across Cosmic Time **[I]**

Brandon Hensley*, JPL/Caltech*

Polycyclic aromatic hydrocarbons (PAHs) and other carbonaceous molecules have been observed across the Universe, from our own Galactic backyard to the first billion years after the Big Bang. This talk summarizes PAHs in a galactic context, focusing on the interrelationships between the observational characteristics of PAHs and the properties of their host galaxies, such as star formation rate and metallicity. I will tie together results from theoretical modeling, simulations, and observations, exploring open questions like the emergence of PAHs in the early Universe, the main processes responsible for creating and destroying PAHs, and how the relationship between PAHs, metals, and star formation evolves with cosmic time. Avenues for answering these questions, including new techniques and new observational facilities, will be highlighted. Finally, I will discuss PAHs in the context of their diagnostic power: how can we learn about galaxy properties by studying its observable PAH signatures?

1.10 PAHs, Mid-IR Emission, Gas, and Dust in Nearby Galaxies **[I]**

Adam Leroy *(1); Ryan Chown ; Oleg Egorov ; Jaeyeon Kim ; Hannah Koziol ; Debosmita Pathak ; Karin Sandstrom ; Jessica Sutter ; and The PHANGS Team*
(1) Ohio State University

Over its first four cycles, JWST has conducted a remarkable campaign imaging mid-infrared emission from local galaxies. These images capture emission from PAHs and small dust grains over large areas, and they often overlap studies of the gaseous interstellar medium and stellar population from ALMA, VLT/MUSE, and HST. I will review some of the highlights from these first few years of observations. These include clear evidence of PAH destruction in HII regions, evidence for impact of the shape of the interstellar radiation field on PAH band ratios in diffuse regions. JWST's high resolution and rich filter suite make it possible to distinguish the radiation field (i.e., heating) from column density as drivers of dust emission. This has led to the use of PAH emission to

construct some of the most sensitive, high resolution, wide field maps of the ISM to date, and I will review the promise and potential pitfalls of this approach. Compact, bright dust emission has also emerged as a key tracer of the most embedded, youngest stellar populations, and JWST resolves star forming regions, tracing out the radiative zone of influence of young stellar populations on the surrounding emission. I will highlight some next steps, as well as synergies with detailed Milky Way work and spectroscopy that achieves much more physical detail over more limited areas.

1.11 PAHs trace atomic gas in Local Group galaxies with variations driven by local ISM and dust properties

Devisree Tallapaneni *(1); Adam Leroy (1); Jérémy Chastenet (2); Eric W. Koch (3); Erik Rosolowsky (4); Jiayi Sun (5); Lindsey Hands (6); Harrisen Corbould (4); LGLBS*
(1) The Ohio State University, (2) Ghent University, (3) National Radio Astronomy Observatory, (4) University of Alberta, (5) University of Kentucky, (6) University of California, San Diego

High-spatial-resolution observations of atomic gas are challenging to obtain. However, high-spatial-resolution infrared observations of PAH emission using JWST are now widespread and have been suggested as a way to trace the atomic gas. PAH observations could be a powerful probe of atomic gas structure, but this hypothesis must first be tested in locations where we can map both PAH emission and atomic gas at high resolution. Local Group galaxies M33 and M31 provide ideal testbeds for this analysis. Both are HI dominated over most of their area and, owing to their proximity, enable multiwavelength observations at high physical resolution. Leveraging new VLA HI survey data together with CO observations from IRAM and ALMA, full infrared SED coverage, and PAH observations from Spitzer, SPHEREx, Herschel, and JWST, we show PAH emission does trace atomic gas in these galaxies. We find that PAH and HI emission are correlated at all radii, but that the slope of the relation (and thus the PAH/HI ratio) varies. This means additional, environmental information is needed to use PAH emission to trace atomic gas. After accounting for both atomic and molecular gas, we show for M33 that variations in the PAH/N$_{\rm H}$ ratio can be explained by the underlying dust and ISM physics. In all radial bins, the intensity of the radiation field is the primary factor driving this variation. The dust-to-gas ratio becomes important in the inner galaxy, while the PAH-to-dust fraction contributes at large radii. Given these physically driven variations, we discuss the implications of using PAHs generally as a tracer of atomic gas structure and apply our results to JWST observations of PAH emission from M33 to construct a $\sim$2 parsec resolution map of neutral gas structure.

1.12 Using JWST Photometry to Trace PAH Destruction in HII Regions

Jessica Sutter *(1); The PHANGS Team*
(1) Whitman College

New high-resolution photometry from JWST-MIRI allows us to map the emission of polycyclic aromatic hydrocarbons (PAHs) in exquisite detail. As the PAHs play an important role in regulating heating and electron density in the interstellar medium (ISM), the distribution of the PAHs provides a key indicator of ISM conditions. To better trace PAHs across full galaxy disks, we have developed a MIRI-photometry based proxy for the PAH-fraction of the total dust mass: RPAH. RPAH is defined as the sum of the PAH-tracing F770W and F1130W bands divided by the F2100W band, which traces larger dust grain emission. We present trends in RPAH with galactic radius, metallicity, gas content, and galaxy environment in 19 $D < 20$ Mpc galaxies from the Physics and High Angular resolution in Nearby GalaxieS (PHANGS) JWST sample (Cycle 1 Treasury Program #2107, PI J. Lee). At these distances, JWST is able to resolve individual giant molecular clouds and star forming regions, allowing us to see how the PAH distribution varies across ISM phases. Through comparisons to Hα emission from MUSE, CO emission measured by ALMA, and HI data from the VLA, we find that RPAH is fairly constant across different ISM conditions with the exception of Hα bright star forming regions where RPAH drops significantly. This is evidence of PAH destruction within HII

regions, where hard radiation from young stars destroys these small grains. Outside of the destruction within HII regions, very little impacts the PAH fraction, showing that PAHs are prevalent and evenly distributed throughout the ISM. These observed trends have implications for where we expect PAHs to play a prominent role in heating the ISM, and where these small dust grains are being destroyed by hard radiation fields.

1.13 Infrared Spectroscopy of Aromatics - A Laboratory Perspective **[I]**

***Sandra Brünken**, HFML-FELIX and Radboud University*

The unprecedented spectral resolution, spatial detail, and sensitivity of the JWST are transforming our view of aromatic molecules in space, allowing to reveal subtle variations in the mid-infrared emission bands commonly attributed to polycyclic aromatic hydrocarbons (PAHs), and pointing toward a richer chemical diversity than previously recognized. Interpreting these observations requires comprehensive laboratory spectroscopic data for a broad range of PAH and other aromatic molecules than typically considered. In astrophysical environments, chemical reactions and energetic processing can produce a variety of aromatic structures, including ionized and electronically excited species, molecular fragments, and non-classical PAHs containing pentagonal rings or other structural irregularities formed during reactions and fragmentation processes. Expanding experimental methods to provide spectroscopic data on such diverse classes of aromatics is therefore essential for connecting astronomical observations with specific molecular carriers. This talk presents a laboratory perspective on infrared spectroscopy of PAHs and aromatics in the gas phase. Particular emphasis will be placed on broadband vibrational spectroscopy across the molecular fingerprint region using infrared action spectroscopy with free-electron lasers, with a focus on cationic and anionic PAHs and related species. Studying their anharmonic vibrational structure provides a link from the experimentally measured absorption to the astronomically observed emission spectra. Perspectives on novel action spectroscopic methods will be provided.

1.14 Infrared Spectroscopy of the T1 state of Naphthalene

***Priyanka Arvind Paunikar** (1,2); Hugo Maurer (3,4); Lars Reems (5,4); Alessandra Candian (5,4); Sandra Brünken (1,2); Jos Oomens (1,2); Piero Ferrari (1); Wybren Jan Buma (3,4)*
(1) HFML-FELIX, (2) IMM, Radboud University, The Netherlands, (3) HIMS, (4) University of Amsterdam, The Netherlands, (5) API

Aromatic Infrared Bands (AIBs) reflect the chemical complexity of the interstellar medium (ISM). These bands correspond to IR emission from UV-processed polycyclic aromatic hydrocarbons (PAHs), and arise from the vibrationally hot electronic ground state of various PAHs. In the specific case of neutral PAHs, which have a singlet ground state (S0), this means AIBs originate from S0. However, aromatic molecules like PAHs can also undergo intersystem crossing (ISC) to a triplet state after UV excitation, which in some cases is a dominant route. This suggests some PAHs in the ISM may become trapped in the long-lived T1 state, potentially affecting the interpretation of AIBs. Therefore, spectroscopic information on triplet-state PAHs is needed to assess their contribution to the emission features. While the infrared spectra of neutral PAH in the S0 state are well-studied both computationally and experimentally, IR data for the T1 state remain unavailable. Such data are important for identifying these species and understanding their physicochemical properties. In this work, we address the lack of experimental IR data for neutral PAHs in their T1 state by measuring their spectra. For the first time, we report the triplet-state spectral signatures of neutral naphthalene using FELIX and table-top OPO. The anharmonic frequencies reproduce the fingerprint spectrum well, while larger deviations occur in the 3 μm region. Our results demonstrate a general approach for obtaining triplet-state IR spectra of molecules with efficient ISC, providing measurements that can be used to benchmark and enhance IR emission models. With JWST's improved spatial resolution, these reference spectra will aid in detecting and identifying triplet PAHs in the ISM.

1.15 High resolution rovibrational and rotational spectroscopy of small aromatic ions

Divita Gupta *(1); Weslley GDP Silva (1); Philipp C. Schmid (1); Lise von Rötel (1); Sven Thorwirth (1); Oskar Asvany (1); Stephan Schlemmer (1)*
(1) Universität zu Köln, Germany

High-resolution laboratory spectroscopy of molecular ions provides key reference data for identifying and understanding chemical processes in the interstellar medium. Small aromatic and heteroatom-containing hydrocarbon ions are particularly relevant because they are thought to act as intermediates in the formation of larger organic molecules during the early stages of star and planet formation. However, the spectra of many of these ions remain unknown due to experimental challenges associated with producing, and probing reactive charged species. I will present recent progress in the high-resolution spectroscopy of several small aromatic ions obtained using cryogenic ion-trap instrumentation combined with action spectroscopic techniques. By probing rovibrational and rotational transitions under cold, well-controlled conditions, precise spectroscopic parameters can be derived that enable astronomical searches and improve our understanding of ion chemistry in astrophysical environments.

Using the leak out spectroscopy approach in a cryogenic ion trap, the rovibrational spectra of cyclopropenyl cation (c-$C_3H_3^+$), the deuterated cyclopropenyl cation (c-$C_3H_2D^+$) and azirinyl cation (c-$C_2H_2N^+$) were recorded. Since the latter two possess a permanent dipole moment, these spectra were used to guide pure rotational measurements through IR/mm-wave double resonance for these molecules. Together, these studies demonstrate the capability of modern cryogenic ion-trap spectroscopy to provide the precise laboratory data required for future astronomical detection of small aromatic ions.

1.16 Laboratory Simulation of Dust Formation and Molecular Evolution in Evolved Stars and the Interstellar Medium In the STARDUST facility **[I]**

José Ángel Martín-Gago *(1); Gonzalo Santoro (2)*
(1) ICMM-CSIC, (2) CSIC

Stardust is a unique, advanced ultra-high-vacuum experimental machine designed to reproduce the conditions of the dust-nucleation zone in the inner envelopes of evolved stars. It is based on ultrahigh-vacuum technology and combines gas-aggregation sources with in situ characterization techniques [1]. The chemistry explored in Stardust relies on low-energy gas-phase atomic aggregation, while the densities of the elements under study can be tuned to closely approach those expected in dust-nucleation regions of evolved stars. Stardust provides a high level of control over the molecular species and grains produced, making it a unique platform to investigate the catalytic role of grain surfaces in the formation of new evolved species. In addition, Stardust can mimic key processes involved in the processing and evolution of dust in the interstellar medium.

Our studies have revealed the critical role of molecular hydrogen in this chemistry. I will summarize recent findings on the formation of gas-phase species and dust analogues related to evolved stars, as well as their evolution toward the interstellar medium under hydrogen-rich conditions [2]. In particular, we have shown the formation of carbon grains and carbon clusters composed of highly saturated aliphatic structures [3], the formation of hydrogenated amorphous silicon and silane [4], and the formation of silicon carbide grains, identifying SiC_2 as a key precursor [5]. Finally, we will discuss recent studies on the irradiation of ice analogues under hydrogenated atmospheres, particularly the formation of polyenes through irradiation of alkanes [6].

[1] Sci. Rep.8, 7250 (2018); [2] Rev of Sci. Inst (2020) 91, 12; [3] Nat. Astron. 2019, 4, 97; [5] Nat. Astron. 2026; [6] The Astrophysical J, 2024, 965, 184

1.17 The role of PAHs in the ISM and in planet-forming disks **[I]**

Sílvia Vicente *(1); Els Peeters (2); Alexander Tielens (3); Wing-Fai Thi (4)*
(1) Institute of Astrophysics and Space Sciences (IA) - Faculty of Sciences of Lisbon University (FCUL), (2) Western University, (3) University of Maryland, (4) Institute for Atmospheric Physics at the DLR

Polycyclic Aromatic Hydrocarbons (PAHs) dominate the heating of gas in the neutral interstellar medium (ISM) and in the surface layers of protoplanetary disks directly exposed to far-ultraviolet (FUV) radiation, either from the young parent star or from neighbouring massive OB stars. The FUV photoionisation of PAHs efficiently heats the gas through the ejection of electrons with excess kinetic energy, a mechanism known as the photoelectric effect. In protoplanetary disks, FUV photons and PAH heating strongly contribute to the 2-D physical structure (temperature and density), chemical composition, and evolution of the disk, thereby shaping the physical and chemical environment in which planets may form. The James Webb Space Telescope (JWST), with its groundbreaking angular and spectral resolution and sensitivity, has initiated a golden age for PAH studies in protoplanetary disks. JWST can spatially resolve the Aromatic Infrared Bands (AIBs) at 3.3, 6.2, 7.7, 8.6, 11.3, 11.9, and 12.7 µm, observed in protoplanetary disks and the ISM in nearby star-forming regions (SFRs), enabling the extraction of PAHs abundance, size, and charge distributions on small spatial scales. In this talk, I will summarise the current state of knowledge regarding the role of PAHs in the ISM and in protoplanetary disks, covering both observational and theoretical aspects, with a particular focus on recent JWST discoveries. I will highlight key open questions and discuss perspectives for future research.

1.18 JWST Edge-on Disk Ice (JEDIce): An analysis of PAHs signatures within the disks

Charles Mentzer *(1); Daniel Harsono (1); Jennifer B. Bergner (2); Jennifer A. Noble (3); Emmanuel Dartois (4); Zhi-Yun Li (5); Nicole Arulanantham (6); Korash Assani (5); Lukas Welzel (7); Klaus M. Pontoppidan (8); Maria N. Drozdovskaya (9); Melissa McClure (7); Karin I. Öberg (10); Yao-Lun Yang (11); Julia C. Santos (10); Will E. Thompson (2); Elizabeth S. Yunerman (10); Aditya M. Arabhavi (8); Alice S. Booth (10); Mayank Narang (8)*
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Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous carbonaceous molecules that trace the interaction between radiation fields and molecular material, providing key diagnostics of disk surface chemistry, ultraviolet processing, and ionization structure. Using recently obtained JWST/NIRSpec and MIRI IFU observations of the edge-on disks ESO-Hα 574, HV Tau C, Oph 163131, Flying Saucer, and LkHα 263C, we analyze N-MIR emission features commonly attributed to PAHs. We first assess the spatial origin of the emission to distinguish disk-associated PAH features from background cloud contamination, exploiting the edge-on geometries and spatially resolved IFU data. For sources where the emission is demonstrably disk-confined, we derive physically motivated band ratios (3.3/11.3, 11.3/7.7, and 3.4/3.3) to constrain PAH representative sizes, ionization, and aliphatic fractions. Where signal-to-noise permits, we construct spatially resolved ratios to trace vertical and radial variations in PAH properties across the disks. Preliminary results indicate predominantly small- to medium-sized PAHs, with regionally dependent ionization states that are either strongly neutral or strongly ionized. Several systems exhibit systematic vertical gradients consistent with irradiation-driven processing in disk surface layers, while mid-plane regions show suppressed aromatic emission, likely due to shielding and grain growth. These findings demonstrate that PAH emission in edge-on disks provides a spatially resolved diagnostic of disk irradiation and chemical stratification. When combined with JWST constraints on gas excitation and ice composition, PAHs emerge as a powerful probe of radiation-driven evolution, ionization balance, and the processing

of aromatic carbon during planet formation.

1.19 Do Clouds and Disks Create Carbon Grains and Supply them to the ISM **[I]**

***Edwin A. Bergin**, University of Michigan*

In this talk I explore the story of solid state refractory carbon throughout the process of star and planet formation. I will outline how the solar system provides clear clues of a genetic link to PAHs isolated, and possibly forming, in cold ($\sim$10 K) gas to that of carbonaceous material studied in meteorites and asteroid return samples. I will also show that it is likely that PAHs are forming at some level in the outer tens of au in protoplanetary disks and discuss evidence supporting this hypothesis. Finally, I will show JWST spectra that demonstrate that some young protostars are ejecting abundant small hydrocarbons at the base of disk winds. The hydrocarbon content within the wind exceeds that of CO requiring hydrocarbon supply from the destruction of carbonaceous grains. There two fascinating implications of these results. (1) Destruction of carbonaceous grains is a pre-requisite for the formation of silicate-rich worlds such as the Earth, and we may be witnessing the initial stages of Earth-like planet formation. (2) More speculatively, if carbon grain destruction is not fully complete we may also be witnessing the release of carbon grains back to the ISM supplied by star formation.

1.20 Aromatic Carbon Across the Solar System: Insights from Sample-Return Missions **[I]**

***Hassan Sabbah**, University of Toulouse*

Carbonaceous material is widespread in Solar System bodies and preserves a record of the chemical links between the interstellar medium, the protosolar nebula, and early planetesimals. Aromatic species, including polycyclic aromatic hydrocarbons (PAHs) and related macromolecular carbon, are an important part of this inventory, yet their origin, diversity, and evolution remain debated. Their signatures are found across the Solar System, from primitive solids to environments such as Titan's atmosphere. Meteorites, interplanetary dust particles, and early space missions established the foundations of our understanding of Solar System aromatics. Carbonaceous chondrites show that extraterrestrial organic matter occurs in both soluble and insoluble forms, the latter dominated by aromatic-rich macromolecular material altered on parent bodies. The Stardust mission extended this framework to cometary samples, highlighting the links between cometary, meteoritic, and interstellar organics. Results from Hayabusa2 and OSIRIS-REx, which returned samples from the asteroids Ryugu and Bennu, reveal minimally altered carbonaceous matter and diverse organics. Notably, Ryugu contains large free PAHs extending up to $\sim$60 carbon atoms [1], providing the first laboratory identification of PAHs in the size range associated with the aromatic infrared bands and establishing a direct link between large interstellar aromatics and primitive Solar System solids. OSIRIS-REx provides a key comparative benchmark between asteroids with distinct alteration histories. Open questions, together with the opportunities offered by future missions and the development of advanced analytical techniques, will be discussed.

[1] Sabbah et al. 2024, Natural Sciences 4: e20240010.

1.21 Aromatics in Meteorites: Origins, Evolution, and Connections to the Aromatic Universe **[I]**

***José Aponte**, NASA Goddard Space Flight Center*

Carbonaceous meteorites preserve a record of the organic chemistry that accompanied the formation and early evolution of the Solar System. Among their diverse organic inventory, aromatic compounds, i.e.; polycyclic aromatic hydrocarbons (PAHs), alkylated aromatics, heterocyclic species, and macromolecular aromatic networks, provide important clues about the chemical heritage of primitive materials and the processes that modified them in asteroidal environments. Yet,

major questions remain regarding their origins, molecular diversity, isotopic signatures, and relationships to aromatic reservoirs observed elsewhere. This invited presentation will provide an overview of the current state of knowledge on aromatic species in meteorites, emphasizing analytical advances and recent findings from carbonaceous chondrites and asteroid-return samples. I will discuss the occurrence, molecular distributions, and isotopic compositions of meteoritic aromatic compounds, with particular attention to evidence for interstellar inheritance, nebular processing, and parent-body aqueous and thermal alteration. Finally, I will highlight key unresolved questions and future opportunities in the JWST era, including links between meteoritic aromatics and aromatic compounds identified in the interstellar medium and protoplanetary environments. By integrating meteoritic analyses with astronomical observations, laboratory astrophysics, and theoretical studies, this presentation aims to place Solar System aromatic matter within a broader cosmic framework and identify promising directions for future interdisciplinary research.

1.22 Beyond Benzene: The Search for Aromatic Molecules on Titan **[I]**

***Conor Nixon**, NASA Goddard Space Flight Center*

Saturn's moon Titan is renowned for the chemical complexity of its atmosphere. Consisting primarily of nitrogen (N_2) and methane (CH_4), it has an intriguing chemistry that is intermediate between the oxidizing environments of the inner solar system worlds and the reducing atmospheres of the giant planets. Photochemical reactions act to produce a cornucopia of complex molecules, primarily saturated and unsaturated hydrocarbons, along with a sprinkling of known nitriles. While our knowledge of the chemical inventory remains sparse, the abundant, light-scattering haze particles in the atmosphere along with low-resolution mass spectrometry from Cassini all hint towards the presence of PAHs. To date, the only aromatic species firmly detected is benzene, and the hunt continues to identify multi-ringed molecules and heterocycles using ground and space-based spectroscopy at IR through radio wavelengths. This presentation first reviews our current knowledge of Titan's atmospheric chemical roster and then discusses recent results from ongoing astronomical campaigns to identify new compounds in the atmosphere. In conclusion future instrumentation and facilities, as well as needs, are summarized.

1.23 The Metallicity Dependence of PAH Emission in Galaxies **[I]**

***J.D. Smith** (1); Cory Whitcomb (2); Karin Sandstrom (3); Brandon Hensley (4); Bruce Draine (5); Thomas Lai (6); Elizabeth Tarantino (7); Martha Boyer (7); Evan Skillman (8); Desika Narayanan (9); Danny Dale (10); Julia Roman-Duval (7); Alberto Bolatto (11); Lee Armus (6)*
(1) University of Toledo, (2) UToledo, (3) UC San Diego, (4) JPL, (5) Princeton, (6) IPAC/Caltech, (7) STScI, (8) UMinnesota, (9) UFlorida, (10) UWyoming, (11) UMaryland

The interplay between free and condensed metals in galaxies substantially drives their evolution and observational properties. Metals drive the cooling of ionized gas and alter the temperatures of stars. Dust mediates the flow of energy through the ISM, setting the conditions of star-forming gas. As the gas metal content declines among and within galaxies, the fraction of metals locked in the solid form, in dust, drops. But dust grains do not all disappear at the same rate. Spitzer left us with an enduring mystery: carbon nano-particles — PAH grains — all but vanish below about one-quarter solar metallicity, well before their larger brethren. A solution to this mystery will directly inform our understanding of the origins of dust and its journey through the ISM.

I'll review the compelling observational evidence for the PAH-metallicity relationship (PZR), and explain how the combination of archival Spitzer data, new multi-instrument JWST observations and recently developed physical models for grain growth and emission are together cracking the mystery of disappearing PAHs. As one of the most observable forms of metals in the Universe, PAH emission will play an important role in revealing the rise of dust and metals at early times. I'll describe how a new class of physically realistic PAH-bearing hydrodynamical galaxy simulations

and future far-infrared facilities like PRIMA can uncover their origins in massive galaxies during the first Gyr of the Universe.

1.24 JWST Captures Growth of Aromatic Hydrocarbon Dust Particles in the Extremely Metal-poor Galaxy Sextans A

Elizabeth Tarantino *(1); Julia Roman-Duval (1)*
(1) Space Telescope Science Institute

The mid-infrared spectrum of star-forming, high metallicity galaxies is dominated by emission features from aromatic and aliphatic bonds in small carbonaceous dust grains, often referred to as polycyclic aromatic hydrocarbons (PAHs). In metal-poor galaxies, the abundance of PAHs relative to the total dust sharply declines, but the origin of this deficit is unknown. We present JWST observations that detect and resolve emission from PAHs in the 7% Solar metallicity galaxy Sextans A, representing the lowest metallicity detection of PAH emission to date. In contrast to higher metallicity galaxies, the clumps of PAH emission are small (0.5-1.5" or 3-10 pc), which explains why PAH emission evaded detection by lower resolution instruments like Spitzer. Ratios between the 3.3, 7.7, and 11.3 μm PAH features indicate that the PAH grains in Sextans A are small and neutral, with no evidence of significant processing from the hard radiation fields within the galaxy. These results favor inhibited grain growth over enhanced destruction as the origin of the low PAH abundance in Sextans A. The compact clumps of PAH emission are likely active sites of in-situ PAH formation within a dense, well-shielded phase of the interstellar medium. We will also present new JWST NIRSpec and MIRI/MRS spectroscopic observations targeting the brightest clump that further constrain the size distribution, ionization state, and formation pathways of PAHs in extremely metal-poor environments. Our results show that PAHs can form and survive in extremely metal poor environments common early in the evolution of the Universe.

1.25 Variations in PAH Feature Strengths Across Nearby Galaxies Driven by Metallicity and Radiation Field Spectrum

Hannah Koziol *(1); Karin Sandstrom (1); Dalya Baron (2); Adam Leroy (3); The PHANGS Team*
(1) University of California, San Diego, (2) Stanford University, (3) The Ohio State University

Polycyclic aromatic hydrocarbons (PAHs) contribute a significant fraction of the total infrared luminosity of galaxies and influence the phase structure of the interstellar medium (ISM) through photoelectric heating, with the smallest, neutral PAHs having the highest efficiency. PAH band ratios provide measurements of the relative size and charge of the PAH population. Previous studies have focused on the 5-17 μm PAH features; now, with JWST, we can constrain the smallest, neutral PAHs that primarily emit at 3.3 μm. I will present measurements of variations in the 3.3, 7.7, and 11.3 μm features driven by metallicity and radiation field hardness across 19 nearby, star forming galaxies. At fixed metallicity, we find a correlation between PAH band ratios and radiation field spectrum, due to harder radiation fields heating PAHs to higher temperatures. We also observe a shift to more neutral PAHs in the presence of AGN, confirming previous observations with the addition of the 3.3 μm feature. Over a metallicity range of $\sim$0.4 dex, we observe a near-linear decrease in the 3.3/7.7 and 3.3/11.3 μm ratios with increasing metallicity that cannot be explained by radiation field effects alone, revealing a shift to smaller average PAH sizes. Our findings demonstrate that the characteristics of PAH populations in low metallicity environments cannot only be explained by the preferential destruction of the smallest PAHs, but instead support an inhibited growth scenario. While there is a lower PAH abundance at low metallicity, the small and neutral PAHs that remain contribute the most to photoelectric heating in these environments.

1.26 The PAH population characteristics in galaxies and AGNs **[I]**

Dimitra Rigopoulou *(1); Ismael Garcia-Bernete (2,3); Fergus Donnan (4); Oscar Veenema (5); Zujia Lu (1); Niranjan Thatte (1); Miguel Pereira Santaella (6,3)*
(1) University of Oxford, (2) CAB, (3) CSIC, (4) UCSD, (5) Univ. of Oxford, (6) IFF

With the advent of the James Webb Space Telescope, we now have access to the entire suite of dust diagnostics at unprecedented resolution. Emission from Polycyclic Aromatic Hydrocarbons (PAHs) in particular, is a powerful tool to study and characterize the ISM in the centres of nearby galaxies and Active Galactic Nuclei. In this talk I will review the state-of-art in our understanding of the PAH population in the vicinity of supermassive black holes. Using mid-infrared spectroscopy we zoom-in the nuclear and circumnuclear regions of a sample of nearby AGN at sub-arcsecond angular resolution. The observations reveal, quite unexpectedly, that PAH molecules are present in the innermost regions of Seyfert galaxies. However, we find that the PAH population in the nuclear regions of AGN have markedly different properties to the PAH population found in the circumnuclear SF regions. Such studies have revealed that nuclear PAH emission mainly originates from neutral PAHs while, in contrast, PAH emission in circumnuclear SF regions favours smaller and more ionised PAH grains. These results provide evidence that the central AGN has a significant impact on the ionization state and size of the PAH grains on scales of a few x100 parsecs. Rather unexpectedly (and surprisingly) we detected PAHs in the AGN-driven outflows of the galaxies studied, thus, establishing PAHs as a tool to probe AGN feedback in the nearby Universe.

1.27 PAH Survival in the M82 Superwind with JWST

Serena Cronin *(1); Alberto Bolatto (1)*
(1) University of Maryland, College Park

By expelling gas and dust to large distances beyond galaxy disks and enriching the circumgalactic medium, galactic winds are key players in the baryon cycle and galaxy evolution. M82 is the archetypal starburst galaxy with a spectacular multiphase galactic wind. With its nearly edge-on geometry and close proximity (3.6 Mpc), M82's wind can be studied in exquisite detail with powerful observatories. Spitzer-era photometry and spectroscopy revealed a wind rich with polycyclic aromatic hydrocarbons (PAHs) extending several kiloparsecs into the halo, yet it remains unclear how this cool material can survive the harsh conditions of the hot, X-ray-emitting wind. To investigate the survival of cool material in hot winds, we present JWST NIRCam and MIRI imaging of the inner $\sim$5 kpc of the M82 wind at $\sim$0.9-6.5 pc resolution using filters that probe PAH emission at 3.3, 7.7, and 11.3 μm. These images reveal a complex network of cool wind filaments, plumes, and bubble walls traced by PAHs. Comparing PAH band ratios with dust models, we find little variation in PAH size and a modest decline in PAH ionization with distance from the intense radiation field of the starburst. Combining these data with archival Spitzer and Herschel observations, we find that the PAH abundance (qPAH) remains constant at $\sim$1% with distance from the starburst out to $\sim$5 kpc. The picture that emerges is one in which PAHs that are successfully launched in the wind are embedded in the surface layers of entrained cool clouds and protected for at least $\sim$20 Myr.

1.28 Cosmic Fullerenes: from Discovery to a new Paradigm **[I]**

Morgan M. Giese *(1); Jan Cami (1); Simon Van Schuylenbergh (1); Els Peeters (1); Charmi Bhatt (1); Dries Van De Putte (1); Michael J. Barlow (2); Jeronimo Bernard-Salas (3); Alessandra Candian (4); Bryan Changala (5); Nick L. J. Cox (3); Harriet Dinerstein (6); Vincent Esposito (7); D. A. García-Hernández (8); Marco A. Gomez-Muñoz (9); Kay Justtanont (10); Kathleen E. Kraemer (11); Eric Lagadec (12); Arturo Manchado (8); Ana Monreal Ibero (13); Raghvendra Sahai (14); Ameek Sidhu (1); Greg Sloan (15); N. C. Sterling (16); Alexander Tielens (17); Jeremy R. Walsh (18); Roger Wesson (2); Joshua Cole Whitman (16); Albert Zijlstra (19)*
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Fullerenes and PAHs share similar molecular and physical properties and are often found in the same astrophysical environments. Yet fullerenes are unique among large molecules detected in space: they are the only such species with distinct vibrational modes that can be unambiguously identified in the IR, giving us an uncontaminated view of how large molecules interact with their environment. Fundamental questions remain, however, about how these molecules form, whether they exist in the gas or solid phase, and what processes drive their excitation and IR emission.

In this review talk, I will give an overview of the observational characteristics of fullerenes, the variety of astrophysical environments in which fullerenes have been detected, and what we currently know – and don't know – about their formation and excitation pathways. I will then discuss how new JWST observations are now transforming our understanding of fullerenes across a range of environments. As a particularly striking example, spatially resolved spectroscopy of the planetary nebula Tc 1 with JWST/MIRI and VLT/MUSE reveals remarkably rich spectra, with clear signatures of neutral C_{60} and C_{70}, resolved ro-vibrational profile structure, and ^{13}C isotopic substitution confirming they are in the gas phase. Intriguingly, the fullerenes reside in the HII region – where they were expected to photo-fragment rather than survive – and we identify several excitation mechanisms operating in this ionized gas. These new observations fundamentally revise our understanding of fullerene physics and have broad implications for large molecules – including PAHs – in space.

1.29 Spatially disentangling carbonaceous emitters in the Iris nebula: from PAHs to C_{60}

Dries Van De Putte *(1); GTO-1192 team ; Karl Gordon (2); Karl Misselt (3); Adolf N. Witt (4); Alberto Noriega-Crespo (2); Pierre Guillard (5); Marion Zannese (6); Meriem El Yajouri (2); Boris Trahin (2); Pierre Dell'ova (7); Maarten Baes (8); Pamela Klaassen (9); GO-8007 team ; Els Peeters (1); Jan Cami (1); Alexander Tielens (10); Alexandros Maragkoudakis (11); Baria Khan (1); Joost Bakker (12); Giel Berden (12); Wybren Jan Buma (13); Jos Oomens (12); Rens Waters (12)*
(1) Western University, (2) Space Telescope Science Institute, (3) University of Arizona, (4) University of Toledo, (5) Institut d'Astrophysique de Paris, (6) Instituto de Física Fundamental, (7) Institut d'Astrophysique Spatiale, (8) Universiteit Gent, (9) United Kingdom Astronomy Technology Centre, (10) University of Maryland, (11) NASA Ames Research Center, (12) Radboud Universiteit, (13) Universiteit van Amsterdam

We present combined MIRI IFU observations (GTO-1192, GO-8004) of the Iris reflection nebula (NGC 7023) that cover the northwest photodissociation region and the central cavity, up to a projected distance of 5" from the central star. NGC 7023 is a rich spectroscopic target for studying photochemical evolution of carbonaceous material in the ISM, considering its moderate continuum, bright aromatic emission bands, and the known presence of C_{60} in the cavity.

We characterize the strong variations observed in the emission band profiles by decomposing the spectra with PAHFIT. We present an overview of the resulting feature maps and organize the bands into three spatial distribution types according to their brightness ratio in the atomic PDR region (ATM) relative to the main dissociation front (DF1). This reveals a pattern where blue subcomponents of the 5.7, 7.7, 11.3, and 12.7 μm bands are brighter near the star, with spatial dis-

tributions strikingly similar to the 17.4 μm band. The 11.0 μm band is unique with an exceptionally high ATM/DF1 ratio. Entering the cavity, the above trends continue to evolve towards the star, with a further increasing 11.0/11.3 μm ratio and profiles with progressively sharper blue peaks. We interpret this sequence as tracing an intermediate evolutionary stage in the process of fullerene formation.

Previous studies reported an anti-correlation between PAH and C_{60} emission and hypothesize that PAH destruction drives C_{60} formation. However, while the PAH emission smoothly decreases, the C_{60} bands exhibit an initial local maximum at a projected distance of around 25", followed by a smooth increase from 15" to 5". The observed ro-vibrational structure of the 18.9 μm profile confirms the emission originates from gas-phase C_{60}, while C_{60}^{+} signatures are very faint, contrary to charge balance models. The difference between the spatial structures of PAHs and C_{60}, and the lack of C_{60}^{+}, may indicate that their emission originates from different regions along the line of sight.

1.30 PAHs Beyond the Local Universe **[I]**

Jed McKinney *(1); Miriam Eleazer (2); Alexandra Pope (2); Anna Sajina (3); Stacey Alberts (4); Irene Shivaei (5)*
(1) UT Austin, (2) UMass, (3) Tufts, (4) STScI, (5) CAB

PAHs make up less than 0.1% of the mass of galaxies but play a transformative role in shaping their evolution by regulating the heating and cooling of interstellar gas. This ultimately sets the formation rate of new stars. Given the rich information encoded by PAHs on heating, cooling, and radiation field conditions, observations of PAHs in the high redshift Universe (z$\sim$2, $\sim$10 Gyr ago) hold the key to understanding the most active galaxy formation epoch. In this talk I will present a general review on studies of PAH emission in high-redshift galaxies, and what they have told us both about the PAHs themselves and also about galaxy formation. I will begin by discussing observations from Spitzer, then move into the era of JWST, and finally touch on how past observatories point us towards future IR missions like PRIMA.

1.31 Spatially resolved PAH Spectroscopy in the era of JWST: From resolved PAH maps at cosmic noon to kinematics of PAH features.

Fergus Donnan *(1); Karin Sandstrom (1); Irene Shivaei (2); Leindert Boogaard (3); Tanio Diaz-Santos (4); Cristina Lofaro (4); Ismael Garcia-Bernete (2); Dimitra Rigopoulou (5)*
(1) University of California San Diego, (2) CAB, (3) Leiden University, (4) FORTH, (5) Oxford

With the advent of JWST, its superb sensitivity and spatial resolution has enabled us to spatially resolve PAHs in unprecedented detail. In this talk I will present two exciting projects utilizing the spatial resolution of JWST spectroscopy – spatially resolved PAH ratios in galaxies at cosmic noon and the kinematics of PAH features in local galaxies. I will present spatially resolved maps of PAH features at cosmic noon for the first time, utilizing MIRI MRS observations of five main sequence galaxies at z$\sim$1 as part of the PAHSPECS program (GO 5279, P.I. Shivaei). I will show PAH ratio maps produced from this data show the opposite radial trend to local galaxies, where PAHs become more neutral and larger with radius, possibly due to PAH destruction winning over the metallicity driven effects that dominate in local galaxies. It is now also possible to measure the kinematics of PAH features and produce velocity maps of PAHs, opening a new window into the dusty ISM. I will show how we can measure PAH kinematics using novel techniques, where we are able to now observe how dust moves in galaxies in comparison with ionized and molecular gas. I will show the first kinematic evidence for dusty outflows from AGN, answering a key question about dust around AGN. I will also show the kinematics of PAHs in M82, where the disk and base of the star-formation driven outflow are present.

1.32 First view on PAHs in massive z=1 main-sequence galaxies with JWST/MIRI MRS

Wuji Wang *(1); Andreas Faisst (1); Thomas Lai (1); Kyle Finner (1)*
(1) Caltech/IPAC

I will present the first results from JWST/MIRI MRS observations of a sample of eight main-sequence galaxies on the high mass end at z=1. Two of the galaxies host AGN and two are going through merging interactions. We detect major PAH emission from 3.3 μm to 11.3 μm, atomic fine structure lines, and molecular H_2 transitions. By utilizing PAH ratio diagnostics and comparison with theoretical models, we qualitatively constrain PAH sizes and ionization states for these typical star-forming galaxies at z=1. The AGN and mergers have a higher fraction of neutral PAHs possibly related to high radiation intensity and/or shocks. Leveraging the IFU data, we find that the PAHs in the central regions tend to be smaller and less ionized than those in the galactic outskirts. We further link our results to the literature PAHs studies. The PAH11.3/PAH3.3 ratios of our star forming galaxies are higher than local ULIRGs but smaller than (U)LIRGs at z$\sim$1.7. I will discuss the implications of these results regarding PAH production, metallicity, and radiation field intensity. The key novelty of this work lies in our ability to directly resolve PAH emission in prototypical galaxies at the end of Cosmic Noon.

1.33 Resolving PAH physics at Cosmic Noon: spatially-resolved hot-dust maps and slitless 3.3 μm spectroscopy with JWST/MIRI

Román Fernández Aranda *(1); Irene Shivaei (1)*
(1) Center for Astrobiology (CAB), CSIC-INTA, Spain

Understanding dust physics in galaxies beyond the local universe requires multi-wavelength, spatially resolved observations — a challenging and rarely undertaken task. Polycyclic aromatic hydrocarbons (PAH) are a primary source of photoelectric heating in the interstellar medium (ISM) and are therefore critical to understanding star formation activity. At Cosmic Noon (z$\sim$1–3), when cosmic star formation peaked, PAH features remain scarcely explored due to observational challenges; only a few examples exist in the literature.

In this talk I will present spatially resolved 6–9 μm PAH maps and 3.3 μm PAH spectra across a sample of tens of galaxies at z$\sim$1–3 using two complementary JWST programs: (i) a deep (up to 20 h) JWST 15 μm MIRI mosaic that reaches unprecedented sensitivity, enabling spatially resolved observations of PAH emission (rest-frame 6–9 μm) at Cosmic Noon; and (ii) deep (up to 23 h) parallel slitless spectroscopy with JWST/MIRI LRS (5–14 μm), which captures the redshifted 3.3 μm PAH feature at these redshifts. Combining these data with ancillary ALMA cold-dust and molecular-gas measurements and JWST near-IR star-formation tracers, this analysis provides the first investigation of resolved dust physics, dust-obscured star formation, and PAH formation/destruction in a statistically significant sample of galaxies during the epoch of peak stellar mass assembly.

1.34 The role of electron cooling in the stability of small carbon-bearing molecules **[I]**

Piero Ferrari*, HFML-FELIX*

In the harsh conditions of the interstellar medium, small carbon-bearing molecules such as carbon clusters, fullerenes and PAHs are exposed to strong UV irradiation, triggering a plethora of physicochemical phenomena that shape the dynamics of molecules in space. In the absence of an external heat bath, the survival probability of an excited molecule is determined by three processes: fragmentation, electron emission and radiative cooling. Under thermally hot conditions, one of these channels typically dominates, but depending on internal energy and molecule-specific parameters, competition can occur. Radiative cooling, which can stabilize a molecule against fragmentation if active, can proceed via two distinct mechanisms, namely direct vibrational cooling (VC) or recurrent fluorescence (RF). In this contribution, I will discuss the past, present and future

of research in RF, focusing on the role this phenomenon plays in determining the dynamics and survival probability of carbon-bearing molecules in space.

1.35 Photostability and Isotope Fractionation in Interstellar PAHs

Annemieke Petrignani *(1); Sandra D. Wiersma (1); Alessandra Candian (1); Joost Bakker (2); Giel Berden (2); Wybren Jan Buma (1); John R. Eyler (3); Jonathan Martens (2); Jos Oomens (2); M. Rapacioli (4); Alexander Tielens (5)*
(1) University of Amsterdam, (2) Radboud University, (3) University of Florida, (4) Université de Toulouse, (5) Leiden University

Polycyclic Aromatic Hydrocarbons (PAHs) are key components of interstellar chemistry, acting as major reservoirs and processors of cosmic carbon and possibly deuterium. We present UV photodissociation and IR multiple photodissociation (IRMPD) studies of ionic and neutral PAHs revealing key aspects of their photochemical behavior. The irregularly shaped dibenzo[a,l]pyrene cation loses hydrogen alone upon irradiation, despite its 'exposed' pendant rings (Wiersma, Candian, Rapacioli, and Petrignani, 2021). Its armchair edges may facilitate hydrogen loss while resisting hydrocarbon loss. This contrasts with phenyl, where isomerization of the carbon skeleton, i.e., facile ring opening, prevents direct H loss, and, instead, leads to loss of small hydrocarbon fragments (Wiersma et al., 2021a). For deuteronated PAHs, fragmentation is preceded by isotopomerisation, causing deuterium enrichment (Wiersma et al., 2020). Upon excitation, H and D atoms scramble across the PAH perimeter with H atoms more mobile and more prone to fragmentation, shielding its isotope. Spectral studies further show several PAHs to possess surprisingly strong, narrow, and largely uncongested bands in the FIR (Wiersma, Candian, Bakker, and Petrignani, 2022), providing useful fingerprints and benchmarks. Together, these results reveal a rich, kinetically controlled photochemistry governed by PAH structure, indicating that photostability is not restricted to compact, condensed families, but can also arise from specific geometries and kinetic barriers. These studies shed light on fundamental processes crucial for interpreting JWST observations, where the ability to trace spatial variations within nebulae enables unprecedented insight into interstellar chemistry.

1.36 Infrared Emission Spectra of Fullerene C_{60}: Experiments and Simulations

Tomonari Wakabayashi *(1); Keito Morimoto (1); Nanase Kohno (1); Hal Suzuki (1)*
(1) Kindai University

Laboratory measurements of infrared (IR) emission spectra of fullerene C_{60} thin films were conducted in a temperature range of 300 – 400°C to observe systematic changes in the relative intensity of four IR-active T_{1u} modes of the molecule. Thin films of fullerene C_{70} and coronene $C_{24}H_{12}$ were also subjected to the same measurements. Temperature dependence of the IR-emission intensity of the T_{1u} modes of C_{60} was simulated on the bases of thermal population of an ensemble of C_{60} molecules in all possible $\sim 10^{21}$ vibrational energy levels up to the excitation energy of 12000 cm^{-1}, using harmonic frequencies and intensities from DFT calculations. The spectral simulation showed a good agreement with the experimental temperature dependence of the IR-emission intensity.

Part of our results has already been published in PRB (2024) [1]. In this presentation, improvements are discussed for the measurable temperature range and the counting scheme of vibrational energy levels. For fine details of the observed band shape for each T_{1u} mode, emission spectra of C_{60} thin films are compared with absorption spectra of matrix-isolated C_{60} molecules in solid parahydrogen at cryogenic temperature, which includes considerations on spectral composites of isotopically substitute species, $^{13}C_x\ ^{12}C_{60-x}$ ($x = 0$–3), [2] and possibly quantized rotational structures accompanied by the vibrational transition [3].

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1.37 In-situ PAH formation in an O-rich Planetary Nebula: The Butterfly Nebula

Nicholas Clark *(1); Els Peeters (1); Jan Cami (1); Greg Sloan (2); Kevin Volk (2); Kathleen E. Kraemer (3); Harriet Dinerstein (4); Mikako Matsuura (5); Patrick J. Kavanagh (6); Charmi Bhatt (1); Raghvendra Sahai (7); Alexander Tielens (8); Isabel Aleman (9); Bruce Balick (10); Michael J. Barlow (11); Jeronimo Bernard-Salas (12); Joris Blommaert (13); Naomi Hirano (14); Olivia Jones (15); Kay Justtanont (16); Joel Kastner (17); Francisca Kemper (18); Eric Lagadec (19); J. Martin Laming (20); Frank Molster (21); Hektor Monteiro (5); Paula Moraga Baez (1); Anita M. S. Richards (22); N. C. Sterling (23); Peter A. M. van Hoof (24); Jeremy R. Walsh (25); Roger Wesson (5); Nicholas J. Wright (26); Albert Zijlstra (22)*

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The James Webb Space Telescope (JWST) has revealed unexpected spatial variations in the mid-infrared emission of the Butterfly Nebula (NGC 6302), a Planetary Nebula that has been oxygen-rich throughout its entire evolution. The nebula surrounds a stellar remnant with one of the highest known effective temperatures in our Galaxy, and this extreme radiation field drives a rich and complex chemistry in the surrounding gas and dust. Among the most surprising products of this chemistry is an abundance of small hydrocarbons such as the methyl cation, and Polycyclic Aromatic Hydrocarbons (PAHs) - whose formation in an oxygen-rich environment poses a fundamental challenge to current astrochemical models. PAHs are thought to form in the circumstellar envelopes of carbon stars through processes similar to soot formation in terrestrial flames, but the oxygen-rich composition of the Butterfly Nebula places severe constraints on the possible carbon chemistry. The strong and spatially varying PAH emission observed across the nebula instead points to in-situ formation and ongoing chemical processing of these molecules. Here we present an analysis of the spatial distribution of the PAH emission features, discuss how the chemical characteristics of the PAHs, such as charge, edge structure, and oxygen content, vary throughout this environment, discuss the physical and chemical conditions that may enable PAH formation, and provide an estimate of the in-situ PAH formation rates. These results offer direct observational constraints on one particular formation channel for PAHs, contributing to a broader understanding of how these molecules arise across diverse astrophysical environments.

1.38 Proto-PAHs: JWST spectroscopy of complex hydrocarbons in objects evolving into planetary nebulae.

Greg Sloan *(1,2); Bernhard Aringer (3,4); Jeronimo Bernard-Salas (5); Charmi Bhatt (6); Jan Cami (6); Nicholas Clark (6); Debayan Das (6); Harriet Dinerstein (7); D. A. García-Hernández (8); Marco A. Gomez-Muñoz (9); Pernille Jensen (10); Kathleen E. Kraemer (11); Arturo Manchado (8); Mikako Matsuura (12); Els Peeters (6); Raghvendra Sahai (13); N. C. Sterling (14); Kevin Volk (1); Glenn M. Wahlgren (15); Albert Zijlstra (16)*

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JWST has obtained infrared spectra of eight carbon-rich objects that have evolved past the asymptotic giant branch and toward the planetary nebula phase. The spectra cover 3 to 22 μm at a spectral resolving power of roughly 2000, and they show a wealth of molecular emission and absorption bands hidden in lower-resolution spectra from the Spitzer Space Telescope. They also reveal more details of the broader spectral features from larger molecules (or particles) of complex

hydrocarbons, including aliphatics and polycyclic aromatic hydrocarbons (PAHs). The near-infrared spectra show a strong contribution from broad aliphatic emission features at 3.4 μm in most of the targets and even aliphatic absorption in a few. The absorption from smaller carbon-bearing molecules is strong enough to affect previous measurements of the strengths and central wavelengths of some of the broader emission features. The feature profiles can differ measurably from more traditional PAH emission spectra. These new spectra will help us disentangle the complex relation between PAHs and simpler non-aromatic carbon-bearing molecules.

1.39 JWST/MIRI Observations of PAH Features around WR140

Riko Senoo *(1); Ryan M. Lau (2); Takashi Onaka (1); Takashi Miyata (3); Takafumi Kamizuka (3); Greg Sloan (4); Itsuki Sakon (3); Hideo Matsuhara (5); Kotomi Taniguchi (6); Emma Lieb (7)*
(1) The University of Tokyo, (2) CalTech/IPAC, (3) Institute of Astronomy, The University of Tokyo, (4) Space Telescope Science Institute, (5) ISAS, JAXA, (6) National Astronomical Observatory of Japan, (7) University of Denver

Binary systems containing carbon-rich Wolf-Rayet (WC) stars are considered one of the key dust-producing sources, particularly in the early universe. WR140 is a well-known dust-producing binary system composed of a WC star and an O-type star. In WR140, dust shells are formed every 7.93 years as the O-type star and WC star approach each other, and multiple dust shells have been observed. Previous research (Lau et al. 2022) used JWST/MIRI/MRS detected the infrared emission features originating from hydrogen-poor carbonaceous material in two dust shells close to the central stars. However, the previous study did not perform spectroscopy on the outer dust shells. The outer dust shells formed earlier than the inner ones, therefore, it is important to observe the differences between the inner and outer dust shells. In this study, slit spectroscopy using JWST/MIRI/LRS was performed on multiple dust shells farther from the central star than in the previous study (the 1st to 7th shells from the innermost and the off-point). As a result, infrared emission features originating from carbonaceous material poor in hydrogen were observed from the inner two dust shells, consistent with the previous study. Conversely, PAH features (such as the 8.6 μm and 11.2 μm features) similar to those observed in the interstellar medium were detected from the outer regions. This presentation will describe the characteristics of the observed 8.6 μm and 11.2 μm features and discuss the possibility that these PAH features originate from organic matter present around WR140.

1.40 Dust extinction in the local universe **[I]**

Marjorie Decleir*, European Space Agency (ESA) at Space Telescope Science Institute (STScI)*

Dust absorbs and scatters a significant fraction of stellar radiation across all wavelengths, and this effect must be accounted for when interpreting observations of astrophysical objects. Multi-wavelength extinction curves not only allow us to account for dust extinction but also provide a direct probe of dust grain properties such as size and composition. In this talk, I will review our current understanding of dust extinction. I will begin by explaining what extinction is, how extinction curves are measured, and what we can learn from them. I will then highlight several key extinction features across the electromagnetic spectrum, in particular aromatic features, and discuss how they reveal clues about grain composition, with emphasis on recent results from JWST. Next, I will show how extinction curves vary across the Milky Way, largely as a function of the total-to-selective extinction ratio, R(V). I will also demonstrate how new measurements in Local Group galaxies are expanding our understanding of dust extinction beyond the Milky Way, revealing its dependence on global and local galaxy properties. Finally, I will conclude with a brief outlook on the future of extinction studies.

1.41 JWST observations of the 2175Å UV Bump at high redshift **[I]**

Katherine Ormerod *(1); Renske Smit (1); Joris Witstok (2)*
(1) Liverpool John Moores University, (2) Cosmic Dawn Center, University of Copenhagen

Dust is a fundamental component of the interstellar medium (ISM), absorbing UV and optical photons and re-emitting in the far-infrared. Some dust attenuation curves exhibit a strong feature known as the 2175Å UV bump, which is generally attributed to carbonaceous dust grains such as polycyclic aromatic hydrocarbons (PAHs) or nano-sized graphite grains. The recent launch of the James Webb Space Telescope has enabled the surprising detection of a handful of UV bump galaxies up to z=7.55, when the Universe was only 700 Myr old, indicating rapid carbonaceous dust enrichment within the first billion years of cosmic time. Interestingly, some galaxies show a shift in the peak wavelength of the UV bump to longer wavelengths than that observed in the MW, which may suggest a difference in high-redshift dust properties. However, this is not seen in all high-redshift UV bumps, suggesting a diversity in dust properties at this epoch. I will present an overview of recent JWST results on the UV bump feature at high redshift, and what these detections reveal about the nature of dust in the early Universe. Finally, I will introduce ongoing and planned follow-up of UV bump galaxies, including multi-wavelength constraints and resolved rest-frame UV observations, which aim to uncover the dust production pathways and physical conditions driving rapid carbonaceous dust formation at early times.

1.42 PAH Evolution in Galaxy Simulations **[I]**

Caleb Choban *(1); Samir Salim (2); Dusan Keres (3); Karin Sandstrom (3); Julia Roman-Duval (4); Hao-Sheng Wang (5)*
(1) Indiana University Bloomington, (2) Indiana University, (3) UC San Diego, (4) Space Telescope Science Institute, (5) University of Virginia

JWST is delivering an observational cornucopia of PAHs across spatial scales and cosmic time. However, galaxy simulations have been caught flat-footed due to their general neglect of PAHs, and interstellar dust in general. The modeling of PAH evolution on galactic scales is still in its infancy, but recent advancements in dust evolution models has spurred on their development. These advances, coupled with radiation transfer codes that self consistently model stochastic heating and emission of PAHs, have also enabled direct comparisons between galaxy simulations and PAH observations. In this talk, I will review the current state of PAH models in galaxy simulations, highlighting their intimate link with developments in dust evolution models and radiation transfer codes. I will discuss the many open questions regarding PAH formation and evolution, and the future paths forward to answer these questions.

1.43 What PAHs reveal about galaxy evolution: insights from cosmological simulations

Massimiliano Parente *(1); Desika Narayanan (1)*
(1) University of Florida

I will present the first ever large box cosmological galaxy formation simulation to self-consistently model the physical and luminous properties of PAHs in galaxy populations across cosmic time. Our newly developed model combines a dust evolution framework that tracks the grain size distribution in galaxies with radiative transfer calculations to predict observable PAH features. Using this model, the commonly observed PAH–metallicity relation is largely driven by grain shattering and accretion processes, and for this reason the dust-to-gas ratio is a more direct tracer of PAH abundance. PAH emission features trace both star formation and molecular gas content, yet are only weakly correlated with the PAH mass fraction. Even very small PAH mass fractions can produce large PAH luminosities in intensely star-forming galaxies, such as those recently observed at cosmic noon with JWST. I will finally discuss how these results can guide future far-infrared missions such as PRIMA.

1.44 PAHs in Dense Cores **[I]**

Gabi Wenzel *(1,2); GOTHAM team ; Edwin A. Bergin (3); Alex N. Byrne (1); Andrew M. Burkhardt (4); Steven B. Charnley (5); Bryan Changala (6,7); Ilsa Cooke (8); Martin A. Cordiner (5); M. Duffy (1); Zachary T. P. Fried (1); Siyuan Gong (1); Martin S. Holdren (1); Andrew Lipnicky (9); Ryan A. Loomis (9); Michael C. McCarthy (2); Brett A. McGuire (1,9); Anthony J. Remijan (9); Christopher N. Shingledecker (10); Thomas Henry Speak (8); D. Archie Stewart (1); Alison E. Wendlandt (1); Reace Willis (8); Ci Xue (1); Shuo Zhang (1)*
(1) Massachusetts Institute of Technology, (2) Center for Astrophysics | Harvard & Smithsonian, (3) University of Michigan, (4) Worcester State University, (5) NASA Goddard Space Flight Center, (6) University of Colorado Boulder, (7) National Institute of Standards and Technology, (8) University of British Columbia, (9) National Radio Astronomy Observatory, (10) Virginia Military Institute

Polycyclic aromatic hydrocarbons (PAHs) are a major reservoir of interstellar carbon, and their identification in space requires a close interplay between laboratory spectroscopy and astronomical observations. In this talk, I will introduce the current understanding of PAHs in cold cores, focusing on recent radio detections of small and medium-sized PAHs and on constraints on the abundance of larger PAHs in these environments. I will summarize key results from radio astronomical observations of sources such as TMC-1, enabled by high-resolution laboratory rotational spectroscopy. These measurements provide the spectral fingerprints needed to identify specific aromatic molecules and assess their role in low-temperature carbon chemistry. I will briefly discuss how chemical modeling informs formation pathways of PAHs, and highlight open questions about the origin of aromatic species in dense cores, outlining future directions for laboratory, modeling, and radio astronomical efforts in the study of PAHs in astrophysical environments.

1.45 Diffuse Interstellar Bands **[I]**

Alexander Ebenbichler*, Western University*

I will present an overview of the properties and characteristics of the diffuse interstellar bands (DIBs), which remain to be one of the most difficult problems in astrophysics and astrochemistry. DIBs are interstellar absorption features observed in optical and near-infrared spectra of reddened stars. They are ubiquitous in the Universe, as they have been observed in various sight lines across the Milky Way and other galaxies. While to this point, more than 600 DIBs have been detected, only five have been assigned to a carrier molecule which is the fullerene C_{60}^+. Multiple studies found that their carriers are gas phase molecules as opposed to dust grains, mainly indicated by the lack of solid state shifts and polarization. I will discuss the various proposed carrier candidates. It has been suggested that some DIB carriers might well be polycyclic aromatic hydrocarbons (PAHs). The high stability of PAHs in ultraviolet-intense environments makes them compelling candidates. But also other species like carbon chains, carbon rings, and small molecules containing transition metals are currently under investigation in laboratories as possible DIB carriers. I will highlight recent results that have opened new approaches to the carrier identification problem. Recent correlation studies suggest that some DIBs might be caused by common carrier molecules, possibly displaying vibrational progressions. Other observational studies focus on the characterization of DIB profiles and their variation to derive parameters like rotational constants of their carriers to constrain the carrier candidates. A joint effort from experimentalists, observers and theorists will be necessary to bring us closer to solving the DIB puzzle.

1.46 Anomalous Microwave Emission **[I]**

Clive Dickinson*, The University of Manchester*

In this review, I will give an overview of Anomalous Microwave Emission (AME) research. AME is an excess of emission observed at frequencies around 10-100 GHz and is a significant foreground to the CMB. Since its first detection in 1997, it has been observed in diverse astrophysical environments and has even been detected in some nearby extragalactic sources. However, we still know very little about what is actually causing it. AME appears to have a peaked spectrum near 20-30

GHz, is strongly correlated with thermal dust emission suggesting a dust origin, and is not strongly polarized. The leading theory is electric dipole radiation from rapidly spinning nanometre-sized grains ("spinning dust"), either very small grains or large molecules with electric dipole moments, PAHs being the leading candidate. However, previous observational data has not allowed a detailed analysis, which so far support both origins. Upcoming data, such as all-sky PAH maps from SPHEREx, should allow us to determine whether there is indeed a connection between PAHs and AME, opening up a new window into the interstellar medium.

1.47 Laboratory Studies of Interstellar Ion Chemistry and Electronic Spectroscopy **[I]**

Ugo Jacovella *(1); Corentin Rossi (2); Anne Rasmussen (2); Bérenger Gans (2); Roland Thissen (2); Jean-Christophe Loison (3); Jan Zabka (4); Juraj Jasik (4)*
(1) ISMO Université Paris-Saclay, (2) Université Paris-Saclay, (3) Université Bordeaux, (4) Heyrovsky institute

Astrochemical models rely critically on laboratory-derived reaction rates, branching ratios, and spectroscopic data, while observational constraints are obtained from molecular abundances inferred through spectroscopic fingerprints detected by telescopes. Progress in understanding interstellar chemistry therefore depends on two complementary approaches: detecting and characterizing new interstellar ions to refine observational constraints, and investigating previously unexplored ion–molecule reactions to provide reliable kinetic and mechanistic input for chemical models.

In this talk, I will present examples illustrating how advanced laboratory techniques can be combined to address these challenges. Our work focuses on ion–molecule reactions and ion spectroscopy, with particular emphasis on isomeric effects. Our experimental toolbox includes ion mobility spectrometry, mass spectrometry, cryogenically cooled ion traps, and laser spectroscopy. Spectroscopic approaches range from action spectroscopy using messenger tagging to direct absorption measurements employing cavity ring-down spectroscopy.

These methods will be highlighted through ongoing efforts to identify molecular ions in diffuse interstellar clouds via their electronic spectra, with a focus on carbon cluster derivatives and polycyclic aromatic hydrocarbon-related species. In parallel, we aim to expand astrochemical reaction networks by investigating new ion–molecule reactions of astrophysical relevance, including studies on the formation of the first aromatic species.

1.48 Isomer-Selected Spectroscopy of Hydrogenated Carbon Cluster Cations and Their Implications for the Diffuse Interstellar Bands

Anne Rasmussen *(1); Zekai Li (1); Corentin Rossi (1); Ugo Jacovella (1)*
(1) ISMO, Université Paris-Saclay, CNRS

To date, more than 340 molecules have been detected in space, the majority through radio astronomy, which is sensitive only to species possessing a notable permanent dipole moment. In the visible-to-near-infrared spectral region, in which the Diffuse Interstellar Bands (DIBs) appear, only one molecular ion has been identified so far, namely the Buckminsterfullerene in its cationic form (C_{60}^{+}). Carbon clusters and their derivatives are therefore strong candidates for additional DIB carriers. Smaller hydrogenated carbon clusters have already been detected in space in their neutral, anionic, and cationic forms, suggesting that related species may also contribute to the DIB spectrum.

Here, we investigate hydrogenated cyclic carbon cluster cations generated by laser ablation of a graphite rod in an atomic hydrogen-rich environment. Drift-tube ion-mobility spectrometry coupled to mass spectrometry is used to determine hydrogenation states and probe isomer distributions. Subsequently, cryogenic ion-trap action spectroscopy combined with time-of-flight mass spectrometry provides high-resolution action-absorption spectra across the visible-to-near-infrared region. The combined mobility and spectroscopic data identify preferred hydrogenation

states and structural isomers, while also providing laboratory reference spectra for comparison with astronomical DIB observations

1.49 The chemical journey of interstellar PAH nitriles

Ilsa Cooke *(1); Sam McGrath (1); Linshan Zeng (1); Takamasa Momose (1); Brendan Moore (1); Pavle Djuricanin (1); Thomas Henry Speak (1); Brett A. McGuire (2); Gabi Wenzel (2); and the GOTHAM team*
(1) University of British Columbia, (2) Massachusetts Institute of Technology

With the number of aromatic nitriles detected in interstellar space rapidly increasing, questions about their formation routes and photostability have been reinvigorated. These aromatic nitriles can serve as proxies for their ”parent” aromatic hydrocarbons, which are often invisible to radio astronomical observations. Recently, our collaboration (GOTHAM) has detected the multi-ring aromatic nitriles cyanopyrene and cyanocoronene in the cold molecular cloud TMC-1, highlighting the importance of targeted laboratory measurements involving the small (< 35 carbon atom) polycyclic aromatic hydrocarbons (PAHs). To understand the presence of these PAHs in the cold ISM, we are using a multipronged approach — combining radio observations, theoretical kinetics calculations, and laboratory measurements. I will present some highlights from our recent work, including chemical interpretations from our observations of PAHs in TMC-1. In addition, I will discuss our recent laboratory measurements of the spectroscopy and photochemistry of aromatic nitriles in para-hydrogen matrices.

1.50 From Gas-Phase Growth to Surface Reactivity: Aromatics in Astrophysical Environments **[I]**

Shane Goettl *(1); Ralf I. Kaiser (1)*
(1) University of Hawaii at Manoa

Polycyclic aromatic hydrocarbons (PAHs) and fullerenes are central components of the aromatic universe, serving as key intermediates between small hydrocarbons and carbonaceous grains across diverse astrophysical environments. In the James Webb Space Telescope (JWST) era, unprecedented spectroscopic sensitivity provides new constraints on the molecular inventory, structure, and evolution of these species. Recent experimental and theoretical studies have advanced bottom-up formation mechanisms of PAHs and fullerenes, both under high-temperature and low-temperature conditions relevant to a diverse array of astrophysical regions. Radical-driven growth pathways, including reactions involving resonance-stabilized and aryl radical species, have emerged as efficient routes to molecular mass growth, providing viable pathways to large aromatic systems. Beyond gas-phase formation, PAHs also act as chemically active surfaces. Their role in processes such as molecular hydrogen (H_2) formation and catalysis establishes an important link between gas-phase chemistry and grain-surface processes in the interstellar medium. At the same time, PAHs and fullerenes are subject to a variety of destruction pathways, including photodissociation, fragmentation, and ion-driven reactions in radiation-rich environments, which critically influence their lifetimes and observable signatures. Despite progress, uncertainties remain regarding competing formation pathways, surface reactivity, and the balance between bottom-up growth and top-down processing. Addressing these challenges requires coordinated experimental, theoretical, and observational efforts to develop a predictive framework for the lifecycle of aromatic carbon in the JWST era.

1.51 Low-energy electron collisions with C_{60}^+ at the Cryogenic Storage Ring

Lucia Enzmann *(1); Leonard Isberner (1,2,3); Klaus Blaum (1); Bhalchandra Choudhari (1); Manfred Grieser (1); Florian Grussie (1); Claude Krantz (4); Holger Kreckel (1); Stefan Schippers (2); Viviane Schmidt (1); Andreas Wolf (1); Oldrich Novotný (1)*
(1) Max Planck Institute for Nuclear Physics, (2) Physikalisches Institut, Justus-Liebig-Universität Giessen, (3) Columbia Astrophysics Laboratory, Columbia University, (4) GSI Helmholtzzentrum für Schwerionenforschung GmbH

The interstellar medium is characterized by a diverse molecular landscape. In particular, carbon-rich molecules such as fullerenes and polycyclic aromatic hydrocarbons (PAHs) are important in astrochemical processes. While the presence of C_{60}^+ in the interstellar medium (ISM) is well-established, its formation and destruction mechanisms remain a puzzle. Low-energy electron collisions are a significant destruction pathway for small molecules in the ISM, but studies on large molecules at those collision energies are limited and challenging. We investigate low-energy electron collisions with C_{60}^+ using the Cryogenic Storage Ring (CSR) at the Max Planck Institute for Nuclear Physics.

The CSR operates at temperatures below 10K and thus offers an ideal environment to study these reactions at conditions mimicking the ISM. By overlapping a stored ion beam with an electron beam in a merged-beams setup, we study electron collisions with C_{60}^+ at energies ranging from a few meV to approximately 85 eV. We observed various collisional processes and determined absolute rate coefficients. In comparison to collisions of smaller ionized molecules with electrons, C_{60}^+ exhibits a dominant non-dissociative recombination channel with high recombination rates at low collision energies. These results provide insight into the destruction mechanisms of C_{60}^+ in the ISM and provides data for modeling the chemistry of complex carbon-rich molecules in space. Building on this work, we have recently measured electron collisions with C_{70}^+. Future experiments at the CSR will focus on studying electron collisions with PAHs, further contributing to our understanding of the complex chemistry in the ISM.

2 Posters

2.1 Vibrational Carbon Character Analysis of Astronomical PAHs

Kevin Fleming *(1); Vincent Esposito (2); Ryan C. Fortenberry (3); Mateus Quintano (4); Elfi Kraka (1)*
(1) Southern Methodist University, (2) Chapman University, (3) University of Mississippi, (4) Federal University of Pernambuco

The attribution of various aromatic infrared bands (AIBs) to the aromatic or aliphatic C–H stretching modes of polycyclic aromatic hydrocarbons (PAHs) may require a serious reassessment. These attributions, made previously on the basis of harmonic frequency quantum chemical calculations of potential PAH AIB carriers, do not account for the anharmonic vibrational mode coupling in the vibrational transitions of these carriers. Such anharmonic coupling can cause the transitions and their corresponding emission bands to have mixed vibrational carbon character (VCC). In this work, vibrational carbon character analysis (VCCA), a method for quantifying the VCC of the vibrational transitions and emission bands of AIB carriers, is introduced. VCCA is applied to indene, one of the smallest astronomically-detected PAHs, and its proposed interstellar precursor 2-ethynyltoluene. Indene's conventionally-defined aliphatic 3.4 μm emission band is revealed to involve strong VCC mixing with nearly 45% non-aliphatic character. Significant VCC mixing is also predicted for indene's conventionally-defined aliphatic 6.85 and 7.25 μm emission bands. Similar behavior is observed for 2-ethynyltoluene, as well. The traditionally-described aromatic emission bands of both molecules at 3.3 and 6.2 μm, however, are found to be primarily aromatic, although smaller amounts of non-aromatic character are present, too. Overall, these findings call for a detailed examination of the VCC mixing of other potential AIB carriers, and VCCA can serve as an effective tool for this purpose. An improved understanding of VCC mixing in these carriers would greatly facilitate the interpretation of the high-quality IR data now provided by JWST and SPHEREx.

2.2 How structure shapes survival: a study of $C_{10}H_8$ isomers

Chiara Beldì *(1); Cate Anstöter (2)*
(1) University of Edinburgh, (2) University of Glasgow

Negatively charged polycyclic aromatic hydrocarbons (PAHs) are believed to play a crucial role in the chemistry of cold interstellar regions, yet their formation mechanisms, abundances and reactivities remain poorly understood due to the difficulties associated with their detection and characterisation. Anion chemistry in the interstellar medium (ISM) is thought to begin with electron capture into a metastable electronic state lying above the ionisation threshold. If sufficiently long-lived, this transient state can relax to the anionic ground state, seeding further chemical complexity. However, probing these short-lived states at the extremely low temperatures of the ISM is experimentally challenging, and available data remains scarce. As a result, computational approaches are essential to uncovering their nature and astrochemical significance. The theoretical description of these states is inherently demanding: they are embedded in the neutral – free-electron continuum and therefore evade description by conventional quantum-mechanical methods. In this study, bound-state approaches are extended to allow the computational characterisation of such metastable resonances. The anionic resonances of three isomers of $C_{10}H_8$ are investigated to reveal how atomic connectivity and structural variation shape the electronic and photochemical behaviour of astrochemically relevant PAH anions.

2.3 Aromatic Heterocycle Destruction in Astrochemically Relevant Analogues

Alexandra McKinnon *(1); Elettra L. Piacentino (2); Sam McGrath (3); Michelle R. Brann (2); Mahesh Rajappan (2); Ilsa Cooke (3); Karin I. Öberg (2)*
(1) Harvard University, (2) Center for Astrophysics | Harvard & Smithsonian, (3) University of British Columbia

Heterocycles are present in nucleobases, some sugars, and some amino acids, and they are hence expected to play an important role in any origins-of-life scenario. Their presence in comet 67P suggests that they form efficiently in molecular clouds and/or protoplanetary disks, but so far they have eluded detection outside of the Solar System despite the exquisite sensitivity of JWST and modern radio telescopes. To better understand in which astrophysical environments we may expect to find aromatic heterocycles, and to constrain when cometary ones originate from, we have undertaken a systematic laboratory study of the response of common aromatic heterocycles to FUV irradiation. In particular we have irradiated pyridine (C_5H_5N), pyrrole (C_4H_5N), and furan (C_4H_4O) ices with FUV light (120-160 nm) in an ultra-high vacuum chamber at low temperatures (10 K - 150 K) and low pressure (10^{-10} Torr) in a range of pure, undiluted ices and ice matrices. In contrast to benzene, all three heterocycles experience considerable photodestruction in undiluted ices at 10 K, and interestingly the dissociation cross section appears to correlate with the molecules' degree of aromaticity. Furthermore, the dissociation rate increases further at higher temperatures and when diluted in astrochemical ice analogues. We use these experimental results to calculate aromatic heterocycle lifetimes in different astrophysical environments, and to theorize what formation mechanisms are responsible for their existence in comets.

2.4 Synthesis and Analysis of Carbon Grains Formed from PAHs Under Astrophysical Conditions for Space Return Samples Applications

Pavithraa Sundararajan *(1,2); Ella Sciamma-O'Brien (1); Michel Nuevo (1); Duncan Mifsud (1,3); Claire Ricketts (1,3); Lora Jovanovic (1,3); Farid Salama (1)*
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Cosmic carbon is fundamental to the formation of COMs and is the primordial building block in prebiotic chemistry. In space, carbon is present in the form of simple diatomic, small hydrocarbon, and large complex molecules like PAHs. PAHs that can withstand harsh UV radiation present in space are thought to be the emitters of the Aromatic Infrared bands (AIBs). PAHs have also been identified in planetary objects (comets, asteroids, meteorites, Titan, etc). It is hence important to constrain the spectral characteristics of PAHs and their derivatives, and the COMs that could be produced from PAHs to aid their identification in space. The main goals of our research are: (i) to synthesize carbon grains made from small hydrocarbons and PAHs under astrophysical conditions using the COsmiC SImulation Chamber (COSmIC) Facility; (ii) to analyze the IR spectra of the synthesized carbon grains with the IR Micro-spectroscopy (I3OLAB lab); (iii) to measure their optical constants using the Optical Constants Facility (OCF); and (iv) to study the size distribution and morphology of these grains using the Scanning Electron Microscopy (SEM) facility, all housed at NASA Ames Research Center. The first results of this multidisciplinary study performed with two nitrogen-substituted PAHs — Quinoline and Acridine — will be showcased in the presentation. In addition, we will discuss the next steps of characterization of the COSmIC samples with Raman micro-spectroscopy. The data generated by this research will be provided to the scientific community through three databases: the Optical Constants database, the Nanograin database, and the NASA Raman spectral database. This work will also provide insights in understanding the link between PAHs, carbon grains and organics in meteorites.

2.5 Substituted PAHs in space: a laboratory study of the electronic signatures of oxanthrene and thianthrene

Maëva Louis *(1); Alexander Tielens (2); Alessandra Candian (1); Annemieke Petrignani (1)*
(1) Universiteit van Amsterdam, (2) University of Maryland

Polycyclic aromatic hydrocarbons (PAHs) are well established components of the interstellar medium [1],[2]. In recent years, a specific focus is given to functionalized PAH derivatives, particularly with the discovery of cyano PAHs [3],[4] or sulfur-bearing cyclic hydrocarbons [5]. These functionalized PAHs show distinct photochemical behaviors that can influence their stability and detectability in space. Among them, oxygenated PAHs (OPAHs) and sulfur-bearing PAHs (SPAHs) have attracted increasing interest due to their potential role in astrochemistry, with studies highlighting their unique electronic, vibrational, and rotational signatures [6],[7]. In this study, we aim to investigate the rovibrational electronic spectra of substituted three ring PAHs, with a specific focus on oxanthrene and thianthrene using both theoretical calculations and high resolution experimental techniques. The incorporation of heteroatoms into PAHs affects their photochemical behavior. These species have efficient intersystem crossing [8],[9], resulting in higher population of triplet states that may impact their stability under astrophysical conditions and increase their chemical reactivity. Special attention is given to understanding the photochemical properties of these molecules.

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2.6 A JWST Study of Polycyclic Aromatic Hydrocarbon Emission in a region of 30 Doradus

Congcong Zhang *(1); Joelene Hales (2); Els Peeters (2); Jan Cami (2); Ameek Sidhu (2); Junfeng Zhen (1)*
(1) Xiangtan University, (2) Western University

Polycyclic aromatic hydrocarbons (PAHs) are responsible for strong mid-IR emission features near star-forming regions. It is well known that low-metallicity environments exhibit weaker PAH emission, but it is not clear how the metallicity affects the properties of the emitting PAH population. We present a detailed study of the PAH emission in a region of 30 Dor, a well-known low-metallicity star-forming environment in the Large Magellanic Cloud (LMC) and we compare it to the PAH emission in the Orion Bar to investigate the characteristics of the PAH population and how the environments affect the resulting IR emission. We analyze JWST observations of 30 Dor that include imaging (NIRCam, MIRI) and spectroscopy (NIRSpec/IFU, MIRI/MRS). We extracted NIRSpec/IFU and MIRI/MRS spectra from 18 apertures that cover the morphological structures present within the observed region of 30 Dor. We characterize the profiles and relative intensities of PAH emission in these apertures. The detailed profiles of the PAH emission bands in 30 Dor are all similar and match with one of the dissociation fronts (DF2) in the Orion Bar, but their relative band ratios show a much larger range than in the Orion Bar. The PAH emission in 30 Dor originates from a population with a lower or similar ionization fraction than in the Orion Bar, and a size distribution that has more small-sized PAHs. Since smaller PAHs typically photo-fragment before larger PAHs, our findings support the hypothesis that the lower PAH emission for lower metallicities is the result of inhibition of growth toward larger PAHs rather than photo-fragmentation.

2.7 Near-Infrared Continuum Emission in the Orion Bar

Takashi Onaka *(1); Emmanuel Dartois (2); Els Peeters (3); Olivier Berné (4); Emilie Habart (5); Christiaan Boersma (6); Jan Cami (3); Asunción Fuente (7); Javier Goicoechea (8); Ozan Lacinbala (2); Yoko Okada (9); Alexander Tielens (10); Dries Van De Putte (3); Francois Boulanger (11); Thomas Pino (2); Yong Zhang (12)*
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Conspicuous excess emission is present in the near-infrared (NIR) region in various celestial objects, including reflection nebulae, planetary nebulae, and nearby galaxies. However, the spatial distribution and spectral shape of the excess emission remain poorly understood.

Using the three-dimensional spectroscopic data of the Orion Bar taken with the integrated field unit of NIRSpec on JWST from the Early Release Science program "PDRs4All", we study the NIR continuum emission spectroscopically and obtain its spatial distribution relative to the aromatic infrared band (AIB) at 3.3 μm in the Orion Bar proto-typical photo-dissociation region (PDR). Contribution from the foreground ionized gas is estimated with the Cloudy code and subtracted. The observed regions are divided into nine physically distinct regions and an average spectrum is derived for each of them. The nine regions, including the ionized gas, atomic PDR, and molecular PDR, clearly show remaining continuum in the region 1–4.5 μm. The continuum at wavelengths longer than 2.7 μm shows good correlations with the 3.3 μm AIB, while the correlation of continuum around 1.2 μm is not significant. We further find that the NIR continuum in the Orion Bar can be approximated by a summation of two blackbodies. The low-temperature component shows a good correlation with the AIB, while the high-temperature component does not.

We discuss possible origins of the NIR continuum, among which recurrent fluorescence from carbon clusters would better explains the observed low-temperature component.

2.8 PAH emission in cluster galaxies: A JWST/NIRCam view of environmental processing

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PAH emission is widely used as a tracer of star formation in galaxies, yet the impact of the extragalactic environment on PAH molecules remains poorly constrained. In this poster, I present an analysis of 3.3 μm PAH emission maps obtained with JWST/NIRCam, on both field and cluster galaxies at $0.2 < z < 0.4$. By combining PAH measurements with UV-to-MIR SED fitting and environmental diagnostics, such as the distance from the cluster centre, I statistically investigate how PAH emission depends on both galaxy properties and the environment.

I also focus on galaxies undergoing ram pressure stripping (RPS), one of the strongest environmental mechanisms in clusters. I show a spatially resolved analysis of PAH emission in both galaxy disks and the stripped tails, reporting the detection of PAH 3.3 μm emission in eight out of nine RPS galaxies in the Abell 2744 cluster. The PAH maps reveal morphologies characteristic of RPS, including disk truncation and elongation, supporting a scenario in which the PAH molecules are stripped together with the gas. Crucially, PAH emission is detected in star-forming clumps embedded in stripped tails up to 40 kpc from the galaxy's main body. This result provides direct evidence that PAH-carrying molecules can survive the stripping process and persist in the intracluster medium.

Finally, I find that star formation rates inferred from PAH 3.3 μm are consistent with those derived from SED fitting (averaged over 100 Myr) with an intrinsic scatter of 0.4 dex, although the relation is age-dependent. The agreement also holds in the stripped tails, suggesting that the young stars remain the primary exciters of PAH molecules even in these extreme environments.

2.9 Catalytic Nucleation of PAHs onto Inorganic Dust Grains

Rebecca Firth *(1); Ryan C. Fortenberry (1)*
(1) The University of Mississippi

The surfaces of inorganic dust grains can act as a catalyst for the nucleation of various organic and prebiotic molecules including polycyclic aromatic hydrocarbons (PAHs). This work shows that inorganic oxide clusters are able to form energetically favorably from diatomic molecules in the circumstellar envelopes (CSEs) of stars. While the inorganic oxide clusters are growing, they are traveling towards the outer edge of the CSE before leaving to float through the interstellar medium (ISM). Heavy metallic elements are much less abundant in the ISM than carbon, thus suggesting the inorganic oxide clusters are more likely to react with carbon-abundant molecules after leaving the CSE. PAHs nucleating onto the inorganic dust grains could provide the basis for the formation of carbonaceous chondrites with calcium and aluminum-rich inclusions (CAIs). Combinations of density functional theory (B3LYP) and explicitly correlated coupled cluster theory [CCSD(T)-F12] with a triple-zeta basis set are used to investigate how the small cyclic aromatic hydrocarbons cyclopropenylidene (c-C_3H_2) and benzene (C_6H_6) can nucleate onto inorganic oxide clusters containing aluminum and calcium.

2.10 Quantum Chemical Predictions of PAH IR Spectra

Nolan White *(1); Ryan C. Fortenberry (1)*
(1) University of Mississippi

A novel semi-empirical method developed in our group is showing that the anharmonic vibrational spectroscopic features for various types of polycyclic aromatic hydrocarbons (PAHs) match notable portions of interstellar IR spectra observed for more than half a century. This quantum chemical study is utilizing various sized PAHs from naphthalene ($C_{10}H_8$) even up to circumbiphenyl ($C_{38}H_{16}$) as the sample set for such astronomical comparison giving consideration to most PAH structural motifs. The computed, numerical quartic force fields coupled to second-order vibrational perturbation theory clearly confirm that PAH C-H stretches are responsbile for the features close to 3000 cm^{-1}. Additionally, mid-IR features of neutral PAHs may be responsible for the baseline in regions typically assigned to PAH cations. Finally, the out-of-plane motions are in line with what previous, scaled-harmonic frequencies have implied for PAHs, but the anharmonicity available in this trained semi-empirical method provides direct evidence to confirm what has been proposed for decades.

2.11 Tracing PAH populations with JWST using weak 5–6 µm bands in the Orion Bar

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Polycyclic aromatic hydrocarbons (PAHs) produce a set of infrared emission bands known as aromatic infrared bands (AIBs) and are widespread in the interstellar medium. These bands are widely used as tracers of star formation and interstellar conditions in both Galactic regions and external galaxies. The unprecedented sensitivity and spatial resolution of the MIRI-MRS on the James Webb Space Telescope (JWST) now allow the Orion Bar photodissociation region (PDR) to be probed in exceptional detail. Here we investigate the weak and rarely studied AIBs at 5.25, 5.75, and 5.90 µm across the key zones of this strongly UV-illuminated PDR to constrain their carriers and their evolution across the PDR.

The 5.25 and 5.75 µm AIBs show a spatial distribution like that of the main AIBs, with emission peaking in the atomic PDR. In contrast, the 5.90 µm AIB exhibits a distinct spatial behavior intermediate between the main AIBs and bands associated with aliphatic material or PAH clusters and very small grains (VSGs). Spectrally, the 5.90 µm AIB has a symmetric profile, whereas the 5.75 and

5.25 µm AIBs display more complex structures. In particular, the 5.75 µm AIB can be decomposed into three components whose relative intensities vary across the Orion Bar.

Correlation analyses and principal component analyses indicate that these components trace different PAH populations: one is associated with fragile PAHs and VSGs in shielded molecular zones, while the others are linked to stable neutral and cationic PAHs in more strongly UV-irradiated regions. These results highlight the diagnostic potential of the weak 5–6 µm AIBs for probing the evolution of PAH populations across photodissociation regions and for interpreting JWST observations of star-forming environments in nearby galaxies.

2.12 Benchmarking Computational Methods for Anharmonic Vibrational Spectra of Substituted Polycyclic Aromatic Hydrocarbons

Rachel Huchmala *(1); Vincent Esposito (1)*
(1) Chapman University

Cyano-substituted PAHs (CN-PAHs) have been detected in TMC-1 in the gas-phase using radio astronomy. The confirmed presence of CN-PAHs in space begs the question of whether they can be detected in the IR with JWST. To do that, accurate reference data are needed to interpret the observational spectra. The same electronic effect induced by the cyano substituent in CN-PAHs that enables radio detection also leads to a unique CN stretch vibrational motion. In this study, various density functional theory (DFT) methods are benchmarked against available gas-phase experimental data for CN-PAHs as well as their NC-PAH isomers. Ethynyl-substituted PAHs are also expected to play a role in carbonaceous molecular growth in space, and so similar computational benchmarking has been undertaken for this family of molecules. Additionally, reactions have been explored for the possible formation mechanism of cyanobenzene in Titan's atmosphere.

2.13 Radiative stabilization of Phenylium: Constraints on exothermicity in radiative assosiation

Arun Subramani *(1); James N. Bull (2); Paul Martini (1); MingChao Ji (1); Henning Zettergren (1); Henning T. Schmidt (1); Henrik Cederquist (1); Mark Stockett (1)*
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Aromaticity appears to be ubiquitous even in harsh astrophysical environments, as increasingly revealed by observations from JWST. However, the formation of the first aromatic ring, benzene, in such environments remains poorly understood. Extensive chemical networks have been proposed to explain its formation under different conditions. In many of these networks, the dominant pathway involves dissociative recombination of $C_6H_7^+$, which is formed through reaction of the phenylium cation with H_2, highlighting the importance of phenylium in benzene chemistry. However, the formation of phenylium through radiative association pathways included in these networks has recently been questioned. Given the detection of benzene (and by extension phenyl) in environments with varying physical conditions and chemical compositions, multiple formation pathways could contribute to its abundance. Constraining these pathways is therefore essential to identify viable routes to benzene formation. In radiative association, an important constraint is whether the newly formed species can be radiatively stabilized while carrying the internal energy released upon formation. To investigate this, storage-ring experiments with phenylium ions were carried out at DESIREE. The cryogenic, ultra-high-vacuum conditions at DESIREE allow ions to be stored and studied in isolation, making the measurements directly comparable to astrophysical environments. The absolute dissociation rate of phenylium was obtained from lifetime measurements. By modelling the measured rates with radiative cooling and dissociation rate coefficients, we find that phenylium can be radiatively stabilized against up to 5.02 eV of internal energy, setting an upper limit on the exothermicity of possible radiative association channels.

2.14 Towards proper astrophysical modelling of large interstellar cyclic species: the case of collisional excitation of cyclopentadiene

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Complex organic molecules, including large cyclic species, are prevalent in interstellar space and play a vital role in various astrochemical processes. Cyclopentadiene (C_5H_6) has recently been detected in several interstellar molecular clouds. While its spectroscopic properties have been accurately measured, collisional rate coefficients for its rotational transitions were previously unavailable. As these transitions are typically targeted in radio astronomical surveys, the lack of collisional data hinders the appropriate interpretation of observed emission lines.

We have conducted a thorough theoretical study to calculate the thermal rate coefficients for the rotational transitions of cyclopentadiene, which are essential for non-local thermodynamic equilibrium (non-LTE) radiative transfer modelling. Accurate quantum scattering calculations were performed to study its collision with helium. In particular, close-coupling and coupled-states methods were employed based on a highly correlated three-dimensional rigid rotor potential energy surface. Our study covers a wide range of rotational states, spanning levels up to $j \leq 25$. The calculated rate coefficients allow proper astrophysical modelling at kinetic temperatures ranging from 10 to 50 K.

Our first radiative transfer simulations showed that most cyclopentadiene rotational levels are thermalised under typical cold cloud conditions, exhibiting minor non-LTE effects. At the same time, we were able to draw some important conclusions regarding the collisional excitation mechanisms of complex cyclic and aromatic interstellar species, which could facilitate a more accurate interpretation of future detections.

2.15 Closing the loop: Mutual neutralization of PAH ions

Mark Stockett *(1); Danial Mohammadi (1); Arun Subramani (1); James N. Bull (2); Henrik Cederquist (1); Michael Gatchell (1); MingChao Ji (1); Paul Martini (1); Åsa Larson (1); Henning T. Schmidt (1); Richard D. Thomas (1); Henning Zettergren (1)*
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The identification of specific PAHs in TMC-1 has challenged state-of-the-art models of interstellar cloud chemistry, which under-predict the observed abundances by orders of magnitude. Numerous laboratory studies have now established that PAHs are rapidly stabilized by thermal photon emission following ionizing collisions with atomic cations, considered the most important PAH destruction channel in molecular clouds. In most cases, the primary mechanism of radiative stabilization is recurrent fluorescence, optical photon emission from thermally excited electronic states. From a laboratory perspective, the next logical step is to determine the fate of the PAH cations resulting from these reactions.

Neutralization of PAH cations would close the loop, leading back to the neutral PAHs identified by radioastronomy. In dense clouds like TMC-1, negative charge is expected to be carried by molecular anions including PAHs. Mutual neutralization (MN) between PAH cations and PAH anions has long been considered a key process in the chemistry of interstellar clouds, but no experimental studies of PAH-PAH MN have been reported.

We have investigated MN between positively and negatively charged ions of indenyl (C_9H_7) using the DESIREE infrastructure for merged ion beams experiments. With its high electron affinity and fully sp^3-hybridized structure, indenyl is useful as a tractable model system for the much larger PAHs generically considered by astrochemical models. We find the majority of MN reactions to be non-dissociative, leading to excitation energies around 4.5 eV, below the $\sim$5 eV dissociation threshold. This supports the notion of PAH recycling, helping to rationalize the anomalously high abundance of PAHs observed in TMC-1.

2.16 One Photon at a Time: A Fast New Framework for Modeling PAH Emission Spectra

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PAH emission spectra encode rich information about the underlying physical properties of PAH populations, including their sizes, compositions, and ionization states. However, interpreting these spectra is complicated by degeneracies between PAH properties and the characteristics of the radiation field responsible for heating them — degeneracies that are difficult to break using existing theoretical models.

We present a novel approach to modeling PAH spectra that leverages the single photon approximation for PAH heating and emission. This method achieves a speedup of over an order of magnitude in the computation of PAH emission spectra compared to existing approaches, dramatically reducing the computational cost of producing theoretical models of PAH emission spectra. This model is now publicly available in the Python library pah_spec. Its computational efficiency opens new pathways for fitting theoretical models to observed data via, e.g., MCMC-style routines, and enables the incorporation of PAH heating into dust radiative transfer frameworks. I will discuss the ongoing implementation of pah_spec in the dust and PAH radiative transfer code, POWDERDAY, and prospective applications to synthetic observations from hydrodynamical simulations.

2.17 The NASA Ames PAH IR Spectroscopic Database / New Library of Anharmonic Computed and Gas-phase Laboratory Spectra

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The importance of anharmonicity to the nature of the astronomical PAH emission bands was recognized soon after their discovery. Anharmonicity predicted, among others, the presence of a combination band at 5.25 μm. Subsequently, this feature was searched for and found, underpinning the presence of PAHs in space. The bedrock laboratory studies to interpret and analyze astronomical PAH observations, ultimately enabling their use as probes of and establishing the inherent roles they play in defining their astrophysical and astrochemical environments, all presented anharmonicity. As the astronomical PAH field evolved, it became clear that the PAH population in space has a size range that extends far beyond what is possible to study experimentally. This motivated the development of pioneering quantum-chemical techniques to compute the requisite spectra. However, these techniques, out of necessity, relied on the harmonic approximation. Nonetheless, the need to address anharmonicity eventually caught up as the high-fidelity observations by the James Webb Space Telescope (JWST) require commensurate computational data that fully embrace it. Leveraging improvements in computational techniques, ever growing raw compute power, and laboratory advancements to obtain gas-phase reference data, computing anharmonic spectra of small PAH is now feasible, with extension to larger PAHs in the future. This poster reports on the release of a new anharmonic computed and high-resolution gas-phase laboratory-measured library to the NASA Ames PAH IR Spectroscopic Database (PAHdb). PAHdb can be accessed at www.astrochemistry.org/pahdb, where these new data can be browsed and downloaded. PAHdb and these new data provide the JWST community with the means to get the most out of their observations.

2.18 Producing naphthalene in Titan's atmosphere

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The atmosphere of Saturn's largest moon, Titan, features a rich hydrocarbon photochemistry that efficiently converts the primordial methane to larger unsaturated organic species. Hyperspectral imagery of Titan from the NASA/ESA Cassini-Huygens mission consistently features day-

side 3.38 µm emission feature in the upper atmosphere attributed to PAH's with up to 18 rings [1], and in-situ mass spectra of Titan's ionosphere suggest the presence of a range of PAH and nitrogen-containing PAH species with up to 24 C atoms, or 5 to 6 rings [2]. However, the chemical reactions leading to PAH formation in Titan's atmosphere are currently unknown; the largest species explicitly represented in the current state-of-the-art Titan photochemical models are substituted benzene species. We have reviewed the literature on potential naphthalene-forming reactions and identify several candidate reactions that produce naphthalene or molecules with the naphthalene skeleton. The most promising reactions for producing the naphthalene skeleton are phenylethynyl ($C_6H_5C_2$) addition to ethylene (C_2H_4) or propylene (C_3H_8) to produce naphthalene or methylnaphthalene, respectively; repeated additions of ethynyl radicals to benzene to form ethynylnaphthalene (3 C_2H + $C_6H_6 \rightarrow C_{10}H_7C_2H$); and reaction of acetylene with a phenylacetylene cation to produce a naphthalene cation (C_2H_2 + $C_6H_5C_2H^+ \rightarrow C_{10}H_8^+$). These reactions are being incorporated into a photochemical model of Titan's atmosphere [3], and we will present preliminary results.

[1] López-Puertas, M., et al., 2013. ApJ 770, 132. Stikkelbroeck, F., 2025. Master's Thesis. Univ Amsterdam. [2] Haythornthwaite, R.P., et al., 2021. Planet. Sci. J. 2, 26. [3] Vuitton, V., et al., 2019. Icarus 324, 120–197. Lavvas, P., et al., 2025. EPSC-DPS2025-220.

2.19 Energetic processing of hydrocarbon ices: application to Titan

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The Cassini-Huygens mission detected large amounts of positive ions in the moon's ionosphere via mass spectrometry that have been identified as PAHs and PAH derivatives [1]. Remote-sensing infrared measurements have also suggested the presence of PAHs/PANHs with up to 10–11 rings in the atmosphere [2,3]. These species are considered key ingredients for the formation of the aerosols responsible for Titan's orange haze layer. They can also end up closer to the surface, where they would condense, as happens to benzene (C_6H_6) and other hydrocarbons. However, the fate and role of condensed PAHs in Titan's lower atmosphere remain unclear. We used the AQUILA chamber at the ECRIS Facility at HUN-REN ATOMKI to investigate the energetic processing of pure ices of phenanthrene ($C_{14}H_{10}$), acetonitrile (CH_3CN), and their mixtures by 10 keV H^+ (protons), simulating cosmic ray processing of the ice. Pure phenanthrene and acetonitrile samples show different behaviours: phenanthrene ice undergoes compaction while bombardment of acetonitrile produces new chemical species. Interestingly their mixture $C_{14}H_{10}$:CH_3CN shows the formation of the same species as for the acetonitrile-only ice, but at lower abundance, suggesting that phenanthrene molecules within the mixture partially protect the acetonitrile from the bombardment. The results of this study have implications for our understanding of hydrocarbon-ice evolution in Titan's lower atmosphere.

2.20 Attack on Titan: PAH contribution

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The atmosphere of Titan is a key environment for studying complex organic chemistry in a cold, oxygen-poor and nitrogen-rich environment. Photochemistry of CH_4 triggers a rich chemistry, leading to the detection of several organic molecules, including benzene. In addition, Polycyclic Aromatic Hydrocarbons (PAH) molecules have been invoked to explain the signal leftover from the non-LTE modelling of CH_4 in VIMS limb data. In this work, we reanalyse Cassini VIMS limb spectra using version 4.0 of the NASA Ames PAHdb. We model the PAH emission mechanism,

considering the solar irradiance spectrum at the date of the observations and extending the photo-absorption cross-section down to the near infrared. A Non-Negative Least Square (NNLS) fitting is used to obtain information on average PAH size that best fits the VIMS data at different heights and uncertainty is evaluated using a Monte Carlo technique. We follow up with Non-Negative Least Chi-square minimization fitting to gain insight on the type of single PAHs that could reproduce the VIMS residual features.

Even considering a larger database of PAHs with different sizes, the average number of aromatic rings of the best-fitting PAHs is only slightly higher than the 10-11 rings found in the earlier study. Also, surprisingly, the largest PAHs are found at higher altitude, up to 1000 km, which is counterintuitive given that PAHs are believed to be the seeds for aerosols formation and their size should increase as the altitude decreases. When looking at which single PAH molecule best fit the data, we find the asymmetric, catacondensed PAHs are preferred. These findings challenge existing models of PAH growth and survival in Titan's atmosphere and call for new modelling efforts.

2.21 Tracing Photochemical Evolution in the ISM using the 11.2 μm / 3.3 μm size diagnostic

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Polycyclic aromatic hydrocarbons (PAHs) are important tracers of the chemical and physical evolution of the interstellar medium (ISM), including high-energy environments such as star-forming regions in galaxies and protoplanetary disks. It is therefore vital to probe the relationship between ISM phases and the PAH populations within them.

In this work, we use JWST NIRSpec and MIRI-MRS observations to investigate PAH size variations across the photo-dissociation region (PDR) of the reflection nebula NGC 7023. We employ the well-established 11.2 μm / 3.3 μm ratio as a size diagnostic. Because PAH size is regulated by the local radiation field, NGC 7023 – with its multiple H_2 dissociation fronts– provides an ideal environment to examine how PAHs evolve from exposed atomic regions into shielded molecular gas. JWST's unprecedented spatial and spectral resolution reveals substructure in the 11.2 μm band due to a carrier that behaves independently of PAHs and that we attribute to very small grains (VSGs) and/or PAH clusters (Khan et al. 2025), previously undetectable with Spitzer. By removing this non-PAH contribution, we obtain for the first time a clean measurement of the 11.2 μm PAH feature for use in the 11.2 μm / 3.3 μm diagnostic. We find that smaller PAHs are progressively destroyed as the radiation field strengthens in the atomic region, leaving behind larger PAHs. The smallest PAHs gather at the first H_2 dissociation front, marking the transition from atomic to molecular gas, while the largest PAHs reside deeper in the molecular cloud. These results demonstrate that, with JWST and the removal of VSG contamination, the 11.2 μm / 3.3 μm ratio provides an uncontaminated probe of PAH photochemical evolution in high-radiation environments of the ISM.

2.22 Constrain star formation criteria by comparing statistics of ISM structures in simulations with PHANGS observations

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The complex structure of the ISM, comprised of filaments and cavities, is driven by feedback from stellar winds, SNe, and galactic dynamical processes. With the advent of JWST, the ISM in nearby galaxies can now be resolved on spatial scales of $\sim$10 pc, providing critical constraints for feedback models in galaxy simulations. However, JWST observes PAH emission features, which are not a direct tracer of the gaseous ISM in galaxy simulations. Therefore, it is essential to generate PAH emission maps from these simulations. In this work, we post-process FIRE cosmological

zoom-in simulations with the radiative transfer code SKIRT to forward-model MIR photometric images (e.g., MIRI F770W). These synthetic observations provide the first PAH emission images of simulated galaxies on JWST-resolution scales. Using the persistent homology package Perch, we identify PAH-traced ISM structures based on their topological features and compare with observations from the PHANGS–JWST survey of the nearby spiral galaxy NGC 628. By statistically characterizing the ISM structures in PAH maps from both simulations and observations, we quantify how PAH emission traces the underlying ISM structure and assess its potential to constrain star formation and feedback models in zoom-in galaxy simulations.

2.23 Changes in PAH spectral class and molecular properties in the Red Rectangle with JWST

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The Red Rectangle is a carbon-rich proto-planetary nebula associated with the post-AGB binary HD 44179 and characterized by oppositely directed outflows. This unique environment provides an excellent laboratory to study the evolution and processing of carbonaceous material, including polycyclic aromatic hydrocarbons (PAHs). We present JWST MIRI MRS observations obtained along the southwest whisker of the Red Rectangle. The spectra reveal PAH emission with aromatic infrared band (AIB) Class A profiles, where the 7.7 µm complex peaks near 7.6 µm. In contrast, ISO observations of the central region of the nebula show Class B profiles with the 7.7 µm complex peaking near 7.8 µm. This change in AIB profile class indicates a modification of the molecular structure of the emitting PAHs. The JWST observations further reveal variations in PAH charge state, size, and molecular properties across the field of view, including along the outflow, along the whisker (the edge of the outflow), and in regions outside the outflow. These observations provide new insight into PAH evolution in the complex outflow environment of the Red Rectangle.

2.24 Gas-phase IR spectra of anionic fullerenes

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We report new experimental infrared spectra for the anionic fullerenes C_{60}^-, C_{70}^- and C_{84}^- in the 400-1800 cm^{-1} region. The spectra were recorded using IR multiple-photon detachment spectroscopy in an ion trap mass spectrometer using the tunable IR radiation from FELIX. For anionic C_{60} and C_{70}, our results are consistent with previously reported spectra obtained in the gas phase and/or in rare-gas matrices, but are generally of better quality. The experimental IR spectra of the three fullerene radical anions suggest that there may not be a generic fingerprint IR spectrum for anionic fullerenes but that each species possesses a distinct spectrum. The gas-phase spectrum of the C_{60} anion aligns well with theoretical predictions at the B3LYP/6-31++G** level of theory, whereas significant deviations are observed for the C_{70} anion, confirming previously reported matrix-isolation spectra. This lack of agreement has previously been attributed to the presence of low-lying electronic states in the radical anion and comparison with theoretical spectra at alternative levels of theory are presented. For the C_{84} radical anion, no previous spectra are available as far as we are aware. Harmonic frequency calculations at the B3LYP/6-31++G** level were conducted for the 24 isomers obeying the isolated pentagon rule. The match between experiment and theory is generally good and allows us to constrain the number of possible isomers of C_{84}^- in our experiment.

2.25 Tracing Fullerene-Linked Dust Variation in Tc 1 with JWST

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We have observed the archetype fullerene-rich planetary nebula Tc 1 with the MIRI/MRS on JWST. We study the dust environment in detail, and link dust variation to fullerene formation processes. Understanding the dust processing in sources like Tc 1 is crucial to gaining insights into the formation of aromatic molecules in space. The mid-infrared spectra of this spatially resolved source reveal that the fullerene emission is not co-spatial with the dust emission. Two broad plateau-like features can be distinguished in the mid-IR spectrum: one at 6–9 µm and one at 9–13 µm. Spectral variations of the 9–13 µm plateau reveal at least three distinct components, peaking at 9.5 µm, 11 µm and 12 µm respectively. SiC produces most likely at least one of those components (11 µm) and we find evidence that a second component (12 µm) is likely produced by SiC grains too. The variation in relative strength of these two components across the field of view hints at dust processing taking place in Tc 1. The third component of the 9–13 µm plateau — peaking at 9.5 µm — has a strong correlation with the SiC component(s) and is thus likely produced by similar material. The 6–9 µm plateau does not change shape spectrally across the entire field of view, indicating it is produced by stochastically heated material. We discuss the ramifications of these results for the formation of aromatic molecules.

2.26 Survival of Polycyclic Aromatic Hydrocarbons in the ionized environment of Tc 1

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We detect Polycyclic Aromatic Hydrocarbons (PAHs) in the HII region of the fullerene-rich planetary nebula (PN) Tc 1. JWST/NIRSpec and MIRI/MRS observations reveal the 3.3, 6.2, and 11.2 µm Aromatic Infrared Bands (AIBs) across this region. Their relative strengths (3.3/11.2 and 6.2/11.2) imply a population slightly smaller than in the Orion Bar. Additionally, the charge distribution shows a radial gradient from predominantly charged species close to the central star to predominantly neutral near the edge of the bright core. We estimate the timescale for photo-fragmentation and find that PAHs with more than $\sim$54 C atoms survive in Tc 1 over the kinematic age of the bright core of the nebula, whereas smaller PAHs are destroyed. For these surviving PAHs, photo-

ionization is the dominant channel upon photon absorption; however, the high electron density in the HII region drives rapid recombination, retaining a moderately ionized population close to the central star and a predominantly neutral population near the edge of the bright core.

2.27 IGRINS and JWST Spectroscopy of the AIB-Emitting Planetary Nebula NGC 6644

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We report results from a high spectral resolution (R = 45,000) near-infrared (H and K band) slit-scan spectroscopic map of the planetary nebula NGC 6644, obtained with the 2.7m Harlan j. Smith Telescope at the University of Texas' McDonald Observatory. The high velocity (+199 km/s) and subsolar metallicity of NGC 6644 imply that it originates from an old Galactic population. The 15" x 15" map, taken with the Immersion Grating Infrared Spectrometer IGRINS (Sawcyznec, Kaplan, Mace, et al. 2025, PASP, 137, c4505S and references therein), is centered on the bright, compact (3") central torus which was observed with the NIRSpec IFU and MIRI-MRS on JWST under program GO-07965 (P.I. E. Peeters), but also includes the spatially extended bipolar lobes oriented previously reported by Hsia, Kwok, Zhang, et al. (2010, ApJ, 725, 173H). The IGRINS data reveal a gradient in the centroid velocity across the central torus in ionized species, while the bipolar lobes show similar radial velocities, suggesting that their expansion is primarily in the plane of the sky. The 2.12 micron 1-0 S(1) line of H_2 is relatively weak in both the IGRINS and JWST spectra. Other features seen include [Fe II] and [Fe III] lines that provide potential diagnostics of the UV radiation field and physical conditions (e.g., Kaplan, Dinerstein, & Jaffe 2026, AJ, 171, 219). These tracers will be compared with properties of the aromatic features such as band ratios and profiles. We confirm the presence of a strong emission line of Se (Sterling, Porter, & Dinerstein 2015, ApJS, 218, 25S), indicative of enhanced abundances of neutron-capture species due to s-processing within the AGB progenitor star.

This work received support from grants NSF AAG 2307117 and STScI GO-07965.003-A and 07965-022-A.

2.28 PAH Spectral Diversity in NGC 7027 and the Evolution of Aromatic Carriers

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Polycyclic aromatic hydrocarbons (PAHs) constitute a significant fraction of the Universe's carbon budget, playing a key role in the cosmic carbon cycle and dominating the mid-infrared spectra of many astrophysical environments. Although PAHs likely form in the circumstellar envelopes of carbon-rich evolved stars, their subsequent evolution remains poorly understood. How pristine circumstellar hydrocarbons evolve into the PAHs observed in the interstellar medium remains unclear. We analyze JWST MIRI MRS spectral cubes (5–18 μm) of the young, carbon-rich planetary nebula NGC 7027 to investigate the evolution of aromatic carriers in a circumstellar environment. These observations reveal, for the first time in a single source, spatially resolved variations in PAH spectral profiles across classes A, AB, and B in all major PAH bands (6.2, 7.7, 8.6, and 11.2 μm). The spectral variations correlate with morphological structures in the nebula. Decomposition of the 6–9 μm features shows strong correlations among the red components of the 6.2, 7.7, and 8.6 μm bands, while the blue components of the 6.2 and 7.7 μm bands correlate separately. In contrast, the blue component of the 8.6 μm band behaves independently. These correlations point to distinct PAH subpopulations with different molecular structures. Decomposition of the 11.2 μm band confirms two components, with the broader 11.25 μm component attributed to emission from very small grains or PAH clusters. The variation of PAH profile classes with proximity to the central star

suggests that class B PAHs represent more processed species, while class A PAHs remain relatively pristine, challenging current notions of the spectral evolution of PAHs.

2.29 PAHs 101: A One-Stop Shop Benchmark in M101

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At metallicities below 0.2$\times$ solar, the abundance of PAHs relative to total dust mass drops precipitously, with differences in shielding, ISM density, UV field strength, and grain growth and destruction and mechanisms all proposed to cause this decline. With an exquisite array of ancillary data and a dramatically-steep metallicity gradient, the nearby, massive spiral galaxy M101 provides a controlled, single-galaxy laboratory for untangling the effects of local properties on PAH feature variations and the drivers of the decline with metallicity. Here I present a preliminary look at the results of a comprehensive imaging program with JWST/NIRCam and MIRI in 6 fields across M101 that span $>$1 dex in metallicity, neutral and ionized gas density, and UV field strength. With $\sim$3500 high S/N PAH measurements (at a binned GALEX-like resolution of 2″), we can remove confounding variables by examining how PAH strengths and ratios vary with just one parameter (e.g., metallicity) while others are held fixed. I show preliminary feature ratio maps across our 6 fields, along with semi-quantitative results relating emission from PAHs, warm dust, and ionized gas.

2.30 PAH Sizes and Ionization on the Cosmic Noon Main Sequence with MIRI/LRS

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Pre-JWST, the 3.3 µm PAH feature - a key PAH grain size and ionization tracer - was only accessible in the brightest galaxies beyond the local Universe, limiting our ability to understand the effects of evolving interstellar conditions with redshift on PAHs. Now, JWST's unprecedented sensitivity provides the power to effectively trace interstellar conditions with the 3.3 µm PAH to cosmic noon and beyond in typical, main-sequence star-forming galaxies. We present the initial results of a MIRI/LRS slit-stepping program to obtain efficient, spatially resolved measurements of the 3.3 and 6.2 µm PAH features in 22 main-sequence galaxies near redshift 1: this is the first sample to probe the 3.3 µm PAH at $log(L_{IR}) < 11.5$ outside the local Universe, and the only JWST program so far to do so in a spatially resolved manner. We discuss our observational design, data reduction considerations, and custom cube-building procedure; the intensities and ratios of the PAH features in our sample compared to local galaxies at similar IR luminosity; and their implications for the grain size distribution and ionization conditions of PAHs at high redshift as a function of the radiation field strength within galaxies.

2.31 Spectroscopy and photochemistry of aromatic molecules in para-hydrogen matrices.

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With the successful launch and application of the James Webb Space Telescope (JWST), a new source of high-resolution infrared (IR) data is becoming readily available. However, this data is only useful in conjunction with further experimental and theoretical work to support it. Matrix isolation is a useful experimental tool for examining the spectroscopy and photochemistry of molecules of interest. Para-hydrogen (p-H_2) is a unique medium for matrix isolation in comparison to other common media such as argon, krypton and neon. At cryogenic temperatures conversion from the ortho-hydrogen (o-H_2) isomer becomes more efficient and forms a "quantum" solid on cold surfaces. The p-H_2 isomer has anti-parallel nuclear spin states and occupies a lower energy rotational state ($J = 0$) meaning it has no net nuclear spin and minimal anisotropic effects. Weak intermolecular interactions and broad optical transparency allow for narrow well-resolved lines in IR

spectroscopy. In addition to this, the relatively large zero-point lattice vibrations of p-H_2 molecules grant more spatial freedom to guest molecules and provide an environment akin to the interstellar gas phase when it comes to studying their photochemistry. In our work we have studied a number of aromatic molecules, focussed mainly on polycyclic aromatic hydrocarbons (PAHs) and their nitrile derivatives. We obtain high resolution (0.1 cm^{-1}) FTIR spectra, as well as studying their photochemistry when irradiated with vacuum ultra-violet (VUV) light sources in a cold ($<$10 K), low pressure ($\sim 10^{-7}$ Torr) environment. Helping us to understand the photo-kinetics leading to their dissociation and the mechanisms for the formation of photo-products.

2.32 Spectroscopic validation of JWST PAH photometric prescriptions

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The 3.3, 7.7, and 11.3 μm infrared emission features are key tracers of the carbonaceous dust content and physical conditions in photodissociation regions (PDRs) and star-forming galaxies. With JWST, numerous photometric prescriptions have been proposed to isolate these features from NIRCam and MIRI broadband imaging, yet their accuracy relative to spectroscopic ground truth has not been systematically assessed across all three bands. We present such an assessment using JWST/NIRSpec and MIRI/MRS integral field unit (IFU) spectroscopy of local PDRs such as NGC 7023 (Misselt et al. 2025) and the Horsehead Nebula (Abergel et al. 2024), as well as the nearby galaxy NGC 7469 (PDRs4All XVI., Van De Putte 2025). Using PAHfit decomposition (Van De Putte et al. 2024, 2025, 2026), we construct synthetic photometry to evaluate published prescriptions within continuum-subtraction frameworks. For each band, we define multiple spectroscopic ground truths spanning individual sub-features to the full PAH complex, enabling us to identify which physical component each prescription recovers.

2.33 Uncovering new pathways to rich carbon chemistry in planetary nebulae

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The intense UV radiation fields in planetary nebulae (PNe, singular: PN) make them unique testbeds for studying the formation and evolution of a wide variety of molecules, including polycyclic aromatic hydrocarbons (PAHs) and fullerenes. JWST/MIRI observations of PN NGC 6302 have revealed two unexpected carbon species that uncover missing pieces in our astrochemical models. NGC 6302 is a butterfly-shaped PN containing several solar masses of O-rich gas. Its exceptionally hot central star ($T_{\rm eff} \sim 220000$ K) is obscured at optical wavelengths by a thick, dusty torus. Despite its O-rich environment, we detected CH_3^+, which is a key driver of organic chemistry in irradiated environments. Spatially resolved observations reveal that CH_3^+ is widespread across the central re-

gion and is co-located with PAHs, CO, H_2, and HCO^+. This suggests that CH_3^+ may be crucial for the formation pathway of PAHs and other carbon-bearing species. Moreover, we detected CO_2 ice and (cold) gas in the torus. The dense torus shields against intense UV radiation and enables ice chemistry, making this a unique site for the formation of complex organic molecules. Strikingly, the CO_2 gas-to-ice ratio exceeds that of young stellar objects by more than an order of magnitude, pointing to distinct ice formation or processing mechanisms in evolved stellar environments. The ice absorption profile exhibits a double-peak profile characteristic of pure, crystalline CO_2 ice. These detections reveal that chemical networks in PNe are far more extensive than current models predict, and incorporating CH_3^+ and CO_2 ice will be essential for understanding carbon chemistry in PNe and ISM enrichment by low-mass evolved stars.

2.34 Probing Aliphatic Signatures of PAHs in the Orion Bar

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Polycyclic Aromatic Hydrocarbons (PAHs) are carbonaceous molecules in the interstellar medium (ISM) widely considered carriers of the prominent mid-infrared emission bands observed in many astrophysical environments (Tielens 2008). These bands occur at 3.3, 6.2, 7.7, 8.6, 11.2, and 12.7 μm and vary from source to source, suggesting that the carriers of the unidentified infrared (UIR) bands depend on local physical conditions (Geballe 1997). Such variations indicate different PAH structures, including neutral, cationic and anionic PAHs, species substituted with heteroatoms (N or O), functional groups such as CN, OH, and CH^3, as well as hydrogenated or superhydrogenated forms (Buragohain et al. 2020; Yang, Li & Glaser 2020; Mishra et al. 2025). Besides the major bands, weaker features have been reported across the 3–20 μm region. One feature near 3.4 μm is commonly attributed to aliphatic C–H stretching modes from aliphatic side groups or superhydrogenated PAHs. This wavelength range lies within the coverage of the James Webb Space Telescope (JWST) Near-Infrared Spectrograph (NIRSpec). Here we analyze JWST/NIRSpec observations of the Orion Bar to investigate possible aliphatic hydrocarbon features and the relative contributions of aromatic and aliphatic structures. In addition, theoretical spectral analysis of PAH molecules is used to interpret the observed features and identify possible molecular carriers. The high sensitivity and spectral resolution of JWST enable the detection of weak features and the study of aliphatic-to-aromatic variations across regions with different physical conditions, providing insight into the chemical processing and evolution of PAHs under varying radiation environments.

2.35 The role of PAH in the dynamics of gaseous bubbles in nearby galaxies.

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Numerous bubble-like structures have been observed in nearby disk galaxies through the 7.7 μm band of PAH emission (Watkins et al. 2023). These bubbles are thought to repeatedly compress the interstellar medium (ISM) and promote the formation of atomic and molecular clouds; however, their origin has not yet been clearly established. In this study, we investigate the creation of bubbles by the expansion of supernova remnants (SNRs). We perform hydrodynamical simulations of multiple supernova explosions with dust destruction processes and radiation processes in shock waves and examine the dynamical evolution of SNRs and the role of PAH in bubble observations in detail. Based on these results, we develop a statistical model of bubble size histogram that takes into account the density distribution of the galactic disk and the star cluster mass function. We find that the resulting bubble size distribution strongly depends on the underlying galactic gas density distribution. This result provides a framework for constraining the density structure of galactic disks from the observed distribution of bubble sizes.

2.36 Missing Molecules: Implications of the Non-detections of Phenylpropiolonitrile and Phenyldiacetylene in TMC-1

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Phenylpropiolonitrile ($C_6H_5C_3N$) and phenyldiacetylene ($C_6H_5C_4H$) both exhibit several characteristics that make them favorable candidates for astronomical detection. However, neither molecule has been identified in TMC-1. The reported abundances of the C_3N and C_4H radicals in TMC-1 exceed those of the CN and C_2H radicals, respectively. At the same time, both $C_6H_5C_3N$ and $C_6H_5C_4H$ possess larger respective permanent dipole moments than benzonitrile and ethynylbenzene, both of which have already been detected in TMC-1. Furthermore, our investigations of the addition-elimination reaction potential energy surfaces for the reactions of C_3N and C_4H with benzene have revealed that each pathway proceeds barrierlessly. Together, these factors make the non-detection of $C_6H_5C_3N$ and $C_6H_5C_4H$ a surprising result. Motivated by this, we investigated alternate reaction pathways for C_3N and C_4H reactions with interstellar benzene which have revealed thermodynamically favourable annulation routes at low temperatures. Considering the available pathways for these two reactions, we made theoretical predictions for the kinetically favored products. We anticipate that reactions of polycyclic aromatic hydrocarbons with C_3N and C_4H are likewise important routes in dense molecular clouds.

2.37 Quantum chemical insights into the formation of cyanoacenaphthylene in cold interstellar environments.

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Following the initial detection of benzonitrile in the dense core in Taurus, TMC-1 a number of bare and cyano "tagged" polycyclic aromatic hydrocarbons (PAHs) have been discovered, facilitated by the GOTHAM and QUIJOTE surveys. The detection of both cyanonapthalenes and cyanoacenaphthylenes inspired this work to explore chemistry linking these molecules and their untagged bare parent molecules. In particular, the non-statistical column densities found for the different isomers of cyanoacenaphthylene is in marked contrast to the statistical abundances of 1, 2 and 4-cyanopyrene. Additionally, the currently available column densities for 1 and 2-cyanonapthalene in TMC-1 leave the ratio of these species as an open question supporting either equal abundances or a 60:40 ratio favouring 1-cyano.

The addition of cyano radicals (CN) provides a route to the formation of CN "tagged" PAHs, where this reaction is the dominant route to the formation of the CN tagged aromatic, the abundance of the parent aromatic can be inferred from the abundance of the tagged aromatic nitrile. Reactions introducing C_2 containing groups (C_2H and C_2H_2 addition to naphthalene and naphthyl) have the potential to yield acenaphthylene from naphthalene. Here we present a computational investigation using classical capture theory and ab-initio potential energy surfaces, calculated at the CCSD(T)-F12/cc-pVDZ-F12//wB97X-D4/def2-TZVPP level, in the master equation solver MESMER to predict low-temperature (< 50 K), low-pressure ($[H_2] < 105$ cm^{-3}) rate coefficients. This work provides insights into the formation of cyanonapthalene, acenaphthylene and cyanoacenaphthylene under conditions cold interstellar conditions.

2.38 Carbonaceous Nanodust Produced by WR140 Endures in its Extreme Stellar Environment

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Carbon-rich Wolf-Rayet (WC) binaries can evolve to a dust formation phase in less than a few million years, yet their contribution to the dust and PAH budget of the early and local universe has long been overlooked. Recent JWST observations have revealed that the carbonaceous material

produced by these stars survives for hundreds of years and therefore likely enriches the ISM with dust and aromatic molecules. The textbook example of such a dust producer is WR140. In this work, we investigate the bulk dust properties to explore the carbonaceous nanodust associated with the PAH emission features detected by MRS. By calculating the dust color temperature using MIRI Images, we find direct evidence of dust grains that are not in thermal equilibrium with the stellar radiation field. This confirms that there is a population of nano-sized dust grains that are heated by the intense stellar radiation, resulting in high, stochastic, temperature spikes. The dust surrounding WR140 remains in this transiently heated regime out to over 50,000 au from the central binary. This implies that the PAH-like molecules created by WR140 are robust; they survive the intense stellar environment and high velocities. Additionally, we modeled the dust emission with DustEM, employing a hydrogen-poor amorphous-carbon grain model. Our models show that the dust mass ratio of very small grains ($a \sim 0.002$ µm) to larger grains ($a \sim 0.15$ µm) remains relatively constant as a function of distance from the stars. These results confirm that the dust pushed toward the ISM by WR140 is composed, in part, of H-poor nanodust. It is evident that WR140 is a unique laboratory for studying the survivability of aromatic nanodust in an environment that may represent a major source for such molecules in the early universe.

2.39 Chemometric Decomposition of Polycyclic Aromatic Hydrocarbon (PAH) Emission In JWST/MIRI Spectra of The Orion Bar Using PAHdb

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Polycyclic aromatic hydrocarbons (PAHs) are the major contributors to the mid-infrared emission observed in photodissociation regions (PDRs). Interpreting spatial variations of these emission bands as changes in PAH population properties remains challenging due to the complexity of the observed spectra. While the interpretation can be supported by databases of simulated and measured PAH emission spectra, using such databases introduces its own set of challenges due to a large chemical diversity. In this study, we present a spectral decomposition method based on a reduced subset of the NASA Ames PAH IR Spectroscopic Database (PAHdb) and apply it to JWST/MIRI observations of emission features in the Orion Bar PDR. A chemically constrained PAH spectra library was produced by filtering species according to number of carbon atoms, charge state, and heteroatom content. To reduce redundancy while preserving the spectral diversity, principal component analysis (PCA) and a K-means clustering approach were used to organize the PAH spectra from the database into groups that represent the spectral variations. We then set up a fitting procedure and applied it to the continuum subtracted Orion Bar spectra using a non-negative least square (NNLS) method. Using the fit results, we derived the spatial distribution of PAH populations with different sizes and charge states. The method recovers meaningful spatial trends and provides an efficient way to trace PAH population properties across the observed region.

2.40 PDRs4All: JWST Reveals New 15–20 µm Aromatic Infrared Bands in the Orion Bar

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Polycyclic aromatic hydrocarbons (PAHs) give rise to prominent infrared emission bands and are a major reservoir of interstellar carbon. Through processes such as photoelectric heating, these molecules influence the thermal balance of the interstellar medium and contribute significantly to its energy budget. Understanding how PAH emission varies across different environments is therefore important for interpreting infrared observations of star-forming regions and galaxies. Aromatic infrared bands (AIBs) in the 15–20 µm wavelength range are thought to arise primarily from skeletal vibrational modes of large PAHs, yet their origin and behaviour across photodissociation regions (PDRs) remain poorly understood. We analyze JWST MIRI MRS observations of the Orion Bar to investigate the AIBs and better constrain the processes influencing their variance

across the PDR structure. The Orion Bar is well suited for this study because its proximity and nearly edge-on geometry allow spectral variations to be traced across the transition from exposed atomic gas to shielded molecular layers, probing physical scales on which chemical processing can occur. JWST MIRI MRS observations reveal previously identified bands in the 15-20 μm range, including the prominent 16.4 and 17.4 μm bands, in addition to three distinct, previously unreported AIBs. The spatial distributions of the bands suggest that multiple carriers contribute to emission in this region; some bands peak in the atomic PDR, while others are strongest in the more shielded molecular layers. Correlation analysis indicates that the charge state plays an important role in shaping the observed emission. These results provide new insight into the processing of large PAHs across PDRs that are exposed to strong ultraviolet radiation.

2.41 Aromatic infrared emission bands in carbon-poor/oxygen-rich planetary nebulae

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The formation and processing of polycyclic aromatic hydrocarbons (PAHs) in evolved stars and the subsequent enrichment of the interstellar medium, is important for understanding the cycle of dust and organic matter.

We present new results on the presence and properties of aromatic infrared bands (AIBs), and their carriers, in the circumstellar environments of a ten oxygen-rich / carbon-poor planetary nebulae (PNe) for which spatially resolved moderate resolution infrared spectra have been obtained with the Spitzer infrared spectrograph, IRS.

The 11.3 μm AIB is observed in emission at different positions in the (bipolar) outflows of the four carbon-poor (C/O $\sim$0.8—1.0) PNe. A tentative detection in two oxygen-rich (C/O $\sim$0.4-0.5) PNe and a non-detection in four other carbon-poor/oxygen-rich (C/O $\leq$1) PNe are also reported. The 11.3 μm AIB intensity decreases with the inverse of the distance squared to the central star, indicating excitation by absorption of single UV photons. Its characteristic profile with an extended red shoulder implies a large fraction of evaporating very small grains (eVSGs) and some neutral PAHs. However the observed 6.2, 7.7 and 8.6 μm AIBs are weak, which differs from spectra attributed to eVSGs, especially in carbon-rich PNe.

These new results, obtained using archival Spitzer IRS/SH data, suggest a different composition (and/or charge state) for the eVSG populations in carbon-poor PNe. Given that eVSGs are considered precursors to PAHs, these findings provide strong motivation to further investigate the extended environments of carbon-poor PNe in the near-to-mid infrared, leveraging the high spatial and spectral resolution capabilities of JWST.

This work was supported by the ERC Synergy Nanocosmos.

2.42 A Spoonful of Stardust: The PAH-metallicity relation & the smallest and stubbornest dust grains

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With deep Spitzer/IRS and JWST/NIRcam radial strip maps across the nearby galaxy M101, we explore the physical origins of the observed deficit of PAHs at sub-solar metallicity (i.e., the PAH-metallicity relation or PZR). These maps allow us to trace the evolution of all PAH features from 3–18 μm as metallicity decreases continuously from solar ($Z_\odot$) to $\sim$30% $Z_\odot$. The total PAH to dust luminosity ratio remains relatively constant until reaching a threshold of $\sim$2/3 $Z_\odot$, below which it declines smoothly but rapidly. The PZR has traditionally been attributed to preferential destruction of the smallest grains in the hard radiation environments found at low metallicity. In this scenario, a decrease in emission from the shortest wavelength PAH features is expected. In contrast, we find a steep decline in long wavelength power below $Z_\odot$ with the shorter wavelength PAH bands carrying

an increasingly large fraction of power at low metallicity. We use recent grain models to reproduce the observed PZR trends, including these variations in fractional PAH feature strengths. The model that best reproduces the data employs an evolving grain size distribution that shifts to smaller sizes as metallicity declines. We interpret this as a result of inhibited grain growth at low metallicity, suggesting continuous replenishment in the interstellar medium is the dominant process shaping the PAH grain population in galaxies. Surprisingly, even as ΣPAH drops significantly relative to the total infrared luminosity (TIR) as metallicity declines, 3.3 µm/TIR alone rises, potentially indicating the mass fraction of the smallest PAH grains increases as the total dust content in galaxies drops. This may be evidence that the smallest PAHs are uniquely robust against destruction and inhibited growth effects.

2.43 Molecular Complexity in Highly Evolved Carbon Stars at Low Metallicity

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The Large and Small Magellanic Clouds (LMC/SMC) offer unique laboratories for studying carbon chemistry in matal-poor environments analogous to the early Universe. We present JWST NIRSpec and MIRI spectroscopic observations of seven carbon-rich objects spanning the AGB-to-planetary nebula (PN) transition. Low metallicity makes elemental abundance more prone to the elements formed within these stars, hence, evolved stars tend to be abundant in carbon atoms, as they are synthesized in these stars. The JWST spectra reveal features of several carbon- and nitrogen-bearing molecules, including CO, CN, C_2H_2, HCN, HC_3N, C_4H_2, CH_3C_2H, and benzene that we investigate to characterize the formation conditions and growth of molecular complexity in metal-poor environments. Simple species such as CO and CN constrain the physical conditions and elemental abundances that govern the chemistry, while the detection of more complex species in two proto-PN objects reveals the molecular pathways through which carbon is channeled into increasingly large structures. Together, these observations connect the physical and chemical conditions in circumstellar envelopes to the formation of aromatic molecules, including PAHs and fullerenes, at metallicities that challenge our current understanding of molecular formation efficiency.

2.44 Interstellar Hydrocarbons and Dust: Connecting Laboratory Analogues to Computational Models

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Hydrocarbons in the interstellar medium (ISM) are chemically and structurally diverse, and which types contribute to observed spectra remains poorly understood. In this study, we bridge laboratory spectra of a carbonaceous interstellar dust (ISD) analogue with computed spectra of its representative molecular models. The ISD analogue produces absorption features at 3.3-µm, 3.4-µm, 5.8-µm, 6.2-µm, 6.9-µm, 7.2-µm, and UV absorption near 217.5 nm, indicating strong chemical similarity with ISD. A combination of ^{13}C NMR and FTIR spectroscopy links sp^2 and sp^3 carbon abundances to the IR absorption features. Although the ISD analogue is dominated by aromatic carbon as indicated by laboratory measurements, the significantly weak 3.3-µm aromatic C–H feature suggests that its absorption coefficient may be small in ISD, and that the observed 3.3-µm aromatic C–H feature in the diffuse ISM may primarily originate from PAHs rather than from ISD. We constructed model hydrocarbon molecules that satisfy the estimated composition and bonding structure (sp^2/sp^3) of the ISD analogue. The computed spectra using DFT reproduce features

that match those in the ISD analogue IR spectra, while differences from experimental intensities likely reflect the limitations of using isolated small hydrocarbon molecules to represent dust in computational studies. The differences between experimental and computed UV spectra imply a molecular-size influence on UV absorption. This combined theoretical–laboratory UV–IR spectral comparison framework provides new constraints on hydrocarbons in the ISM while highlighting limitations in determining their compositions, structures, and sizes and the remaining uncertainties in interpreting ISM observations.

2.45 Separating the PAH cations from neutrals

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The aromatic infrared bands (AIBs), with prominent features at 3.3, 6.2, 7.7, 8.6, and 11.2 µm, are key diagnostics of the physical and chemical conditions in many astrophysical environments. Individual AIBs encode information about the size, charge, and molecular structure of the PAH family — yet in practice, any observed spectrum reflects a mixture of PAHs with a wide range of molecular properties. As a result, the observed spectra do not straightforwardly reveal the properties of any individual component of the PAH family. Having a good understanding of the neutral and cationic contributions and the charge balance is of particular importance to determine the influence of PAHs on heating and chemistry in the ISM. We present preliminary results of a program aimed to break this degeneracy by studying PAHs in reflection nebulae. Because the PAH charge balance is sensitive to the local radiation field, a sample of reflection nebulae illuminated by stars of different spectral types naturally spans a range of ionization conditions — from predominantly neutral to predominantly ionized PAHs. We have obtained JWST observations of a set of such nebulae from the Van den Bergh catalogue, which we are currently analyzing to empirically determine the spectral signatures of neutral and cationic PAHs and develop a robust method for quantifying the PAH ionization fraction.

2.46 Characterizing Star Clusters Born Between the Galaxies in Stephan's Quintet

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Stephan's Quintet is a local compact galaxy group system that exhibits significant star formation activity. A history of tidal interactions between its four member galaxies and a recent collision between an intruder galaxy and the original group are associated with active star formation, particularly in many shocked regions in the intragroup medium. Using an existing star cluster candidate catalog constructed from Hubble Space Telescope (HST) UV/optical images, we integrate flux measurements from 5 near-infrared filters (F090W, F150W, F200W, F277W, and F356W) obtained from JWST NIRCam observations in 2022. Leveraging the extended photometric baseline from HST and JWST, we perform spectral energy distribution (SED) fitting using CIGALE to derive reliable estimates of age, mass, and extinction for a high confidence sample of 1588 clusters. We confirm earlier results that very young star clusters ($\sim$a few Myr) are predominantly located along previously identified shock regions near the merging galaxies, while older ($>$100 Myr) and globular clusters are more widely distributed. Our analysis shows that near-IR photometry, particularly those bands that cover PAH features, emission lines and dust continuum emission, helps break the age-extinction degeneracy, reclassifying many clusters as younger and moderately dust-extincted. We find that the two prominent epochs of star formation, around 5 and 200 Myr, correspond to the two major interaction events that gave rise to the observed extended tidal features. The F356W-F277W colour, sensitive to PAH and dust continuum emission, is used to identify regions hosting embedded cluster candidates for spectroscopic follow-up.

2.47 PAHs and star formation at the central region of nearby nuclear ring host galaxies: JWST NIRCam observations.

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The regulation of star formation (SF) in the central regions of galaxies is governed by a complex interplay between gas inflow, turbulence, and stellar feedback. In the dusty environments of nuclear rings, traditional Ha tracers suffer from severe attenuation, while high-resolution CO maps often exhibit complex morphologies shaped by rapid gas dynamics, making it challenging to isolate the immediate onset of star formation. To overcome these limitations, we utilize JWST NIRCam observations to investigate PAH emission and star formation of nearby nuclear ring host galaxies. Given that PAH molecules are highly sensitive to the local radiation field and evolve on short timescales ($>$ 1 Myr), they offer a unique temporal advantage in analyzing SF-ISM interactions within the short dynamical cycles of nuclear rings. By resolving these features at $\sim$10 pc scales , we examine how the rapid evolution of PAHs correlates with GMC destruction and the emergence of young massive stars. This approach allows us to quantify feedback efficiency and test whether the intense SF in these rings follows a ”pearls on a string” or ”popcorn” scenario.

2.48 PAH Survival in Metal-Poor Environments: Spatially Resolved Emission in a Blue Compact Dwarf with JWST

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We present JWST NIRSpec and MIRI integral-field spectroscopy of the nearby blue compact dwarf galaxy II Zw 40, offering the first spatially resolved view of polycyclic aromatic hydrocarbon (PAH) emission in a blue compact dwarf galaxy at $\sim$10 pc resolution. With a metallicity of only one-quarter solar, II Zw 40 provides a crucial laboratory for studying small dust grain survival in metal-poor environments. Our observations reveal the 3.3 μm PAH band as the dominant aromatic feature, while the 6.2 and 11.3 μm bands appear notably weaker. A strong correlation between the PAH 3.3/11.3 ratio and neon line diagnostics suggests that radiation field hardness plays a key role in regulating PAH size distributions. Despite clear signatures of grain processing, the 3.3 μm feature accounts for more than 10% of the total PAH power—substantially higher than in typical star-forming galaxies—indicating a power shift toward smaller PAHs. The absence of 17 μm emission, typically associated with large PAHs, alongside the enhanced 3.3 μm signal, points to processes beyond photodestruction. These results establish that in low-metallicity dwarfs, PAH populations are shaped by a combination of photon-driven destruction and inhibited growth — a dual pathway that likely governs dust evolution across the low-metallicity universe.

2.49 Mapping MIR PAH Emission Features in Nearby Galaxies

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Polycyclic Aromatic Hydrocarbons (PAHs) are important mediators of the energy budget of the interstellar medium (ISM), and their population characteristics impact the efficiency of photoelectric heating in the ISM. By measuring their mid-infrared emission features, we can constrain the relative size and charge of the PAH population. The 11.3/7.7 band ratio, in particular, traces the ionization state of the PAH population. Leveraging the large archival spectral dataset of Spitzer, we have developed a novel method for measuring the 7.7 and 11.3 μm PAH emission features and

thermal dust continuum in high angular resolution JWST MIRI imaging. We present maps of these features in 19 nearby, star-forming galaxies and compare variations of PAH abundance, 11.3/7.7 μm, and stellar and thermal dust continuum shape to environmental factors such as specific star formation rate and metallicity. We find that the PAH emission relative to hot dust continuum drops in regions with depressed star formation. We also find little variation in the 11.3/7.7 ratio with metallicity and galactocentric distance, suggesting that the ionization of the PAHs does not change at high metallicity. Ultimately, a relatively constant ionization state of the PAH population suggests that the photoelectric heating efficiency is generally unchanged in these galaxies.

2.50 H_2 promotes the formation of Silicon Carbide in evolved stars

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Asymptotic Giant Branch stars (AGBs) are the main source of cosmic dust in space. In carbon rich stars (C-rich), the dust is mainly composed of amorphous carbon and silicon carbide grains, although the physical and chemical processes governing their formation remain insufficiently understood. In the case of silicon carbide several molecular precursors have been proposed.

We will present our latest results on the formation of silicon carbide dust grains using laboratory astrochemistry and kinetic modelling [1]. We observe that molecular hydrogen, the most abundant gaseous species in the circumstellar envelopes of AGBs, plays a crucial role in the formation of silicon carbide dust and identify SiC_2 as its molecular precursor. In particular, we only observe SiC_2 formation when the ratio of H_2 to atomic C/atomic Si is comparable to that of C-rich AGBs whereas in the absence of H_2 SiC_2 is not detected. We also observe that in the presence of H_2 the production of silicon carbide dust is very highly enhanced. Finally, the dust analogues are composed of three populations of nanograins, namely, aliphatic amorphous carbon, partially crystalline hydrogenated silicon, and amorphous silicon carbide (both hydrogenated and non-hydrogenated), reflecting the competition between different chemical pathways. We rationalize the experimental results on the basis of thermochemical calculations and chemical kinetics modelling.

Our findings reveal the central role of molecular hydrogen in the formation of SiC_2 and silicon carbide dust and contribute to a deeper understanding dust formation processes in evolved stars, from atoms to molecules, clusters, and ultimately dust grains.

[1] Tajuelo-Castilla et al. 2026 Nature Astronomy (accepted; doi: 10.1038/s41550-026-02854-1).

2.51 The 3.3 μm PAH Feature as an SFR Indicator: First Results from POPPIES

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The 3.3 μm polycyclic aromatic hydrocarbon (PAH) feature has long been proposed as a tracer of star formation, but its reliability as an indicator of the star formation rate (SFR) remains poorly constrained due to the limited sensitivity of previous infrared facilities. The advent of the James Webb Space Telescope (JWST) now allows the detection of this feature in large samples of galaxies across a wide range of redshifts.

In this poster, we present preliminary results from the POPPIES survey (Public Observation Pure Parallel Infrared Emission-Line Survey; PI: Jehyan Kartaltepe), a 400-hour JWST programme in Pure Parallel mode that combines wide-field slitless spectroscopy with NIRCam and multi-band imaging over approximately 1000 arcmin^2. From the currently available data (we examined 49 fields on the sky out of 110), we have identified a sample of approximately 90 sources at redshift $z < 0.51$, which show PAH emission at 3.3 μm.

To assess the robustness of the 3.3 μm PAH as an SFR indicator, we selected a subsample of 6 targets showing both PAH emission and at least one hydrogen recombination line among Brβ, Pfζ, Pfε, Pfδ, Pfγ and Brα. This allows a direct comparison between SFR estimates derived from hydrogen recombination lines and those inferred from the PAH feature. The spectra were fitted using the CAFE spectral decomposition code (Diaz-Santos et al. (2025)), adapted for JWST/NIRCam F444W slitless spectroscopy. We discuss the prospects for calibrating the 3.3 μm PAH feature as a robust tracer of SFR with the POPPIES survey.

2.52 Laboratory Infrared Spectroscopy of Ethynyl-bearing $C_{11}H_8$ PAH Species via IR-UV Ion Dip Spectroscopy for Astrochemical Applications

Danial Moh *(1); Mark Stockett; Jérôme Loreau; Piero Ferrari; Kevin Anthony Kaw; Ewald Janssens; Peter Lievens*
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Pentagon-bearing polycyclic aromatic hydrocarbons (PAHs) such as indene (C_9H_8) are hypothesized to be key intermediates in the bottom-up synthesis of fullerenes in space. The Hydrogen-Abstraction-Ethynyl-Radical-Addition (HAERA) mechanism predicts that indenyl radicals react with ethynyl radicals (C_2H) to form ethynyl-substituted indene derivatives ($C_{11}H_8$), a molecule class with predicted peak fractional abundances of $\sim 1.8 \times 10^{-10}$ in TMC-1. Despite their astrochemical relevance, the infrared (IR) spectra of most $C_{11}H_8$ isomers remain experimentally uncharacterized, limiting the interpretability of aromatic infrared band (AIB) observations by JWST. We present laboratory IR spectroscopy of $C_{11}H_8$ species (m/z 140) in the gas phase generated by electrical discharge of bromobenzene and 1,2-dibromopropane precursors in a supersonic molecular beam, using IR-UV ion dip spectroscopy, which selectively ionizes and probes $C_{11}H_8$ species using the free electron laser for infrared experiments (FELIX). In our experiments, the discharge products were characterized using time-of-flight mass spectrometry, allowing identification of multiple PAH species. For the m/z 140 channel, we have done a systematic survey of $C_{11}H_8$ isomers across the full 25 μm - 5 μm (600 - 2200 cm^{-1}) range, covering all diagnostic PAH vibrational modes including the terminal ethynyl groups. The resulting experimental IR reference spectra, matched systematically against DFT calculations (B3LYP/N07D) and anharmonic VPT2 calculations, will provide critical benchmarks for interpreting JWST AIB.

2.53 LAIBrary: from molecular spectroscopy to simulated astro-PAH spectra

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The Aromatic Infrared Bands (AIBs) are now being observed by the James Webb Space Telescope with unprecedented spectral and spatial details. This provides a strong motivation for comparably detailed modeling of the photophysics of specific carriers under UV irradiation and generation of synthetic IR spectra for AIB analysis. In particular, the carriers, usually considered to be polycyclic aromatic hydrocarbons (PAHs), emit through cooling cascades involving a large temperature range over which the IR spectrum changes.

We have developed CosmicPAH-IRDB (https://cosmicpah-irdb.irap.omp.eu), a new database dedicated to the evolution of PAH IR spectra (experimental and theoretical) as a function of temperature. The analysis of selected bands is conducted using CosmicPAHmift, a specialized spectral fitting tool that extracts key parameters such as band position, width, and intensity. Simple empirical anharmonic functions describing these parameters are derived. They are suitable for use in our (or other) emission models to generate synthetic IR spectra, simulating realistic emission from specific PAHs under specific UV radiation fields.

The aim of the LAIBrary project is to provide a collection of such spectra, which can be combined, for comparison with the observed AIB spectra. We present here the tools, database features, and

recent advancements in our modeling efforts (available at the cosmic PAH portal https://cosmic-pah.irap.omp.eu/).

Acknowledgments: this project was supported by CNES and the PN PCMI of CNRS, CEA and CNES.

2.54 A Molecular Absorption Coincident with the λ4689 Å Diffuse Interstellar Band

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The diffuse interstellar bands (DIBs) are the longest unsolved mystery in molecular spectroscopy. They are a series of over 500 absorption features in near-IR, visible, and near-UV light, observed through all lines of sight within the interstellar medium (ISM). Despite over a century of research, only one molecule has been conclusively identified as carrying any DIBs: ionised buckminsterfullerene (C_{60}^{+}) [1].

These unknown molecules are generally assumed to be carbonaceous radicals and cations present in molecular clouds where they account for a large percentage of the cosmic carbon budget. Their identification will provide further insight into the chemical and physical environments of the ISM and the cosmic lifecycle of carbon.

Small polycyclic aromatic hydrocarbons (PAHs), and the molecules they grow into, are of interest in these experiments, as their discovery in the ISM may reveal information on the chemical pathways which form these, and eventually larger, molecules. Interstellar conditions conducive to PAH processing were replicated in this experiment with the use of a jet-cooled molecular beam within a vacuum chamber and a high voltage plasma discharge, with these molecules being analysed with laser induced fluorescence (LIF), dispersed fluorescence (DF), and resonance-enhanced multiphoton ionization (REMPI) spectroscopy.

This research reveals that the electronic transition of a PAH growth product, a neutral radical of a substituted bicyclic hydrocarbon, is coincident with a weak DIB, λ4689, as pictured in the included figure, and hence may be present in the ISM. This may mark the second identified DIB carrier discovered from over a century of systematic research. This poster will include a detailed methodology of this experiment, comparisons to interstellar data, other non-detections, and astrochemical implications.

[1] E. K. Campbell, M. Holz, D. Gerlich, J. P. Maier, “Laboratory Confirmation of C_{60}^{+} as the Carrier of Two Diffuse Interstellar Bands,” Nature 523, 322–323 (2015).

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