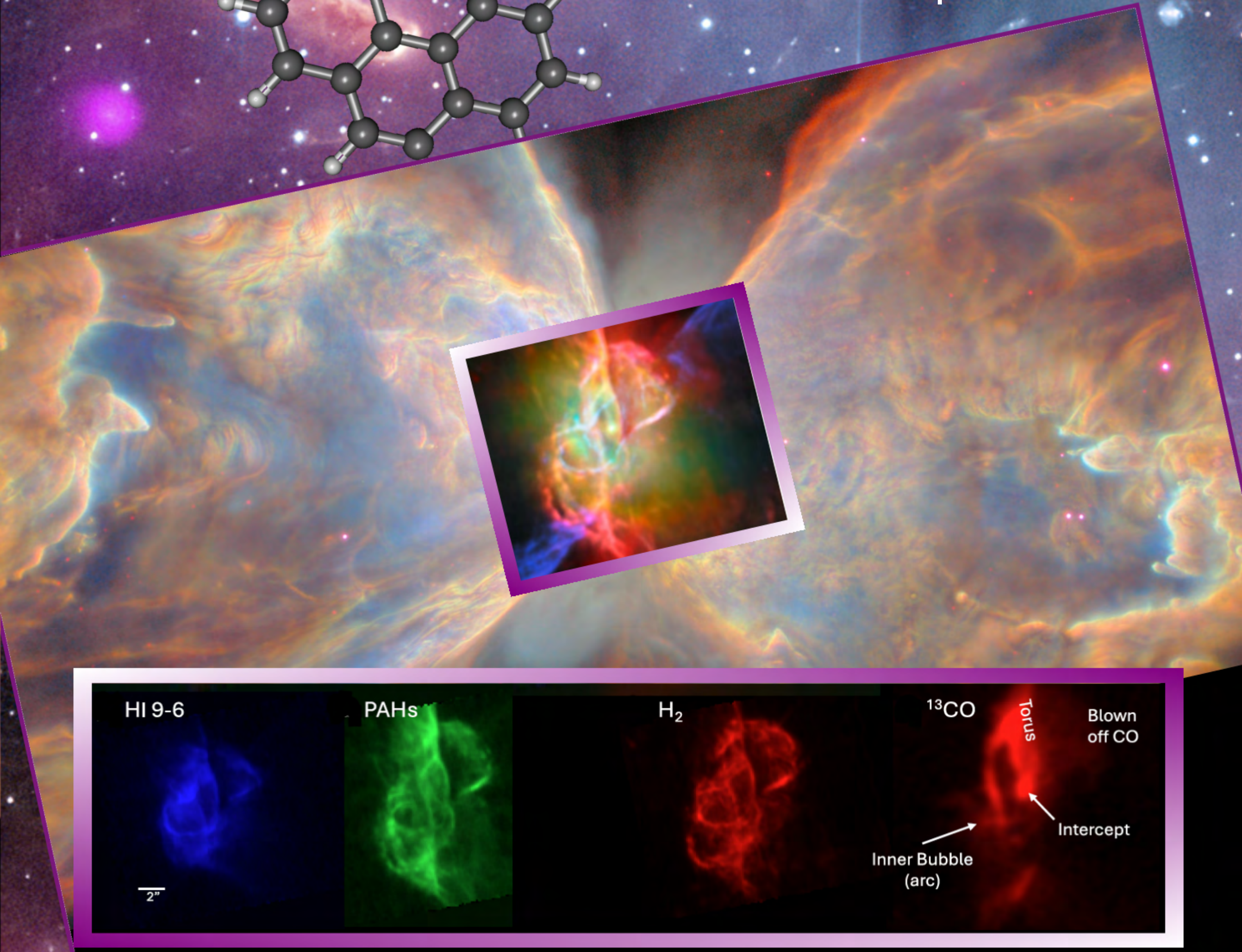
AstroPAH

A Newsletter on Astronomical PAHs

Issue 121 • September 2025



PAHs at the Heart of the Butterfly

Editorial

Dear Colleagues,

For this 121st issue, let us start with a visit to the Butterfly Nebula, NGC 6302, for our Picture of the Month. The mosaic map shown on the cover of our newsletter was obtained from JWST mid-infrared emission and ALMA submillimeter data, and helps us look deep inside its core, even through dust-obscured regions. A complex structure, influenced by the very hot central star, is revealed by the different species emission, from highly ionized ions to molecules as H_2, CO and PAHs.

We have two In Focus articles this month! The first one is an interview with Dr. Athena Flint (our newest AstroPAH editor!). As you'll see her research fits our Picture of the Month quite well as it links smaller carbonaceous species (such as the ones imaged by ALMA on the cover) to larger ones such as PAHs, detected by JWST. Her computational approach, involving machine learning, provides a fresh perspective on the complexity of astrochemistry. We warmly welcome Athena to our editorial team. The second In Focus article presents the Global Astrochemistry Lecture Series (GALS), a set of online lectures open to students and scientists from all over the world and aimed at providing a broad overview of scientific issues, problems, achievements, and open questions in astrochemistry and the chemical origins of life.

The abstracts collected in this new issue of AstroPAH display a breadth of PAH research: from refined semi-empirical and machine learning approaches to computing anharmonic spectra, to laboratory studies of hydrogenation and radical–radical chemistry, to new astronomical surveys of PAHs in disks, star-forming regions, and active galactic nuclei.

Finally, our Announcement section highlights the 15th anniversary of the NASA Ames PAH IR spectroscopic database (PAHdb)!

Thank you all for your contributions!

AstroPAH can help you promote your research. Send your contributions to our email.

The Editorial Team

Next issue: 23 October 2025.
Submission deadline: 10 October 2025.

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PAH Picture of the Month

NGC 6302 is a mixed-chemistry bipolar planetary nebula (PN) ionized by a very hot central star (∼220,000 K). Its central region was mapped in the mid-infrared with JWST (H^+, H_2 and PAH emission maps are shown) and in ^{13}CO with ALMA, showing a complex structure at the nebula's core (Matsuura et al. 2025).

Credits: Image in the background from: ESA/Webb, NASA & CSA, M. Matsuura, ALMA (ESO/NAOJ/NRAO), N. Hirano, M. Zamani (ESA/Webb), N. Bartmann (ESA/Webb). H I, H_2, PAHs and CO images reproduced from Matsuura et al. (2025), with the authors' permission.

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An interview with

Dr. Athena Flint

Dr. Athena Flint is a computational astrochemist and a recent graduate of the University of Mississippi. Dr. Flint was born and raised in rural Southern Illinois before attending Yale University, where they spent time teaching and conducting research at the intersection of machine learning and chemistry. At the University of Mississippi, they focused their research on the formation mechanisms and spectroscopic signatures of dust precursors such as PAHs and silicates. Outside of their own research, they are interested in politics, law, and how technology and society interact. In their free time, Dr. Flint enjoys reading and playing video games, watching tennis, basketball, and college football, spending time with their cats, and befriending their friends' pets. Cyclopropenylidene (c-C_3H_2) is their favorite astromolecule.

How did you get into PAH related / astrochemistry research?

As a kid I was really into physics and astronomy. Growing up in the middle of nowhere, free of the impacts of light pollution, meant that I was able to see the cosmos in all its glory on clear nights. As I approached college, I was apprehensive about pursuing either in my degree, as I felt inadequately prepared by my high school education. However, I found I had quite the knack for chemistry, and only after pursuing this for about a year in college did I realize that I wasn't actually very interested in many of the popular research pursuits in chemistry. Many of them intersected too strongly with biology for my taste - my high school biology teacher attempted to teach us the Krebs cycle once and that was enough for me for a lifetime. I knew that my research interests lay elsewhere, but I didn't know how to reconcile the fact that I wanted to be doing research as a chemist but focusing my efforts on astronomical problems. I learned about astrochemistry through an event the ACS was running during my sophomore year of college, decided to look more into it, cold-emailed a few people, and ended up doing summer research at the University of Mississippi, where I returned for my PhD.

PAHs weren't even on my radar when I got into astrochemistry. I did some work related to early astrochemistry with HeH^+ as an undergrad, and was wanting to get into oxygen astrochemistry as a graduate student. I picked up a project centering around cyclopropenylidene chemistry when I began my PhD and it inspired me to think about the massive amount of pre-PAH carbon astrochemistry that is understudied but could be meaningfully contributing to the presence of these aromatic species that were then just beginning to be observed in larger numbers. Truthfully, I also enjoyed how strange some of the prevalent astromolecules such as c-C_3H_2 are in contrast to chemical species commonly encountered on Earth. In space, a highly-strained cyclic carbene is considered stable while it would be highly reactive here. Studying astrochemistry and PAHs in particular means that I get to think about chemistry in a way that most chemists don't, which has been really exciting for me.

What are your current research goals?

Presently, I'm trying to pursue some offshoots of my past work. I recently took a look into a few polycyclic antiaromatic hydrocarbons, and we've been looking at how those structural motifs might persist in the spectral signatures of larger astromolecules. The current project I'm finishing up, which was heavily contributed to by one of my undergrads, concerns the azide radical - although it's a long shot, I've been hoping someone would observe it in Titan's atmosphere for years.

What is the importance of quantum chemistry in understanding the Universe?

With the massive amount of data we have coming at us from all angles (observational, modeled, etc.) in recent years, it seems like many astrochemists, including myself, are getting wrapped up in some decision paralysis as it pertains to our next research directions. What makes it a little easier for computational astrochemists is that there are certain questions that an experimentalist may not be able to answer for years to come but that we can answer next month, next week, or even tomorrow depending on the complexity of the problem. While we in the computational sphere can never have all of the answers, I would like to think that the insights that we are able to provide with quantum chemistry highlight certain astrochemical processes and species that are deserving of further study.

Which open question in Laboratory Astrophysics would you like to see answered in the near future? What are, in your opinion, the present forefronts of astrochemistry research?

Sulfur chemistry is, obviously, a hot-button issue in astrochemistry at the moment. Tangentially, exoplanetary astrochemistry is one of the areas where JWST has delivered on its promises, and I believe we will see a lot of interesting work continuing to come out of observational and modeling groups that will shape the field of astrochemistry as we know it (however, I disagree with some opinions that the observation of dimethyl sulfide necessarily correlates with the presence of extraterrestrial life). As someone involved in PAH-related work, this may be biased, but the other current major research area in my opinion is the work being done to determine the PAH/carbon inventory in space, specifically in the ISM. I find it rather remarkable how quickly the largest observed PAHs have increased in size, yet their observed concentrations don't appear to diminish - as it stands, the sky is not the limit for our study into these species, but rather the tools we have at our disposal to better understand them. I am very hopeful that sometime in the next 2-5 years someone may be able to determine why some of them, specifically anthracene and phenanthrene, either don't form in the ISM or are getting consumed as quickly as they are made.

What was the most important advice somebody gave you?

It's not necessarily a single piece of advice, but my advisor has drilled into me various ways to improve my science communication skills over the years. I'm a notorious rambler and tend to construct my writing more like prose than something meant to quickly and effectively present my work and my analysis of it, something that is probably evident here. Shortening my sentences, tightening my introductions, and making sure that everything I write serves a purpose has helped me write some manuscripts that I'm really proud of when, previously, I didn't really enjoy the writing process. If you also couldn't tell, I'm not a "thesis statement + 3 supporting paragraphs" person, I tend to let everything flow sequentially, which isn't the most effective information delivery process for scientific manuscripts.

Other than this, the most important piece of advice I've ever been given (also by my advisor) concerns the impact of using humor when giving research presentations. It might not truly be "advice" since I was already using it in practice. People will pay so much more attention to what you're saying, and if it's delivered casually (rather than being very scripted-in) it will hook the audience even more. They enjoy listening to research talks where the speaker is confident enough in themselves and their knowledge to create that casual, conversation-like environment. It takes practice to master, and I have certainly had some critics of the way I choose to present my work, but I really value the confidence in myself that it's helped me build and the conversations that I've gotten to have because of it.

How do you balance your professional and personal life?

I feel like I've done a pretty good job of maintaining a work-life balance, especially when it's so common for graduate school to force students away from having one. When it was possible, I stuck to the 9-5 workflow as closely as I could. It made the times where I couldn't stick to those hours a lot easier because I was much less burnt out to begin with. I may not be the best person to answer this question though, since some PhD students try to treat their labmates as coworkers and their advisor as just their boss in order to keep their personal and professional lives separate. My graduate research group was kind of like one big family, and I spent (and still do spend) a lot of my free time with members (official and honorary) of my research group.

What do you do outside of work?

I spend a lot of time with my cats, Cosmo and Wanda. I didn't learn until after adopting them that cats can be very fickle creatures that get stressed out at any number of things, including your absence. We all look forward to our time spent together in the evenings. My friends and I are known for pinballing around the square in Oxford - going to get tacos, going to the bookstore (or multiple), and ending up at the frozen yogurt shop. I'm a big music nerd and love hunting for used records at record stores and antique malls. I enjoy spending time with my family when I can, especially my nephew, who just hit 10 and is just as obsessed with space as I was when I was his age.

Global Astrochemistry Lecture Series (GALS)

“Astrochemistry: From the Big Bang to Life”

by Alexey Potapov[1], Robin Garrod[2], Wolf Geppert[3] & Martin McCoustra[4]

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Our Universe is full of molecules, from the simplest – molecular hydrogen – all the way up to the complex molecular structures essential to the chemistry of life on Earth. A large and diverse array of chemical species has been detected not only on planets but in interstellar clouds, in regions of star formation, in protoplanetary disks, and in comets, asteroids and meteorites within the Solar System. But how and when was all this material formed, and how does it evolve over time? How much molecular content is inherited from one stage of star and planet formation to the next? What role does the chemistry of the Universe through cosmic time play in the origins of life? A major unanswered question remains whether the molecules essential to life were produced on the early Earth (endogenous origin), or whether they were produced in the parent interstellar medium or planet-forming disk and delivered to Earth via asteroids, comets and their meteoritic remains (exogenous origin).

To answer all these questions, an interdisciplinary combination of knowledge in cosmology, astrophysics, astrochemistry, astronomy, and biochemistry together with fundamental research in the areas of astronomical observations, chemical modelling, and laboratory experiments are required. The Global Astrochemistry Lecture Series (GALS) was created to help students and young researchers to understand both the basics and some of the finer details of these disciplines as well as synergies between them, providing the tools and perspective needed to address the most pressing problems in astrochemistry.

Historically, GALS grew out of the Heidelberg Summer School 2022 “Astronomy, astrochemistry and the origin of life” organized by Dima Semenov and Alexey Potapov, where Robin Garrod and Martin McCoustra participated as lecturers. Evenings with immodest amounts of drinks spent together by the latter three led to the idea of GALS – a series of online lectures open to students and scientists from all over the world and aimed at providing a broad overview of scientific issues, problems, achievements, and open questions in astrochemistry and the chemical origins of life. Although there exist lecture courses at individual institutions that deal with topics in or relevant to astrochemistry, the team recognized that there were, at that time, no widely accessible courses covering all aspects of the field. Students around the world were, in general, unable to access a dedicated course on astrochemistry. Based on the interest shown in the summer school, it was also clear that there was a desire from more advanced researchers already working in astrochemistry or related fields to be able to take a course in astrochemistry that would complement their knowledge base. Noting this clear gap in the landscape of astrochemistry instruction, the team set out to construct a course taught by the world's experts, to help senior undergraduate and postgraduate students, as well as early career scientists, expand their interests and develop a firm understanding of the area, sufficient to choose an appropriate direction for their future career. The team sought also to provide this course online, and at no cost, to ensure engagement from participants around the world, regardless of their funding support.

The team invited Wolf Geppert as a member of the SOC and organized the first series in summer semester 2023. GALS 2023 consisted of 14 lectures. Figure 1 shows the first GALS advertisement. Attendance was good, with typically 70 or more joining each online lecture. Engagement from the attendees was also good, with a lengthy Q and A session with a broad range of questions following every lecture. All this, combined with the large volume of positive feedback that we received from the participants, indicated that it was a successful project. It was therefore an easy decision to make GALS a regular annual event.

Global Online Lecture Series

Topics
Big Bang
Stellar nucleosynthesis
Cosmic life cycle of matter
Astrochemical processes
Astronomical observations
Astrochemical modelling
Laboratory astrochemistry
Interstellar Medium
Protoplanetary disks
Exoplanetary atmospheres
Solar system
Prebiotic synthesis

Astrochemistry:
From the Big Bang to Life

Lecturers
Edwin Bergin
Dieter Braun
Ludmila Carone
Paola Caselli
Robin Garrod
Wolf Geppert
Eric Herbst
Martin McCoustra
Alessandro Morbidelli
Hans Olofsson
Alexey Potapov
Barbara Ryden
Alexander Tielens
Catherine Walsh

March 29 – June 28 2023

Register Now at
www.astrochemistry.de

***Figure 1** – First GALS advertisement.*

GALS in summer semester 2024 was supported by the COST Action ”Nanospace” (CA21126) and accredited by the Faculty of Sciences, University of La Laguna (ULL, Spain). The course consisted of 18 lectures, had an online examination, and carried a credit weighting of 3 ECTS. Attendance at the series in 2024 averaged about 100 students.

GALS starting from summer semester 2025 has a new format: 14 core lectures and 4 special lectures. There will be a new topic for the special lectures every year. For 2025, we chose the James Webb Space Telescope (JWST). Attendance at GALS 2025 averaged about 75 students.

Core Lectures

1. Basics of astrochemistry
2. Big Bang and formation of the elements
3. Environmental conditions in space
4. Origin of planetary systems
5. Astrochemical observations
6. Astrochemical reaction networks
7. Laboratory astrochemistry. Gas-phase processes
8. Laboratory astrochemistry. Solid-state processes
9. Chemistry in the interstellar medium
10. Chemistry in protoplanetary disks
11. Chemistry in (exo)planet atmospheres
12. Chemistry in the Solar System
13. Exogenous synthesis of biomolecule precursors
14. The Origins of Biochemistry and Life

Past and Future Special Topics

- 2025: JWST
- 2026: Ices
- 2027: Protoplanetary Disks
- 2028: Astrocatalysis

GALS 2026

The next round of GALS will be in summer semester 2026. In 18 lectures from the world-leading experts, we will discuss the history of the early molecular universe starting from the Big Bang; environmental conditions and key physico-chemical processes in space; astronomical observations (from ground to space) of objects of astrochemical interest; chemical models describing astrophysical environments and their reaction networks; key laboratory techniques and approaches for studying astrochemical processes; chemistry in specific environments, such as the interstellar medium, protoplanetary disks, and atmospheres of (exo)planets; exogenous synthesis and delivery of biomolecule precursors;

and, finally, evolution of these precursors on the early Earth. The special topic in 2026 will be “Ices”. We will discuss the observations and laboratory work on the composition and evolution of ices in astrophysical environments and their importance for our astrochemical heritage.

We will continue to provide the GALS course at no cost to attendees. Moreover, we seek a university partner that could accredit GALS as ULL did in 2024. Official accreditation and credit weighting will make GALS more attractive and popular.

We must first thank all the colleagues who, through their participation in GALS as lecturers, have ensured the success of this novel activity. That success could not have been guaranteed had we not had the practical support of several colleagues and friends to manage the actual delivery of the online sessions. We are also grateful for financial support from the many people who have supported and hopefully will continue to support GALS through the GALS crowdfunding platform, to the COST Action “Nanospace”, and to the European Astrobiology Institute. .

GALS webpage:

https://www.astrochemistry.de/online-course/

GALS crowdfunding planform:

https://gofund.me/d82cbc20

Acknowledgements

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Abstracts

The JWST/MIRI view of the planetary nebula NGC 6302 – I. A UV-irradiated torus and a hot bubble triggering PAH formation

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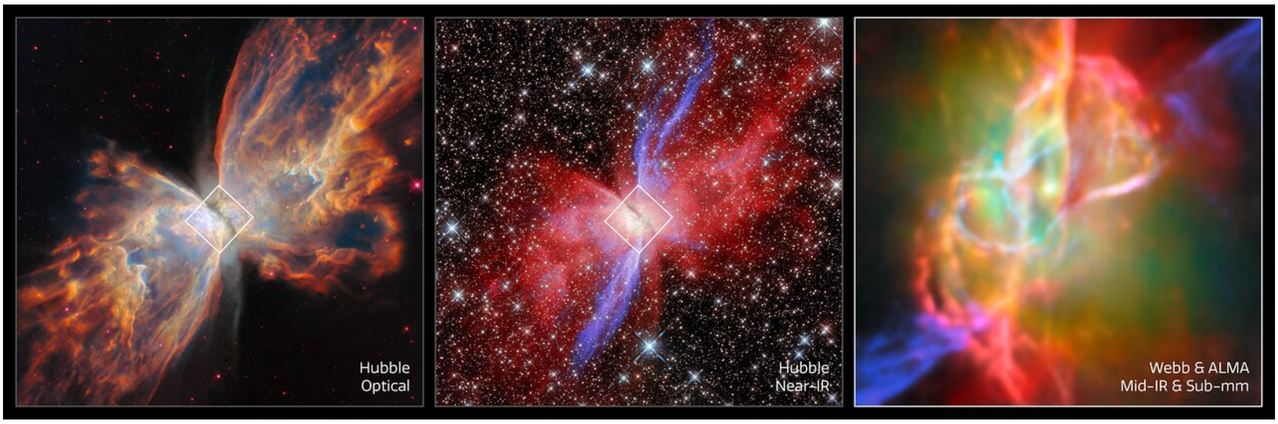
NGC 6302 is a spectacular bipolar planetary nebula (PN) whose spectrum exhibits fast outflows and highly ionized emission lines, indicating the presence of a very hot central star (~220 000 K). Its infrared spectrum reveals a mixed oxygen and carbon dust chemistry, displaying both silicate and polycyclic aromatic hydrocarbon (PAH) features. Using the James Webb Space Telescope Mid-Infrared Instrument and Medium Resolution Spectrometer, a mosaic map was obtained over the core of NGC 6302, covering the wavelength range of 5–28 µm and spanning an area of ~18.5 arcsec × 15 arcsec. The spatially resolved spectrum reveals 200 molecular and ionized lines from species requiring ionization potentials of up to ~205 eV. The spatial distributions highlight a complex structure at the nebula's centre. Highly ionized species such as [Mg VII] and [Si VII] show compact structures, while lower ionization species such as H^+ extend much farther outwards, forming filament-defined rims that delineate a bubble. Within the bubble, the H^+ and H_2 emission coincide, while the PAH emission appears farther out, indicating an ionization structure distinct from typical photodissociation regions, such as the Orion Bar. This may be the first identification of a PAH formation site in a PN. This PN appears to be shaped not by a steady, continuous outflow, but by a series of dynamic, impulsive bubble ejections, creating local conditions conducive to PAH formation. A dusty torus surrounds the core, primarily composed of large (µm-sized) silicate grains with crystalline components. The long-lived torus contains a substantial mass of material, which could support an equilibrium chemistry and a slow dust-formation process.

Press Releases: ESA JWST website and ALMA Website



Credit: ESA/Webb, NASA CSA, M. Matsuura, J. Kastner, K. Noll, ALMA (ESO/NAOJ/NRAO), N. Hirano, J. Kastner, M. Zamani (ESA/Webb)

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Reparameterized Semi-Empirical Anharmonic IR Spectra of Neutral PAHs: Benchmarking and Predictions for PAHs with more than Five Rings

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Recently-developed, reparameterized PM6 methods can reproduce experimental polycyclic aromatic hydrocarbon (PAH) IR spectra with nearly the same accuracy as the state-of-the-art quantum chemical methods but for notably less computational cost. The use of the $O(n^3)$ semi-empirical method (as opposed to $O(n^4)$ for density functional theory or $O(n^7)$ for the most accurate coupled cluster theory) allows for full, explicit, quartic force field (QFF), anharmonic computations on PAHs. The anharmonicity also predicts the combination band and overtone frequencies in addition to the fundamentals. As such, anharmonicity is essential for the best predictions of PAH spectra, and semi-empirical methods trained to compute anharmonic PAH IR spectra are the best bet at tackling such computations for large numbers of large PAHs. Beyond these benchmarks, this approach is utilized to predict the anharmonic IR spectra for five-, six-, and eight-ring PAHs in benzo[a]pyrene ($C_{20}H_{14}$), naphtho[2,1,8-qra]naphthacene ($C_{24}H_{14}$), and naphtho[2,3-b]anthanthrene ($C_{30}H_{16}$), respectively, for the first time. The larger PAHs give a double-peak in the C$-$H stretching region around 3000 cm^{-1} (3.3 µm), whereas benzo[a]pyrene still reports a large single peak, adding support for the notion that larger PAHs are more common than smaller ones in many astronomical regions. Notable IR intensities are also predicted below 1000 cm^{-1} (10.0 µm) where out-of-plane fundamental frequencies arise. The behavior in these two regions combined with the low (but non-zero) mir-IR features are consistent with the previous hypothesis that PAH cations are responsible for most of the astronomically-observed mid-IR features as neutral species like those studied here are not. Hence, this cheaper method is in line with the current best methods of quantum chemical PAH vibrational spectra predictions, is orders of magnitude faster opening the door for explicit anharmonic computations of larger PAH IR spectra, and is already providing insights into PAH behavior where only harmonic computations have previously been possible.

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Superhydrogenation of indene at low temperatures

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Context. The hydrogenation of polycyclic aromatic hydrocarbons (PAHs) is crucial to understanding molecular hydrogenation formation in the interstellar medium (ISM). This process also helps to elucidate the weakening of the aromatic bonds in PAHs, which may function as a carbon reservoir, facilitating the formation of interstellar complex organic molecules (iCOMs) through top-down chemistry. Tunneling can significantly promote the hydrogenation process in a low-to-moderate temperature range (approximately 10–200 K), which could also be important in warmer regions of the ISM, such as photodissociation regions (PDRs).
Aims. We aim to present the hydrogenation sequence of the newly observed PAH molecule, indene, for the first time and clarify the tunneling rule at temperature in PDR and dark molecular-cloud conditions. In addition, we report fit parameters to be utilized in astronomical modeling.
Methods. The hydrogenation sequence was studied using simple hydrogenation rules based on tight-binding methods and confirmed by barriers from density functional theory (DFT). The binding energy, activation energies, kinetic rate constants, and tunneling corrections –based on the Bell and Eckart models and supported by the accurate instanton method– were calculated using DFT. To make our kinetic studies useful to modelers, we implemented a Monte Carlo method-based program to generate and optimize random initial fit parameters (α, β, γ, and T_0) to achieve the statistically best fit.
Results. We find that indene hydrogenation proceeds with saturation of carbon atoms in the pentagonal ring first, followed by hydrogenation of the benzene unit. Indene hydrogenation follows rules similar to those of other PAHs, such as pentacene, coronene, and corannulene, with binding energies for odd-numbered hydrogenation steps ranging from 0.5 to 2 eV and barriers around 0.13 eV for the first, fifth, and seventh hydrogenation steps. The third hydrogenation step is the rate-limiting step, with a barrier of 0.24 eV, similar to what is found for other PAHs. Even-numbered hydrogenation steps have lower barriers and lead to more stable intermediates as a result of radical-radical recombination. The hydrogenation sequence follows a scheme that strongly depends on the PAH's shape, the number of aromatic rings, and the presence of five-membered rings, aiming to preserve the aromaticity as much as possible. Furthermore, we observe that tunneling plays an important role in the hydrogenation of indene at temperatures between 30 and 75 K, which corresponds to the temperatures of dust in PDRs. Finally, our implementation includes fit parameters that reproduce our model with a high degree of accuracy, achieving a static precision of 0.99 (R^2) and an RMS error of 10^{-2}.

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Star formation rate estimations of a mid-infrared sample of X-ray selected nearby Active Galactic Nuclei

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We investigate the activity of active galactic nuclei and the circumnuclear star formation properties in a nearby ($z \leq 0.1$) sample of 125 hard X-ray (14–195 keV) selected active Galactic Nuclei (AGN) from the *Swift*/BAT 70-month survey catalogue. Using the 11.3 µm polycyclic aromatic hydrocarbon (PAH) emission feature measured with the *Spitzer*/IRS instrument as a proxy for recent star formation, we examine the relationship between AGN power and circumnuclear star formation rate (SFR). We explored the SFR properties of both type-1 and type-2 AGN populations within our sample. A positive correlation is found between hard X-ray luminosity ($L_{14-195\,\mathrm{keV}}$) and SFR for our sample but not for type-2 AGN alone. In comparing type-1 and type-2 sources, we found no significant differences between our sample's low- and high-luminosity populations. For a subset of 50 AGN, we also provide *AKARI*/IRC measurements of the 3.3 µm PAH emission feature, which were used to estimate SFR. Although some correlations are present, these samples' two types of AGN cannot be clearly distinguished based solely on their luminosity or SFR properties, as indicated by their PAH emission.

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When the Wall Fell: Study of Polycyclic Aromatic Hydrocarbons in T Chamaeleontis using JWST

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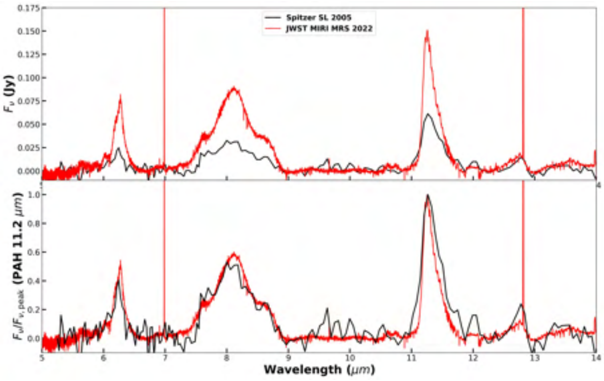
We investigate the polycyclic aromatic hydrocarbon (PAH) emission features of T Cha, a G8-type T Tauri star that has exhibited “seesaw”-type mid-infrared continuum variability over nearly two decades due to the destruction of the disk’s inner wall using *JWST*/MIRI and *Spitzer* observations. We report the first detection of weak PAH emission at 6.2, 7.7, and 8.6 µm in the *Spitzer*/IRS spectrum from 2005 (see Figure). The inner wall destruction in the 2022 *JWST* epoch allowed more ultraviolet photons to reach the outer disk, increasing the flux levels of PAH bands allowing their detection well above the continuum. The 11.2 µm PAH flux increases by a factor of three, yet its profile shape remains remarkably stable, and the 6.2/11.2 µm flux ratio has increased, but the charge state of the PAH population remains 75% neutral. The PAH features exhibit a “class C” spectral profile, with redshifted peaks and broadened wings consistent with emission from low-mass T Tauri disks, while the weak 12.7/11.2 µm ratio points to a lower abundance of duo- and trio-hydrogen modes, implying a predominantly zigzag carbon structure. A faint “class A” sub-component in the 6.2 and 7.7 µm bands may indicate additional PAH processing by ultraviolet radiation from accretion hotspots. Placement on PAH charge–size grids locates T Cha in the low-ionisation, small-size regime ($N_C \leq 30$), signifying a largely neutral PAH population in multiple epochs spanning 18 years. Through multi-epoch, high-resolution data from *JWST* and *Spitzer*, we identify T Cha as a benchmark source for probing disk evolution and PAH processing, emphasizing the potential of temporal monitoring with *JWST*.



Continuum-subtracted spectra of T Cha from JWST/MIRI and archival Spitzer SL *observations. Top: Comparison of spectra showing prominent emission features between 5–14 µm. Bottom: Same spectra normalized to the peak of the 11.2 µm PAH feature, emphasizing the ratios have not changed significantly in 18 year timescale.*

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Polycyclic Aromatic Hydrocarbons in the circumstellar medium of Herbig Ae/Be stars

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We present a comprehensive mid-infrared spectroscopic survey of 124 Herbig Ae/Be stars using newly processed *Spitzer*/IRS spectra from the newly released CASSISjuice database. Based on prominent dust and molecular signatures (polycyclic aromatic hydrocarbons, silicates, and hydrogenated amorphous carbons), we classify the stars into five groups. Our analysis reveals that 64% of the spectra show PAH emission, with detections peaking in the stellar effective temperature range 7000–11000 K (B9–A5). Silicate features appear in 50% of the sample and likewise diminish at higher temperatures. Additionally, we find that future PAH studies can focus on Herbig Ae/Be stars with a spectral index $n_{2-24} > -1$ and flared morphologies to maximize PAH detections. The 6.2 µm PAH band is the most frequently observed in our sample, shifting blueward with increasing stellar temperature, and this is the largest sample yet used to test that peak shift. The weaker 6.0 µm feature does not shift with 6.2 µm, implying a distinct origin of C=O (carbonyl) or olefinic C=C stretching relative to C–C vibrations. We examined the 11.0/11.2 µm PAH ratio using high-resolution *Spitzer* spectra for the first time in a sample of Herbig Ae/Be stars, finding a range of ionization conditions. This study provides a strong foundation for future *JWST* observations of intermediate-mass pre-main-sequence stars.

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Molecular Mass Growth Processes to Polycyclic Aromatic Hydrocarbons through Radical–Radical Reactions Exploiting Photoionization Reflectron Time-of-Flight Mass Spectrometry

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Polycyclic aromatic hydrocarbons (PAHs) represent critical building blocks in molecular mass growth processes to carbonaceous nanoparticles, referred to as interstellar and circumstellar grains along with soot particles in astrophysical environments and combustion systems, respectively. Recent advancements on elucidating elementary steps to PAHs have utilized reactions of aromatic radicals, resonantly stabilized free radicals, and aliphatic radicals with closed shell hydrocarbons. However, the role of radicalradical reactions (RRRs) leading to PAHs has remained largely unexplored on the molecular level due to preceding experimental challenges in producing sufficiently high number densities of radical reactants for isomer-selective detection of products from bimolecular and termolecular reactions. This Account offers the latest developments in our knowledge on the mechanisms and pathways to PAHs via RRRs probed in a chemical microreactor at temperatures as high as 1600 K. Product preservation in a molecular beam coupled with synchrotron vacuum ultraviolet photoionization reflectron time-of-flight mass spectrometry and photoelectron photoion coincidence spectroscopy enabled isomer-selective detection of PAHs of up to three rings by their photoionization efficiency curves, which were fit with a linear combination of reference curves for identification. Experiments were combined with computational fluid dynamics modeling of the physicochemical processes in the microreactor, as well as high-level electronic structure calculations to reveal the reaction pathways of each system. Six distinct reaction mechanisms were discovered in this work: propargyl addition—benzannulation (PABA), methyl addition—ring expansion (MARE), cyclopentadienyl addition—naphthylization (CPAN), fulvenallenyl addition—cyclization—aromatization (FACA), benzyl addition—aromatization (BAA), and phenyl addition—pentacyclization (PAP). By systematically varying the number of carbon atoms in the radical reactants, molecular mass growth processes involving reactions between radicals with odd numbers of carbon atoms access aromatics carrying one, two, or three six-membered rings, whereas reactions between even- and odd-carbon-numbered radicals produce aromatics combining five- and six-membered rings. Our investigations reveal unconventional cycloadditions on excited state triplet surfaces, additions of radicals to low spin density carbon-centered radicals, spiroaromatic and fulvene-type intermediates, and highly strained bicyclic reaction intermediates, challenging current perceptions of PAH molecular mass growth processes. All of the listed mechanisms, except for FACA, feature endoergic reactions or barriers which lie above the separated reactants and therefore might be central to circumstellar environments of carbonrich stars and planetary nebulae as their descendants, but they play no role in the gas phase of cold molecular clouds where temperatures as low as 10 K dominate. Overall, this work provides detailed reaction mechanisms of PAH growth processes, advancing our knowledge of the chemistry of carbonaceous matter in the universe

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Computing Anharmonic Infrared Spectra of Polycyclic Aromatic Hydrocarbons Using Machine Learning Molecular Dynamics

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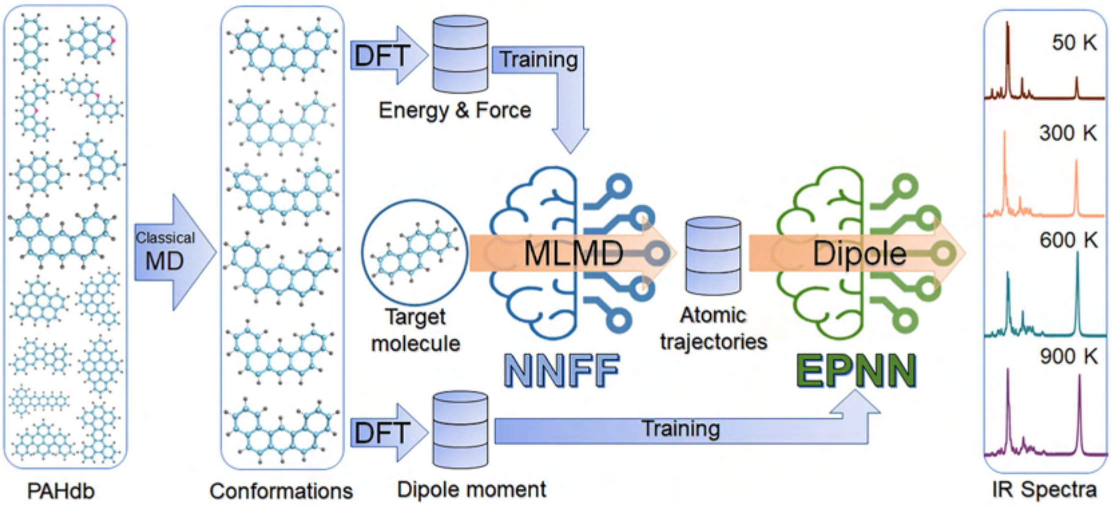
We developed a machine learning-based molecular dynamics (MLMD) method to calculate the infrared (IR) absorption spectra of polycyclic aromatic hydrocarbons (PAHs). In contrast to traditional quantum chemical methods, MLMD naturally accounts for anharmonicity and temperature effects in each molecule's spectrum, achieving accuracy comparable to quantum chemistry at a fraction of the computational cost. Its efficiency scales linearly with system size, enabling calculations for very large molecules. Using MLMD, we computed the anharmonic IR spectra of 1,704 PAHs, some containing up to 216 carbon atoms, across different temperatures. These results demonstrate that MLMD can rapidly generate large and reliable spectral datasets.



Schematic of the workflow for computing anharmonic IR spectra.

The source code and MLMD model for calculating anharmonic PAH spectra are freely available with the publication. The model is ready to use out of the box, without requiring additional training, and will be continuously updated to further enhance its predictive performance.

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15th Anniversary

The NASA Ames PAH IR Spectroscopic Database

Advertised by Christiaan Boersma and the PAHdb Team

Around the mid 1980's the mysterious mid-infrared (IR) emission observed towards a variety of astronomical objects compared favorably to absorption spectra of polycyclic aromatic hydrocarbons (PAHs). The Kuiper Airborne Observatory, flying from Ames, provided some of the first pioneering observations of these puzzling bands that appeared to be widespread throughout the Milky Way. However, there were few IR spectra of PAHs under astronomically relevant conditions to develop them into new probes of the Cosmos. To address this, a program was started at Ames in 1990 to build a library of PAH spectra. Steady progress was made with measuring the spectra of PAHs at low temperatures in solid matrices.

PAHdb launch photo from July 30th, 2010 with, from left to right, Lou Allamandola, Christiaan Boersma, Jan Cami, Els Peeters, Andrew Mattioda, and other team members inset at the top.

As the PAH field evolved it became clear that the astronomical PAH population consists of members with a size range extending well beyond what is possible to study under laboratory conditions. Therefore, Ames pioneered an approach to employ state-of-the-art quantum-chemical techniques to compute these essential PAH spectra, revolutionizing astronomical PAH studies.

The world's foremost collection of genuine PAH spectra created this way at Ames was assembled into the NASA Ames PAH IR Spectroscopic Database (PAHdb), which saw its public release July 30, 2010. PAHdb has since been an important contributor to IR PAH astronomy, supporting missions like the Infrared Space Observatory (ISO), the Spitzer Space Telescope, and the James Webb Space Telescope (JWST). PAHdb is now routinely used as a probe of physical and chemical conditions in a multitude of astronomical objects. With JWST we have entered another Golden Age of IR astronomy where PAHs are again at the forefront and PAHdb is the go-to for those who want to fully mine the treasure of information in their data.

Starting out with some 550 computed and 60 laboratory-measured PAH spectra in 2010, PAHdb has grown to hold almost 11,000 computed and 84 laboratory spectra. Beyond this, PAHdb has expanded to also provide the laboratory and computed spectra of PAH clusters—analogs of interstellar dust particles. A major step has been the recent addition of computed PAH spectra that take anharmonicity into account as well as laboratory-measured, high-resolution spectra of PAHs in the gas-phase. These data are necessary to match the spectral fidelity of JWST and are set for public release by the end of 2025. Further expansion will include the anharmonic computed PAH IR spectra of PAHs in emission as well as PAH ultraviolet absorption spectra to support the forthcoming Habitable World Observatory (HWO). PAHdb continues to support current NASA missions like JWST and SPHEREx (Spectro-Photometer for the History of the Universe, Epoch of Reionization and Ices Explorer).

PAHdb's website enjoys some 50 unique visitors a day, citations to its seminal papers grows every year, a recent JWebbinar organized by the Space Telescope Science Institute (STScI) on PAHdb was extremely well received, and the STScI added PAHdb to its JWST Laboratory Astrophysics Resources and Tools from the Community webpages. Clearly, PAHdb is ready for another 15 years of service to support astronomical PAH research!

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PAHdb Webpage: www.astrochemistry.org/pahdb

Other Resources:

PAHdb at JWST Laboratory Astrophysics Resources

PAHdb at JWST Tools from the Community

AstroPAH Newsletter

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