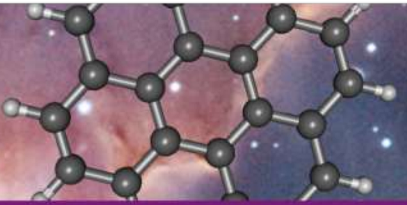
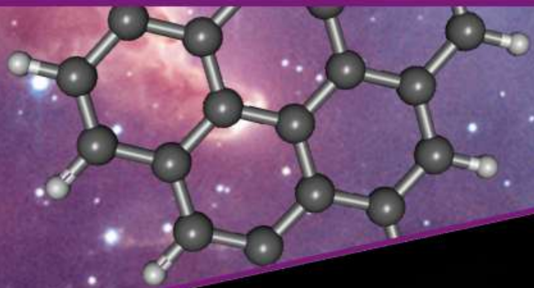
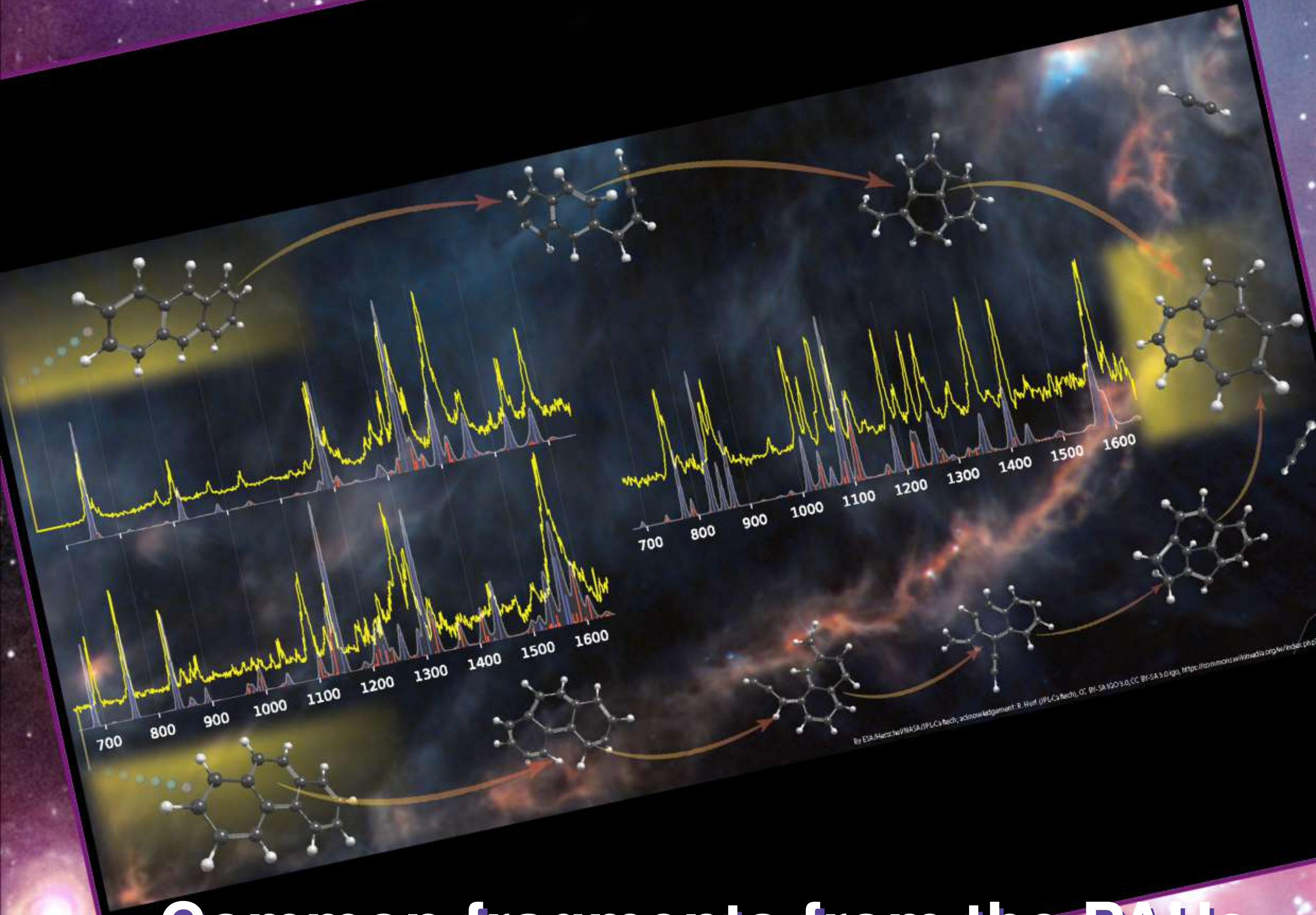


AstroPAH
A Newsletter on Astronomical PAHs

Issue 95 • February 2023





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Common fragments from the PAHs anthracene and phenanthrene

Editorial

Dear Colleagues,

Welcome to our new AstroPAH volume! We are back from our usual January break. We hope all of you are healthy and doing well!

We had the pleasure to interview Dr. Leah Dodson for our In Focus section. Dr. Dodson is an Assistant Professor in the Department of Chemistry and Biochemistry at the University of Maryland, whose research focuses on the reactivity, spectroscopy, and dynamics of exotic chemical systems.

As always, we received many exciting abstracts from you ranging from PAH dissociative ionization to interstellar hydrogenated carbon clusters, including a large number of abstracts from Karin Sandstrom's group at the Center for Astrophysics and Space Sciences at the University of California. Thank you everyone!

We also want to draw your attention to two conference announcements. The mini-symposium 'Infrared Spectroscopy in the JWST Era' at the 76th International Symposium on Molecular Spectroscopy (ISMS) in June in Illinois, USA, and the IAU Symposium 384 on Planetary Nebulae, which will be held in September in Poland. Registration for both conferences will be open soon.

Finally, the Optical Constants database (OCdb) is available online! This database provides peer-reviewed published optical constants of organic materials and ices relevant to astrophysical and planetary environments. The currently available optical constants cover a broad wavelength range from 0.27 to 200 μm. Laboratories generating optical constants are encouraged to contribute their published data in order to increase their visibility and availability. You can find more information in the Announcements section.

If you are on Instagram, be sure to check out our next PAH of the Month!

We hope you enjoy reading our newsletter, and we thank you for your dedication and interest in AstroPAH! Please continue sending us your contributions, and if you wish to contact us for a future In Focus, Picture of the Month, or other ideas, feel free to use our email. See you next month!

The Editorial Team

Next issue: 23 March 2023.
Submission deadline: 10 March 2023.

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PAH Picture of the Month

Infrared action spectra and fragmentation pathways upon (dissociative) ionization of the PAH isomers anthracene and phenanthrene leading to the formation of acenaphthylene cation upon acetylene loss. More information can be found in the manuscript by Banhatti et al.

Credits: Shreyak Banhatti. Background picture by ESA/Herschel/NASA/JPL-Caltech, CC BY-SA 3.0 IGO; Acknowledgement: R. Hurt (JPL-Caltech).

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In Focus

An Interview with Dr. Leah Dodson

Dr. Leah Dodson is an Assistant Professor in the Department of Chemistry and Biochemistry at the University of Maryland. She started her independent career at Maryland in 2019, where her group studies the reactivity, spectroscopy, and dynamics of exotic chemical systems inspired mostly by discoveries in astrochemical sciences, but also extended to atmospheric and combustion chemistry.

She received her BS in Chemistry (2010) at Case Western Reserve University where she worked with Carlos Crespo-Hernández to study the photodegradation of pharmaceutical pollutants in natural water sources. She then moved to the California Institute of Technology where she obtained her PhD in Chemistry (2016) with Mitchio Okumura studying the spectroscopy and kinetics of reactive species in atmospheric and combustion systems. Her doctoral work capitalized on collaborations with multiple government labs, and she took several trips to the Advanced Light Source in Berkeley, CA to work with David L. Osborn and his team from Sandia National Laboratories studying photoionization spectroscopy and reaction kinetics via multiplexed synchrotron-based approaches. Her graduate work was supported by two research fellowships from the EPA (STAR) and Sandia (Campus Executive). After completing her degree, she moved to Colorado where she was a NIST NRC Postdoctoral Fellow working with J. Mathias Weber to develop cryogenic ion spectroscopy techniques at JILA.

What inspired you to become a scientist?

I can't say there's anything specific that inspired me. I have wanted to be a scientist for as long as I can remember. I probably learned what a scientist does from watching Bill Nye the Science Guy, and it just seemed like the obvious career choice for me. I love that my job challenges me every single day, and gives me the opportunity to always be learning something new.

How did you get into astrochemistry research?

I am a huge space nerd (I read a lot of sci fi/fantasy) and always loved chemistry. I always hoped that one day I would be able to do astrochemistry, although my formal chemistry training was not specifically in this field. The wonderful thing about starting an independent lab is that you can propose to study whatever you want (within reason given the current funding climate). I was especially inspired by the astrochemistry symposium held at the 2018 Fall ACS Meeting, which had an incredible attendance. It was clear to me attending that meeting that astrochemistry was a vibrant and growing field and I wanted to be part of it.

Can you tell us about your career path, the difficulties you have faced as a scientist to stay in the field and what has guided your current choice?

I have known for a very long time that I wanted to be a professor, and it has been my single-minded focus all of my life. I'm extremely lucky to have landed my faculty position because I really did not have a backup plan. Getting into research very early was imperative, and building a strong network of supportive mentors was also important. I think one of my most important skills I developed that helped me stay in the field is the art of science communication: both written and spoken. If you can't communicate your science, then why are you doing it?

What are your current research goals?

To share our research with the world! The researchers in my group have been working so hard, and I want to see them get accolades for what they have accomplished, especially considering the odds they were up against founding a new research group during a global pandemic. My group builds instrumentation to make measurements for laboratory astrochemistry studies, and all the instruments are working now! It's time to show them off with cool results.

Which open question in Astrochemistry research would you like to see answered in the near future?

The thing I like most about astrochemistry is that astronomers keep coming back to us with crazier and more exotic findings in space that challenge astrochemists to come up with creative new chemical mechanisms. So it's not so much which questions I want to see answered (although I would really like to know what PAHs are really in space and how they got there), but what questions are about to be asked—what mystifying challenges are on the horizon waiting to be revealed? I can't wait to find out.

Astrochemistry is a very multidisciplinary field. Can you comment on how you collaborate and communicate with different experts and what you like about such interactions?

The University of Maryland is extremely fortunate to be located just 7 miles from NASA Goddard Space Flight Center, and my group really takes advantage of our close proximity to the astronomy experts there to keep us updated on current NASA missions, goals, and discoveries. NASA GSFC scientists constantly challenge us to make our science relevant, and to communicate our research in ways that make it clear how our laboratory findings apply

Dodson Group camping trip 2022: Back row (left to right) Julianna Palotás, Shannon Ganley, Korina Vlahos. Front row (left to right) Thomas Howard, Leah Dodson, Darya Kisuryna, Emily Hockey.

to their work. I have also learned a lot about physics instrumentation as a postdoc, and have really capitalized on the developments made in the AMO physics field to create tools for studying chemistry. The key has been to listen, to admit when I don't know something, and to ask questions. As a student, I was often afraid to ask questions because I didn't want people to discover I wasn't knowledgeable on a topic, but now I realize that I missed out on a lot of opportunities to learn something new. Nobody knows everything. As a postdoc, I started forcing myself to ask a question at every talk I attended, and I have never had anyone make me feel out of place or silly.

What was the most important advice somebody gave you?

"More pictures! More pictures of space!" – Carl Lineberger. When I was preparing for my first faculty job interviews, I gave a practice job talk for several people at JILA (where I was for my postdoc) and when we walked through my slides, Carl kept telling me: "This slide is boring, can you find a picture of space to put on it and remove all of that text?" He even offered to send me some pictures of space in case I couldn't find any. But he's right—presentations should have more pictures and less text—and I got the job.

What do you do outside of work?

I like to read sci fi/fantasy and enjoy getting absolutely entrenched in fan theories/analysis about screen adaptations for epic fantasy series. I like to take care of my little garden, go on hikes and visit vineyards with my husband, and I really like food.

How do you balance your professional and personal life?

I am really bad at balancing my professional and personal life. I really love my job, and I don't have a ton of hobbies, so it's very easy to let my professional life take over. My New Year's resolution for 2023 is to keep a separate calendar for my personal life, so that it is very glaring and obvious for me to see when I haven't taken enough time for my personal life. I am doing pretty well so far (for some reason it has involved eating a lot of tacos), but that's easy to say in January.

What advice would you give a grad student who wants a career in academia?

Every job has pros and cons. No job is perfect, and not everyone has the same tolerance level for the negatives of a specific job (nor do they always place the same value on its positives). Academia is no different: take a critical, honest view of the pros and cons and decide for yourself if the advantages outweigh the disadvantages. And ask questions at every talk you attend.

Formation of the acenaphthylene cation as a common C_2H_2-loss fragment in dissociative ionization of the PAH isomers anthracene and phenanthrene

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Polycyclic aromatic hydrocarbons (PAHs) are thought to be a major constituent of astrophysical environments, being the carriers of the ubiquitous aromatic infrared bands (AIBs) observed in the spectra of galactic and extra-galactic sources that are irradiated by ultraviolet (UV) photons. Small (2-cycles) PAHs were unambiguously detected in the TMC-1 dark cloud, showing that PAH growth pathways exist even at low temperatures. The processing of PAHs by UV photons also leads to their fragmentation, which has been recognized in recent years as an alternative route to the generally accepted bottom-up chemical pathways for the formation of complex hydrocarbons in UV-rich interstellar regions. Here we consider the $C_{12}H_8^+$ ion that is formed in our experiments from the dissociative ionization of the anthracene and phenanthrene ($C_{14}H_{10}$) molecules. By employing the sensitive action spectroscopic scheme of infrared pre-dissociation (IRPD) in a cryogenic ion trap instrument coupled to the free-electron lasers at the FELIX Laboratory, we have recorded the broadband and narrow line-width gas-phase IR spectra of the fragment ions ($C_{12}H_8^+$) and also the reference spectra of three low energy isomers of $C_{12}H_8^+$. By comparing the experimental spectra to those obtained from quantum chemical calculations we have identified the dominant structure of the fragment ion formed in the dissociation process to be the acenaphthylene cation for both isomeric precursors. Ab initio molecular dynamics simulations are presented to elucidate the fragmentation process. This result reinforces the dominant role of species containing a pentagonal ring in the photochemistry of small PAHs.

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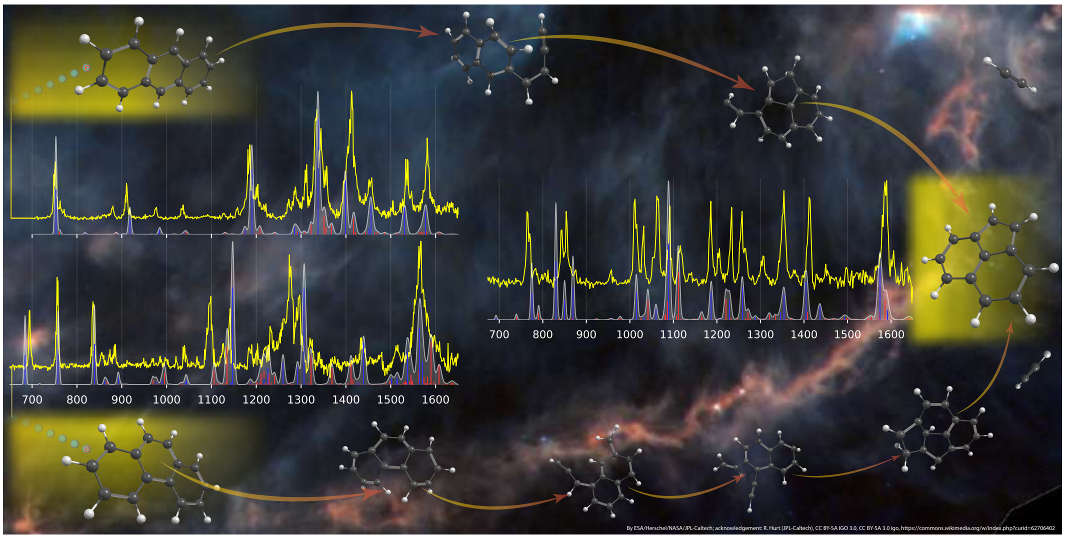
Physical Chemistry Chemical Physics, **24**, 27343 (2022)



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Graphical abstract showing the recorded infrared action spectra and fragmentation pathways upon (dissociative) ionization of anthracene and phenanthrene, leading to the same common C_2H_2-loss structure.

https://doi.org/10.1039/D2CP03835H
https://pubs.rsc.org/en/content/articlelanding/2022/CP/D2CP03835H

Laboratory hydrogenation of the photo-fragments of PAH cations: Co-evolution interstellar chemistry

Congcong Zhang[1,2,4], Xiaoyi Hu[1,2,3], Yanan Ge[1,2], Zhenru Dong[1,2], Yuanyuan Yang[1,2,3], Jia Liu[1,2], Yang Chen[3], Junfeng Zhen[1,2,4], and Liping Qin[1,2]

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To investigate the co-evolution interstellar chemistry, we studied the gas-phase hydrogenation processes of possible photo-fragments of large polycyclic aromatic hydrocarbon (PAH) cations. Our experimental results show that the hydrogenated photo-fragments of hexa-peri-hexabenzocoronene (HBC, $C_{42}H_{18}$) cations are efficiently formed. The predominance of even-mass fragments ($C_{42}H_{2n}{}^{+}$, n = [0–9]) is observed in the photo-fragmentation experiments, while no even-odd hydrogenated mass patterns are observed in the hydrogenation experiments. We investigated the structure of these newly formed hydrogenated photo-fragments and the bonding energies for these reaction pathways with quantum chemistry calculations. We used a molecular kinetic reaction model to simulate the hydrogenation processes of the photo-fragments (e.g. $C_{42}H_{12}{}^{+}$) as a function of the reaction time under the experimental conditions. We obtain the possible structure distribution of the newly formed hydrogenated fragments of $C_{42}H_{18}{}^{+}$ and the infrared (IR) spectra of these possible molecules. We infer that the hydrogenation and photo-dehydrogenation channels are not reversible reaction channels. Hydrogenation tends to be more random and disorderly, with no restrictions or requirements for the carbon reaction sites of PAH species. As a result, under the co-evolution interstellar chemistry network, there is little chance that PAH compounds return to their initial state through hydrogenation processes after photo-dehydrogenation. Consequently, the hydrogenation states and forms of PAH compounds are intricate and complex in the interstellar medium (ISM).

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Astronomy & Astrophysics, **669**, A41 (2023)

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Coincidence study of core-ionized adamantane: site-sensitivity within a carbon cage?

Smita Ganguly[1], **Mathieu Gisselbrecht**[1], **Per Eng-Johnsson**[1], **Raimund Feifel**[2], **Paul-Antoine Hervieux**[3], **Zeinab Alfaytarouni**[4,5], **Reinhold F. Fink**[6], **Sergio Díaz-Tendero**[7,8,9], **Aleksandar R. Milosavljević**[10], **Patrick Rousseau**[11], and **Sylvain Maclot**[2,12]

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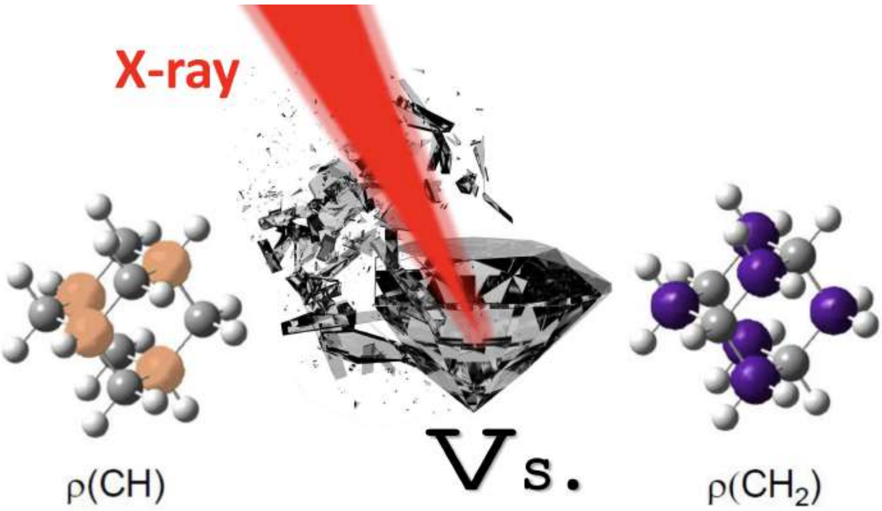
We investigate the fragmentation dynamics of adamantane dications produced after core-ionization at the carbon edge followed by Auger decay. The combination of high-resolution electron spectroscopy, energy-resolved electron-ion multi-coincidence spectroscopy and different theoretical models allows us to give a complete characterization of the processes involved after ionization. We show that energy- and site-sensitivity is observed even for a highly-symmetric molecule that lacks any unique atomic site.



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Physical Chemistry Chemical Physics, **24**, 28994 (2022)

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Bending the rules of PAH hydrogenation: the case of corannulene

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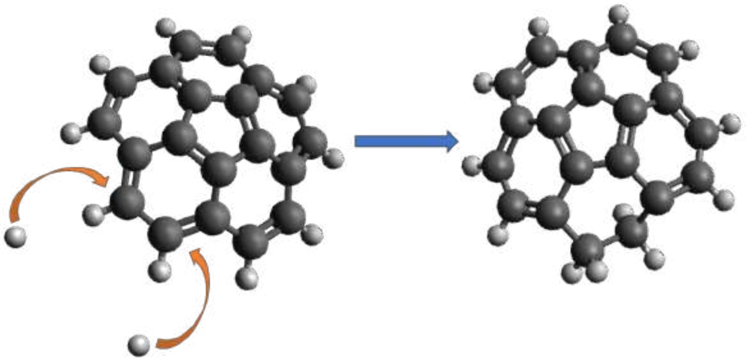
The interaction of a curved polycyclic aromatic hydrocarbon (PAH), corannulene ($C_{20}H_{10}$) with H-atoms leading to the formation of highly superhydrogenated species was studied. In particular, we determined the H-atom addition sequence to a monolayer of corannulene deposited on a graphite surface in order to understand the effect of curvature on the interaction of PAHs with H-atoms. We also investigated why superhydrogenated corannulene species with a certain number of additional H-atoms are more stable than the others. A combination of thermal desorption mass spectrometry measurements and density functional theory calculations was used to reveal and understand the presence of the most stable configurations in the superhydrogenation sequence of corannulene. Specifically, the experiments demonstrate the presence of stable configurations of superhydrogenated corannulene at specific hydrogenation levels of 2, 6, 8, 10, 12, 14, 16, 17 and 18 extra H-atoms. Density functional theory calculations of binding energies and barrier heights explain why some of these configurations are particularly stable and provide new insights into the superhydrogenation of curved PAH molecules under interstellar conditions.



Molecular structure of corannulene ($C_{20}H_{10}$; m/z=250) with the three non-equivalent sites – outer-edge, inner-edge and centre site marked in green, red, and blue, respectively.

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Monthly Notices of the Royal Astronomical Society, **519**, 5567 (2023)

https://academic.oup.com/mnras/article/519/4/5567/6987293

Gas-phase formation and spectroscopic characterization of the disubstituted cyclopropenylidenes *c*-$C_3(C_2H)_2$, *c*-$C_3(CN)_2$, and *c*-$C_3(C_2H)(CN)$

Athena R. Flint, Alexandria G. Watrous, Brent R. Westbrook, Dev J. Patel[1], and Ryan C. Fortenberry

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Aims. The detection of *c*-C_3HC_2H and possible future detection of *c*-C_3HCN provide new molecules for reaction chemistry in the dense interstellar medium (ISM) where R-C_2H and R-CN species are prevalent. Determination of chemically viable *c*-C_3HC_2H and *c*-C_3HCN derivatives and their prominent spectral features can accelerate potential astrophysical detection of this chemical family. This work characterizes three such derivatives: *c*-$C_3(C_2H)_2$, *c*-$C_3(CN)_2$, and *c*-$C_3(C_2H)(CN)$.

Methods. Interstellar reaction pathways of small carbonaceous species are well replicated through quantum chemical means. Highly accurate cc-pV*X*Z-F12/CCSD(T)-F12 (*X*=D,T) calculations generate the energetics of chemical formation pathways as well as the basis for quartic force field and second-order vibrational perturbation theory rovibrational analysis of the vibrational frequencies and rotational constants of the molecules under study.

Results. The formation of *c*-$C_3(C_2H)_2$ is as thermodynamically and, likely, as stepwise favorable as the formation of *c*-C_3HC_2H, rendering its detectability to be mostly dependent on the concentrations of the reactants. Both *c*-$C_3(C_2H)_2$ and *c*-$C_3(C_2H)(CN)$ will be detectable through radioastronomical observation with large dipole moments of 2.84 D and 4.26 D, respectively, while *c*-$C_3(CN)_2$ has an exceedingly small and likely unobservable dipole moment of 0.08 D. The most intense frequency for *c*-$C_3(C_2H)_2$ is ν_2 at 3316.9 cm^{-1} (3.01 µm), with an intensity of 140 km mol^{-1}. The mixed-substituent molecule *c*-$C_3(C_2H)(CN)$ has one frequency with a large intensity, ν_1, at 3321.0 cm^{-1} (3.01 µm), with an intensity of 82 km mol^{-1}. The molecule *c*-$C_3(CN)_2$ lacks intense vibrational frequencies within the range that current instrumentation can readily observe.

Conclusions. Both *c*-$C_3(C_2H)_2$ and *c*-$C_3(C_2H)(CN)$ are viable candidates for astrophysical observation, with favorable reaction profiles and spectral data produced herein, but *c*-$C_3(CN)_2$ will not be directly observable through any currently available remote sensing means, even if it forms in large abundances.

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Astronomy & Astrophysics, Forthcoming Article (2023)

https://doi.org/10.1051/0004-6361/202245643

Efficient stabilization of cyanonaphthalene by fast radiative cooling and implications for the resilience of small PAHs in interstellar clouds

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After decades of searching, astronomers have recently identified specific Polycyclic Aromatic Hydrocarbons (PAHs) in space. Remarkably, the observed abundance of cyanonaphthalene (CNN, $C_{10}H_7CN$) in the Taurus Molecular Cloud (TMC-1) is six orders of magnitude higher than expected from astrophysical modeling. Here, we report unimolecular dissociation and radiative cooling rate coefficients of the 1-CNN isomer in its cationic form. These results are based on measurements of the time-dependent neutral product emission rate and Kinetic Energy Release distributions produced from an ensemble of internally excited 1-CNN$^+$ studied in an environment similar to that in interstellar clouds. We find that Recurrent Fluorescence – radiative relaxation via thermally populated electronic excited states – efficiently stabilizes 1-CNN$^+$, owing to a large enhancement of the electronic transition probability by vibronic coupling. Our results help explain the anomalous abundance of CNN in TMC-1 and challenge the widely accepted picture of rapid destruction of small PAHs in space.

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Nature Communication, **14**, 395 (2023)

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Impact of HAC evolution on the formation of small hydrocarbons in the Orion Bar and the Horsehead PDRs

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We study evolution of hydrogenated amorphous carbon (HAC) grains under harsh UV radiation in photo-dissociation regions (PDRs) near young massive stars. Our aim is to evaluate the impact of the HAC grains on formation of observed small hydrocarbons: C_2H, C_2H_2, C_3H^+, C_3H, C_3H_2 and C_4H in PDRs. We developed a microscopic model of the HAC grains based on available experimental results. The model includes processes of photo- and thermodesorption, accretion of hydrogen and carbon atoms and subsequent formation of carbonaceous mantle on dust surface. H_2, CH_4, C_2H_2, C_2H_4, C_2H_6, C_3H_4, C_3H_6 and C_3H_8 are considered as the main fragments of the HAC photo-destruction. We simulated evolution of the HAC grains under the physical conditions of two PDRs, the Orion Bar and the Horsehead nebula. We estimated the production rates of the HAC' fragments in gas phase chemical reactions and compared them with the production rates of fragments due to the HAC destruction. The latter rates may dominate under some conditions, namely, at $A_V = 0.1$ in both PDRs. We coupled our model with the gas-grain chemical model `MONACO` and calculated abundances of observed small hydrocarbons. We conclude that the contribution of the HAC destruction fragments to chemistry is not enough to match the observed abundances, although it increases the abundances by several orders of magnitude in the Orion Bar at $A_V = 0.1$. Additionally, we found that the process of carbonaceous mantle formation on dust surface can be an inhibitor for the formation of observed small hydrocarbons in PDRs.

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https://doi.org/10.1093/mnras/stac3656
https://arxiv.org/abs/2212.04993

A comprehensive rotational study of astronomical iso-pentane within 84 to 111 GHz

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Department of Physics, Institute of Science, Banaras Hindu University, Varanasi-221005, India

The rotational line survey by ALMA (Atacama Large Millimeter/submillimeter Array) recently revealed the presence of i-C_3H_7CN (i-PrCN) and n-C_3H_7CN (n-PrCN) in 3-mm atmospheric window between 84 to 111 GHz towards the hot core region Sagittarius B2(N) (Sgr B2(N)). This was the first interstellar detection of a linear straight chain molecule. In this light, we report the rotational spectra of C_5H_{12} isomeric group in the same frequency range. We performed quantum chemical calculations for spectroscopic parameters. The pure rotational spectrum of the species has been simulated using the PGOPHER program. The rotational spectrum of this molecule makes it a good candidate for future astronomical detections since the radio lines can be calculated to very high accuracy in mm/sub-mm wave region.

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Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, **290**, 122299 (2023)

https://doi.org/10.1016/j.saa.2022.122299

The 3.3 µm Infrared Emission Feature Profile in HD 44179

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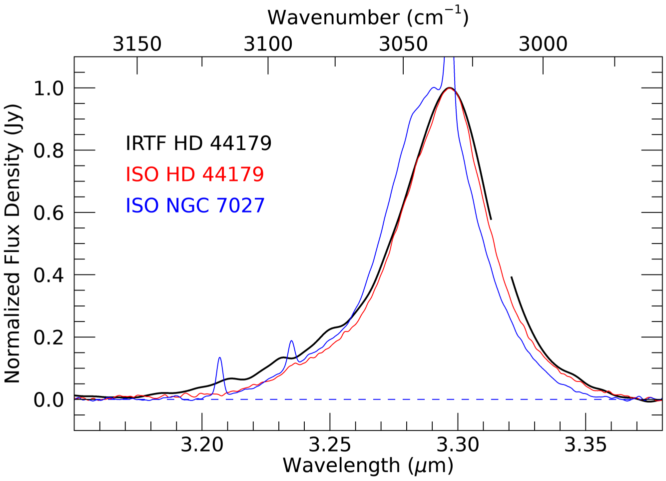
HD 44179 is a post-asymptotic giant branch (post-AGB) star with a biconical nebula known as the Red Rectangle. Previous observations of HD 44179 showed that the width of the 3.3 µm infrared emission feature was narrower within 2 arcsec of HD 44179 and wider further away from the star. This was interpreted as an indication that the 3.3 µm IEF arises from two types of PAHs with spatially-varying relative abundances (Candian et al. 2012, MNRAS, 426:389). With new observations of HD 44179 with the NASA Infrared Telescope Facility (IRTF) we find that the width of the 3.3 µm IEF profile is spatially invariant and conclude that there is no evidence for two spatially-varying components.



Comparison of the IRTF HD 44179 spectrum in the central 2 arcsec (black line) to the ISO spectra of HD 44179 (red line) and NGC 7027 (blue line) spectra after removal of the linear continuum and the plateau emission. The NGC7027 spectrum is from Tokunaga & Bernstein (2022, ApJ, 916:52). The IRTF and ISO spectra of HD44179 are nearly identical except for the short wavelength wing.

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https://iopscience.iop.org/article/10.3847/1538-4357/ac9969/pdf

A plausible molecular mechanism to explain near-IR continuum emission: Recurrent fluorescence

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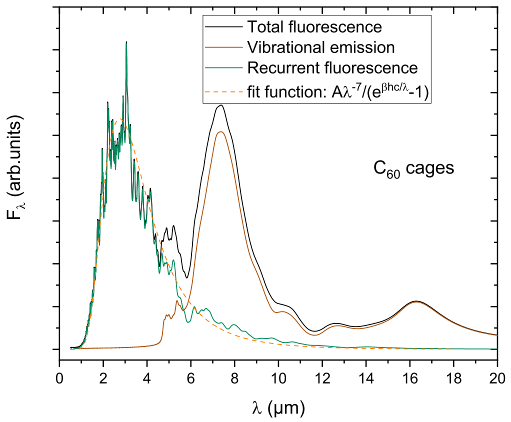
Very small grains and large hydrocarbon molecules are known to convert a fraction of the UV and visible stellar radiation to near and mid-IR photons via stochastic heating and subsequent radiative de-excitation. However, no convincing explanation for the near-IR continuum emission observed in some reflection nebulae and planetary nebulae has been provided so far. We aim to investigate the extent that recurrent fluorescence originating from stellar photon absorption by C_n (n = 24, 42, 60) carbon clusters can account for the IR emission detected in various interstellar environments. To this aim, we modelled the collective emission signature of a carbon cluster sample induced by irradiation from a 20,000 K blackbody source, during which recurrent fluorescence and vibrational emission compete with each other. Our modelling shows that recurrent fluorescence from C_{60} cages and flakes (with little or no sp^1 carbon atoms) and C_{42} cages are able to explain the near-IR continuum emission observed in several reflection nebulae and planetary nebulae. Assuming that the continuum emission observed towards NGC 7023 is due to recurrent fluorescence induced by UV or visible photon absorption in neutral cage carbon clusters containing about 30–60 atoms, the carriers contain about 0.1–1.5% of the interstellar carbon abundance.



Collective emission intensity spectrum from 1000 C_{60} cage carbon cluster sample irradiated by a 20,000 K blackbody excitation.

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Astronomy & Astrophysics, Forthcoming Article (2023)

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Five-membered ring compounds from the *ortho*-benzyne + methyl radical reaction under interstellar conditions

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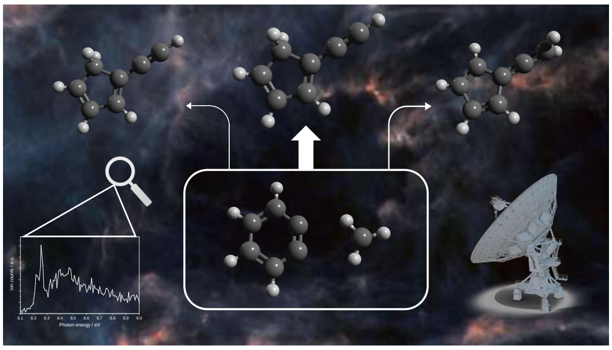
Reactive open-shell species, such as radicals and biradicals, are key intermediates in the formation of (poly)cyclic hydrocarbon species in a variety of interstellar environments, ranging from cold molecular clouds to the outflows of carbon-rich stars. In this work, we identify the products of the *o*-benzyne + methyl radical reaction isomer-selectively by photoion mass-selected threshold photoelectron spectroscopy. We assign the benzyl ($C_7H_7^\bullet$) radical as the sole intermediate of the association reaction. Subsequent hydrogen atom loss from benzyl yields the five-membered ring species fulvenallene (**FA**), 1-ethynylcyclopentadiene (**1ECP**), and 2-ethynylcyclopentadiene (**2ECP**) which have recently been detected in the cold molecular cloud TMC-1. We report a comprehensive C_7H_7 potential energy surface (PES) of the title reaction and show that the products form via direct barrierless addition followed by ring-contraction and hydrogen elimination. A statistical model predicts 89% **1ECP**, 8% **FA**, and 3% **2ECP** branching ratios at 0 K. Astrochemical simulations of TMC-1 incorporating this reaction result in the excellent reproduction of the abundance of a five-membered ring species, **1ECP**, and provide strong evidence for the in situ “bottom-up” formation of small cyclic species in cold cores. Last, we put the results in context of the recent detection of fulvenallene in TMC-1.



*The methyl + ortho-benzyne reaction is found to proceed without a barrier and yield the five-membered ring products **1ECP**, **FA**, and **2ECP**.*

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Time dependent density functional study of nitrogen-substituted polycyclic aromatic hydrocarbons and diffuse interstellar bands

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This work reports theoretical calculations of electronic transitions in nitrogen-substituted polycyclic aromatic hydrocarbon neutrals and cations, using time-dependent density functional theory. The results obtained are compared with the diffuse interstellar bands, a broad group of absorption bands that can be seen mostly in near-ultraviolet and near-infrared wavelengths of the spectrum. It is observed that with nitrogen substituted at the periphery (exoskeletal), these nitrogen-substituted polycyclic aromatic hydrocarbon neutrals and their cation counterparts, similar to their corresponding parent polycyclic aromatic hydrocarbons, absorb in the near-ultraviolet and near-infrared wavelengths, respectively. The analogy then follows a change with nitrogen entering into the structure (endoskeletal) and the nitrogen-substituted polycyclic aromatic hydrocarbon neutrals and cations, unlike their corresponding pure polycyclic aromatic hydrocarbon family, fall in the near-infrared and visible spectral regions, respectively. Based on these and other astrophysical implications, it is concluded that nitrogen-substituted polycyclic aromatic hydrocarbons represent a powerful class of prospective carriers of diffuse interstellar bands.

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ACS Earth and Space Chemistry, **6(12)**, 2867 (2022)

https://doi.org/10.1021/acsearthspacechem.2c00176

Near-infrared spectroscopy of a massive young stellar object in the direction toward the Galactic Center: XCN and aromatic C–D features

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We report near-infrared (2.5–5 µm) long-slit ($\sim 30''$) spectroscopy of a young stellar object in the direction toward the Galactic center with the Infrared Camera on board the AKARI satellite. The present target is suggested to be AFGL 2006 based on its very red color and close location. The spectra show strong absorption features of H_2O and CO_2 ices, and emission of HI Brα recombination line and the 3.3 µm band, the latter of which originates from polycyclic aromatic hydrocarbons (PAHs) or materials containing PAHs. The spectra show a broad, complex absorption feature at 4.65 µm, which is well explained by a combination of absorption features of CO ice, CO gas, and XCN, and HI Pfβ emission. The spectra also indicate excess emission at 4.4 µm. The characteristics of the spectra suggest that the object is a massive young stellar object. The XCN feature shows a good correlation with the Brα emission, suggesting that the photolysis by ultraviolet photons plays an important role in the formation of the XCN carriers, part of which are attributed to OCN^-. The 4.4 µm emission shows a good correlation with the 3.3 µm PAH emission, providing supporting evidence that it comes from the aromatic C–D stretching vibration. The formation of OCN^- is of importance for the formation process of prebiotic matter in the interstellar medium (ISM), while the detection of aromatic C–D emission provides valuable information on the deuteration process of PAHs in the ISM and implications on the hiding site of the missing deuterium in the ISM.

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Spectral variations among different scenarios of PAH processing or formation

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We examine the variations in the spectral characteristics and intensities of PAHs in two different scenarios of PAH processing (or formation): *(1)* small PAHs are being destroyed (or equivalently large PAHs are being formed, referred to as SPR i.e. small PAHs removed), and *(2)* large PAHs are being destroyed (or equivalently small PAHs are being formed referred to as LPR i.e. large PAHs removed). PAH emission was measured considering both the presence or absence of plateau components. The variation in the PAH band intensities as a function of the average number of carbon atoms $\langle N_C \rangle$ has the highest dynamic range in the SPR case suggesting that smaller PAHs have higher impact on the PAH band strengths. The plateaus show overall declining emission with $\langle N_C \rangle$ and their higher dynamic range in the SPR case also suggests that smaller PAHs are mainly contributing to the plateau emission. The 7.7/(11.0+11.2) µm PAH band ratio presents the least amount of variance with the lowest dynamic range, rendering this ratio as the better choice for tracing PAH charge. The 3.3/(11.2+11.0) µm PAH band ratio is the only ratio that has both a monotonic variance and fully separated values among the SPR and LPR scenarios, highlighting its efficiency as PAH size tracer but also allowing the characterization of the dominant scenario of processing or formation in a given region or source. We present new PAH charge – size diagnostic diagrams, which can provide insights on the average, maximum, or minimum N_C within astrophysical sources.

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https://arxiv.org/abs/2302.03678
https://doi.org/10.1093/mnras/stad465

Spectroscopic investigation of interstellar hydrogenated carbon clusters

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Context. The assignment of the mid-infrared (mid-IR) emission features and plateaus observed in C-rich and H-rich regions of the interstellar medium (ISM) is still debated. Such mid-IR assignments must also be related to their contribution to the extinction curve in our galaxy and to the ultraviolet (UV) bump.
Aims. The aim of this work is to investigate the influence of hydrogenation rate on the mid-IR spectra of populations of carbon clusters in order to constraint the n_H/n_C ratios in regions of the ISM where carbon is an important component. Their potential contribution to the extinction curve and in particular to the UV bump is also investigated.
Methods. The absorption IR and optical spectra of tens of thousands of $C_{24}H_n$ (n = 0, 6, 12, 18, 24) isomers classified into structural families — namely flakes, branched, pretzels, and cages — were computed using the density functional based tight binding electronic structure method and its time-dependent version, respectively. Final spectra were obtained by averaging the spectra of many individual isomers.
Results. The shapes and the relative intensities of the bands centered at $\sim$3.25 and 3.40 µm and assigned to the C-H stretch of sp^2 and sp^3 carbon atoms, respectively, present a clear dependence on the n_H/n_C ratio. From a comparison with the astronomical spectrum from the Orion bar H2S1, the most interesting emitting candidates would pertain to the flakes population; this is the most energetically favorable family of clusters, possessing a high content of five and six carbon rings and being mostly planar, with no sp^1 carbon atoms and with a n_H/n_C ratio of lower than 0.5. The same conclusion is drawn when comparing the computed IR features in the [4–20 µm] region with the observed plateaus from some C-rich and H-rich planetary nebulae objects of the Small Magellanic Cloud. The contribution of the same family could be considered for the UV bump. When n_H/n_C increases, only a contribution to the high-energy part of the continuum due to $\sigma \rightarrow \pi^\star$ excitations can reasonably be considered.
Conclusions. These results bring some constraints on the structural features and on the n_H/n_C ratio of the hydrogenated carbon populations emitting in the mid-IR domain in interstellar objects such as protoplanetary and reflection nebulae. The flakes population, with a low n_H/n_C ratio, is an interesting candidate for the carbon population emitting in these regions, but not for that absorbing in the diffuse ISM. None of the populations studied in the present work can account for the UV bump, but they would contribute to a broad extinction rise in this domain. The computed features reported in this article could be used to interpret future astronomical data provided by the James Webb Space Telescope.

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https://doi.org/10.1051/0004-6361/202245472

Polarizability of kekulene, septulene, and nearest non-planar polycyclic aromatic hydrocarbons

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The polarizability of polycyclic aromatic hydrocarbons (PAHs) is an important property that relates to their abundance in natural environments. To assess the differences in the mean polarizability of planar and non-planar polycyclic aromatic hydrocarbons (PAHs), we computationally studied the PAH series of circulenes (kekulene $C_{48}H_{24}$, [13]circulene $C_{52}H_{26}$, and septulene $C_{56}H_{28}$), a number of the nearest helicenes, and their "expanded" isomers. We mean under "nearest" a close number of aromatic rings: 11 ($C_{46}H_{26}$), 12 ($C_{50}H_{28}$), 13 ($C_{54}H_{30}$), and 14 ($C_{58}H_{32}$). For these PAHs, we performed the quantum chemical calculations of thermodynamic and polarizability parameters with the PBE/3ζ density functional theory method, which is widely used in the theoretical chemistry of fullerenes and PAHs. The calculated mean polarizabilities (in Å^3) ranged from 80.1 for [11]helicene to 135.5 for septulene, and while the circulenes and expanded helicenes had similar values, the mean polarizability of the normal helicenes was markedly lower. In all four pairs of helical PAHs, the expanded helicene was energetically considerably more favorable than its standard helicene isomer. Herewith, the ratio of their polarizabilities was equal to 1.3.

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PHANGS-JWST First Results: Measuring PAH Properties across the multiphase ISM

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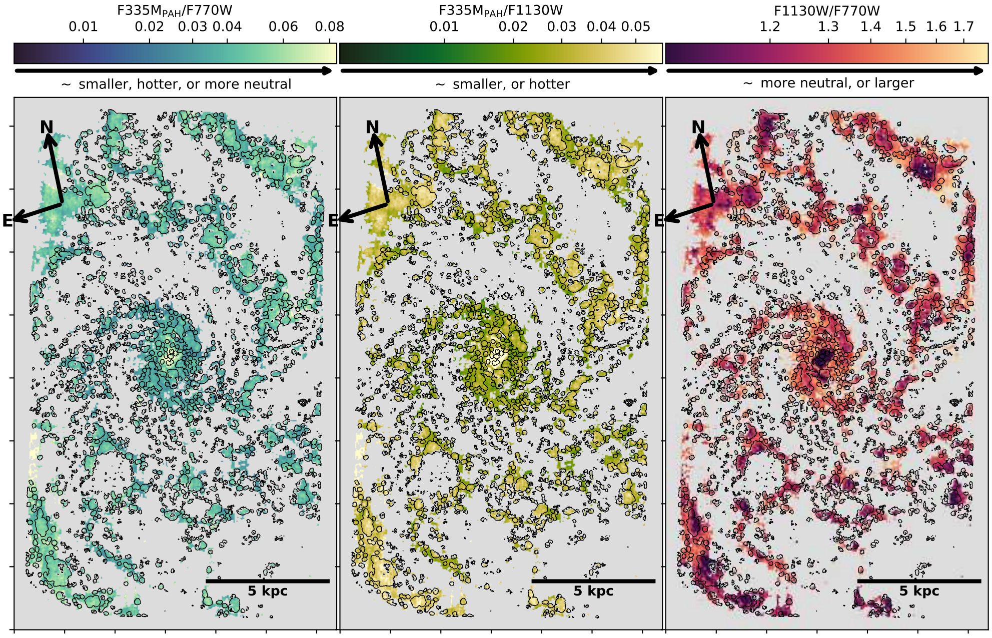
Ratios of polycyclic aromatic hydrocarbon (PAH) vibrational bands are a promising tool for measuring the properties of the PAH population and their effect on star formation. The photometric bands of the MIRI and NIRCam instruments on JWST provide the opportunity to measure PAH emission features across entire galaxy disks at unprecedented resolution and sensitivity. Here we present the first results of this analysis in a sample of three nearby galaxies: NGC 628, NGC 1365, and NGC 7496. Based on the variations observed in the 3.3, 7.7, and 11.3 µm features, we infer changes to the average PAH size and ionization state across the different galaxy environments. High values of $F335M_{PAH}/F1130W$ and low values of F1130W/F770W are measured in HII regions in all three galaxies. This suggests that these regions are populated by hotter PAHs, and/or that the PAH ionization fraction is larger. We see additional evidence of heating and/or changes in PAH size in regions with higher molecular gas content as well as increased ionization in regions with higher Hα intensity.



JWST/MIRI band ratios in NGC 628, overlayed with HII regions contours.

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The Astrophysical Journal Letters, PHANGS-focused issue (2023)

https://ui.adsabs.harvard.edu/abs/2022arXiv221210512C/abstract

PHANGS-JWST First Results: Variations in PAH Fraction as a Function of ISM Phase and Metallicity

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We present maps tracing the fraction of dust in the form of polycyclic aromatic hydrocarbons (PAHs) in IC 5332, NGC 628, NGC 1365, and NGC 7496 from JWST/MIRI observations. We trace the PAH fraction by combining the F770W (7.7 µm) and F1130W (11.3 µm) filters to track ionized and neutral PAH emission, respectively, and comparing the PAH emission to F2100W which traces small, hot dust grains. We find average $R_{\rm PAH}$ = (F770W+F1130W)/F2100W values of 3.3, 4.7, 5.1, and 3.6 in IC 5332, NGC 628, NGC 1365, and NGC 7496, respectively. We find that H II regions traced by MUSE Hα show a systematically low PAH fraction. The PAH fraction remains relatively constant across other galactic environments, with slight variations. We use CO+H I+Hα to trace the interstellar gas phase and find that the PAH fraction decreases above a value of $I_{\rm H\alpha}/\Sigma_{\rm HI+H_2} \sim 10^{37.5}$ erg s^{-1} kpc^{-2} (M$_\odot$ pc^{-2})$^{-1}$, in all four galaxies. Radial profiles also show a decreasing PAH fraction with increasing radius, correlated with lower metallicity, in line with previous results showing a strong metallicity dependence to the PAH fraction. Our results suggest that the process of PAH destruction in ionized gas operates similarly across the four targets.

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https://ui.adsabs.harvard.edu/abs/2023arXiv230100578C/abstract
https://doi.org/10.3847/2041-8213/acadd7

PHANGS-JWST First Results: Mapping the 3.3 µm Polycyclic Aromatic Hydrocarbon Vibrational Band in Nearby Galaxies with NIRCam Medium Bands

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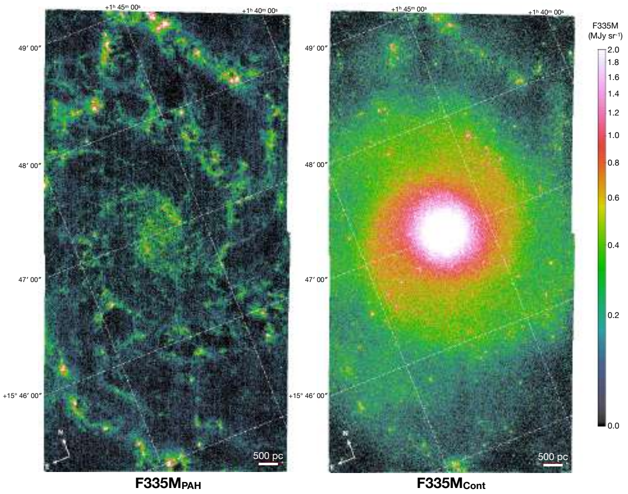
We present maps of the 3.3 µm polycyclic aromatic hydrocarbon (PAH) emission feature in NGC 628, NGC 1365, and NGC 7496 as observed with the Near-Infrared Camera (NIRCam) imager on JWST from the PHANGS-JWST Cycle 1 Treasury project. We create maps that isolate the 3.3 µm PAH feature in the F335M filter ($\mathrm{F335M_{PAH}}$) using combinations of the F300M and F360M filters for removal of starlight continuum. This continuum removal is complicated by contamination of the F360M by PAH emission and variations in the stellar spectral energy distribution slopes between 3.0 and 3.6 µm. We modify the empirical prescription from Lai et al. (2020) to remove the starlight continuum in our highly resolved galaxies, which have a range of starlight- and PAH-dominated lines-of-sight. Analyzing radially binned profiles of the $\mathrm{F335M_{PAH}}$ emission, we find that between 5–65% of the F335M intensity comes from the 3.3 µm feature within the inner 0.5 r_{25} of our targets. This percentage systematically varies from galaxy to galaxy, and shows radial trends within the galaxies related to each galaxy's distribution of stellar mass, interstellar medium, and star formation. The 3.3 µm emission is well correlated with the 11.3 µm PAH feature traced with the MIRI F1130W filter, as is expected, since both features arise from C–H vibrational modes. The average $\mathrm{F335M_{PAH}}$/F1130W ratio agrees with the predictions of recent models by Draine et al. (2021) for PAHs with size and charge distributions shifted towards larger grains with normal or higher ionization.



$\mathrm{F335M_{PAH}}$ **$\mathrm{F335M_{Cont}}$**

PAH 3.3 µm emission and continuum for NGC 628.

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The Astrophysical Journal Letters, PHANGS-focused issue, **944(2)**, 11 pp. (2023)

https://ui.adsabs.harvard.edu/abs/2023arXiv230100854S/abstract
https://doi.org/10.3847/2041-8213/acb0cf

Mini-Symposium “Infrared Spectroscopy in the JWST Era”

at the 76th International Symposium on Molecular Spectroscopy (ISMS)

Urbana-Champaign, Illinois, US
19–23 June, 2023

http://isms.illinois.edu

We are writing to invite you and your students to submit abstracts for a talk in a mini-symposium “Infrared Spectroscopy in the JWST Era” at the 76th International Symposium on Molecular Spectroscopy (ISMS) to be held June 19-23, 2023 in Urbana-Champaign, Illinois.

Our aim is to bring together laboratory and theoretical spectroscopists, observational astronomers, and modelling and database scientists to present the current status and the demands for infrared spectroscopy in the era of JWST. There will be several sessions for this mini-symposium with a focus on the gas-phase and aromatic universe, exoplanetary atmospheres, and ice chemistry in star-forming regions and protoplanetary disks. The invited speakers are Katy Chubb (University of St. Andrews), Klaus Pontoppidan (Space Telescope Science Institute), Ameek Sidhu (University of Western Ontario), Helen Fraser (Open University).

The deadline for ISMS abstract submission is March 1. We encourage you to submit abstracts at your earliest convenience. When submitting your abstract, please choose “Infrared Spectroscopy in the JWST Era” from the drop-down menu under “Abstract Detail”. Do not hesitate to forward this message to your colleagues and group members who might be interested. Please note that ISMS will be held exclusively in person this year with no hybrid/remote option.

More information about ISMS is available on the symposium website. Please feel free to contact either of us if you have any questions. We look forward to seeing you in June!

Sandra Brünken, Sergio Ioppolo, and Rens Waters
— Co-organizers

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IAU Symposium 384

Planetary Nebulae: a Universal Toolbox in the Era of Precision Astrophysics

Cracow, Poland
4–8 September, 2023

https://iaus384-pne.ncac.torun.pl/

Save the date: The next IAU Symposium on planetary nebulae will be held in the beautiful Cracow, Poland, from Sept 4th to 8th, 2023, at the Jagiellonian University, where Copernicus has studied.

Collegium Novum conference room at the Jagiellonian University.

This symposium will explore and stimulate connections between planetary nebulae and research topics in modern astrophysics.

Topics included:

- Planetary nebulae as tracers of stellar evolution: the giant branch-white dwarf connection; mass loss and stellar winds; binary interactions; eruptive events and transients
- Planetary nebulae as hydrodynamics events: shaping of stellar winds, dusty winds, jet launching, jet-nebula interaction; the asterosphere; outflow shaping by binary interactions

- Planetary nebulae as astrochemistry laboratories: molecular evolution; polycyclic aromatic hydrocarbons and fullerenes; dust formation and destruction; photo-dissociation regions
- Planetary nebulae as abundances decoders: atomic physics; photo-ionization and shocks; the forbidden-line vs recombination line abundance discrepancy; primary elemental production and ISM enrichment
- Planetary nebulae as unique tools to study the structure and evolution of galaxies: star formation histories, abundance gradients, structural components and dark matter, galaxy dynamics, hierarchical mass assembly

Registration will be open soon through the conference website. Please check the conference website for more information: https://iaus384-pne.ncac.torun.pl

E-mail for contact: aus384-pne@ncac.torun.pl

Announcements

The Optical Constants database is online!

Advertised by Ella Sciamma-O'Brien

The Optical Constants database (OCdb) website provides peer-reviewed published optical constants of organic refractory materials produced in the laboratory from ice and gas processing (called ice and gas ”tholins”) and optical constants of ices and ice mixtures relevant to astrophysical, planetary, and exoplanetary environments to facilitate both their access by the scientific community and their use for the scientific analysis of observational data returned by space missions and ground-based observatories.

Optical constants are critical input parameters in models to simulate the absorption, reflection and scattering of light due to organic refractory materials and ices in planetary and astrophysical environments and are key to the interpretation of observational data (interstellar medium and molecular clouds, solar system atmospheres and surfaces, protoplanetary disks, exoplanets, comets...).

The database includes optical constants data sets generated by several laboratories and covering a broad wavelength range from 0.27 to 200 µm. *We invite the science community to contribute their published optical constants data sets to OCdb.*

E-mail for contact: ella.m.sciammaobrien@nasa.gov

Webpage: https://ocdb.smce.nasa.gov/

AstroPAH Newsletter

http://astropah-news.strw.leidenuniv.nl
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Next issue: 23 March 2023
Submission deadline: 10 March 2023