



# AstroPAH

A Newsletter on Astronomical PAHs

Issue 104 • December 2023

**Unraveling the subtle dynamics  
between PAHs and water**



# Editorial

**Dear Colleagues,**

Welcome to the last AstroPAH volume of 2023!

The gorgeous illustration in our cover is from Lemmens et al. (2023), where the interaction of PAHs and water is studied. See the abstract on page 12.

In fact, do not miss any of the papers we are including in the Abstract section this month. Beautiful results coming from theory, laboratory and observations!

Dr. Ameet Sidhu is leaving our editorial board. We thank Ameet for her dedication and great work during her tenure in our newsletter. As we wish the best to Ameet in her new adventures, we also welcome Dr. Pavithraa Sundararajan to our editorial board. We interview these two amazing scientists in our In Focus this month.

A Workshop on Astrochemistry will be held in Rio de Janeiro city in July 2024. Although the workshop is focused on the Brazilian community, they welcome all researchers from all countries and in all levels to participate in the event to start new collaborations.

AstroPAH will be back on February 2024, after our traditional January break.

Happy holidays and a wonderful 2024 to all of you!

**The Editorial Team**

**Next issue: 22 February 2022.  
Submission deadline: 9 February 2022.**

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## PAH Picture of the Month

Far-IR action spectroscopy is an excellent tool to investigate microhydrated naphthalene. The low-frequency vibrations unveiled a nuanced interplay between hydrogen bonding and dipole- $\pi$  interactions, resulting in a complex dynamics that represents itself as broad infrared absorption features. More information can be found in the work by [Lemmens et al. \(2023\)](#).

**Credits:** Image by [Lemmens et al. \(2023\)](#).

## An Interview with Pavithraa Sundararajan



**Dr. Pavithraa Sundararajan** is a Marie Curie Postdoctoral Fellow at the Leiden Observatory. She is an experimental Astrochemist. She obtained her PhD in 2020 from the Institute of Molecular Science, NYCU, Taiwan working with the matrix isolation technique to record the Infrared spectra of Polycyclic Aromatic Hydrocarbons (PAHs) in the interstellar medium. At present she is working at the Laboratory for Astrophysics (LfA), Leiden Observatory, Leiden University studying the Photo-dissociation and fragmentation of PAHs in the Photodissociation regions (PDRs) of space.

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### What inspired you to become a scientist?

When I was 10 years old, I saw the first Indian women Astronaut 'Kalpana Chawla' flying to space in the NASA's Space Shuttle *Columbia*. This remarkable achievement gained attention all over the Indian media. From that moment, I witnessed a spark in myself and started reading books, news articles and encyclopedias related to space science. I used to get completely involved when I read or when someone talks to me about outer space. At the age of 14, I made up my mind to work hard towards becoming a scientist. I would call those days *the time of enlightenment* when I truly realized the purpose of my life – to do research in space science for the rest of my life.

### How did you get into PAH-related research?

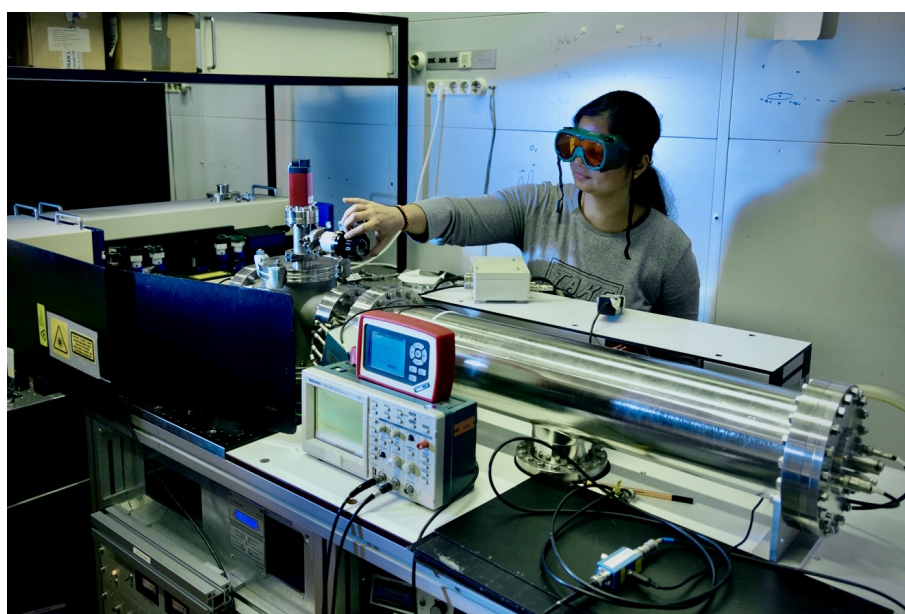
As a Masters student, after performing several short-term projects in Solar Physics,

Astronomical Instrumentation, Meteoritics, etc., I came across the exciting field of Astrochemistry. Ever since my first project in experimental Astrochemistry at Physical Research Laboratory, India, I was determined to pursue a PhD in it. Then I joined NYCU, Taiwan for PhD research where I was awarded the 'Outstanding New Student Scholarship'. For my thesis, I performed matrix isolation experiments to record the high resolution infrared spectra of large PAH molecules that are fragments of buckyball, C<sub>60</sub>. With the same enthusiasm I continued working on PAHs even for my postdoctoral research.

## 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 did Masters in Physics as I believed it is important to have a foundation in it, from where I can understand how the Universe works. Meantime, I also did an internship at the Indian Institute for Astrophysics, Bangalore. Then worked for a year at the Physical Research Laboratory, India as a Project Associate where I gained awareness about a lot of ongoing research topics. My PhD in Astrochemistry was at the Institute of Molecular Sciences, Department of Applied Chemistry, NYCU, Taiwan.

Astrochemistry being an interdisciplinary field, though I gained a Physics background, I had to take up courses and qualifying exams in Chemistry during the first two years of my PhD. As a student, it was challenging for me to adapt to core Chemistry subjects and had to toil to balance between the course work and research. However, at this point in my carrier I feel fortunate to have taken that decision, as both Physics and Chemistry are the essence to experiment and interpret the reactions happening in space. The passion that I have towards research, particularly in performing laboratory experiments, keeps me going even at tough times.



**Figure 1** – The Instrument for Photodynamics of PAHs (*i-PoP*) housed at the Laboratory for Astrophysics (*LfA*), Leiden University.

## What is your current research about?

At present I'm a Marie Curie Postdoctoral Researcher at the Leiden University. I work with Prof. Xander Tielens and perform photo-dissociation experiments with bowl-shaped PAH called 'buckybowls' that are fragments of  $C_{60}$ . Buckyball ( $C_{60}$ ) has a cage-like structure consisting of fused hexagon and pentagon rings and these pentagons leads to curvature of the planar PAH structure and closure upon itself. Pentagon formation is thus a prerequisite for the photochemical transformation of PAHs into fullerenes. They may represent likely intermediaries in the formation routes of  $C_{60}$  in space. The photochemical evolution of PAHs with pentagons and their respective IR spectra are largely unexplored till date. Hence, I'm performing both spectroscopic and spectrometric experiments on these least explored pentagon containing PAHs to understand their role in the interstellar medium.

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

With the unprecedented spectroscopic data from the James Webb Space Telescope, and ever-growing experimental and theoretical spectroscopic databases, I hope Astrochemists (we) can unambiguously identify the PAH(s) responsible for the AIBs. And further continue to implement this knowledge to understand the evolution of carbon chemistry at a larger scale.

## 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?

As an experimentalist, collaboration with observational and theoretical experts becomes an integral part of my Astrochemistry research. It is important for us to understand each other's scientific language to build and contribute a solid research to the community. I find it very interesting to interact with Astronomers, spectroscopist, physical chemists, etc., as each one can endorse a new perspective to an ongoing research.

## How has the COVID-19 pandemic affected your professional life?

I received my doctorate in Taiwan and returned home in February 2020. The COVID-19 lockdown started in March 2020. Though I felt lucky to have defended my thesis before the lockdown and was back with my family, I had no idea back then that I'm going to face the most uncertain period in my professional life. I started applying for postdoc positions well ahead and was already writing few proposals. The severe lockdown conditions at that phase, and the fact that my country was travel red-listed had a heavy impact on almost all my applications. Lack of funding in many laboratories and change in immigration policies because of the pandemic heavily narrowed my chances to get a postdoc position. As a consequence, I had to face a 1.5 years long career break! Even at such hard-hitting times,

I kept contacting scientists and constantly took efforts with a hope that I will get what I deserve. Today, when I look back at those times, I realize that I have only got more stronger and more gritty. I would like to encourage the readers (especially the aspiring scientists) to stay persistent and keep working towards what you want! Never give up!

## What was the most important advice somebody gave you?

The past 10 years in academia has shown me various dimensions involved in career growth. Here are three important advices that I received which helped me a lot:

(i) A good motivation is necessary for everyone, especially for students, to keep performing better. I would like to share the words that my aunt tells me when I feel sad or discouraged *“Tough times never last, but tough people do!”*.

(ii) Another important advice that I have received from a best friend of mine who had overcome imposter syndrome is that *“There are days when we feel energized and accomplish many tasks, and there are days when we just have to keep one foot in front of another and slowly walk forward. Learn to accept both!”*.

(iii) The third one is not an advice but a strong realization after working with several research groups across the globe: *“The success in scientific research is mainly an outcome of consistent commitment and ethical teamwork”*.

## How do you balance your professional and personal life?

Work-life balance is important for any profession. When at work I'm mindful of the effective working hours. I make a checklist with priorities for the whole week and try my best to get it done. But in research, we often get sidetracked with many ideas, travels and discussions. As long as I am satisfied with the science I do in a week I don't feel guilty, and accept that this is how research works. I also try my best not to compromise on my personal time.

## What do you do outside of work?

On sunny days, I usually take a nature walk, or go on a picnic with friends, or spot a good ice cream shop and try one flavor per week! Haha! In spring, I enjoy cycling along the tulip fields in the Netherlands. My favorite hobbies in winter are pencil sketching and doodling; I believe they are equivalent to meditation.

## What does it mean for you to be part of the AstroPAH editorial team?

Ever since I started working on PAHs (since 2015), AstroPAH newsletter has been one of the go to place for me to stay updated. I feel privileged to be a part of the AstroPAH editorial team that has readers at a global level. I'm eagerly looking forward to working with the editorial team and gain amazing experiences.

# In Focus

## An Interview with Ameek Sidhu



**Dr. Ameek Sidhu** completed her PhD in Astronomy with a specialisation in Planetary science and space exploration under the supervision of Profs Els Peeters and Jan Cami at Western University in 2019. She later continued with them for a postdoc where she worked on the data observed with the JWST. Her research focuses on investigating the emission from large carbonaceous molecules, particularly polycyclic aromatic hydrocarbons and fullerenes in the interstellar medium from an observational and theoretical standpoint.

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### What inspired you to become a scientist?

Since I was young, I have heard about Kiran Bedi, the first Woman Indian Police services officer, and Kalpana Chawla, the first Indian Woman to go to space, and their stories are truly inspiring. I never thought of becoming a scientist but rather a person who can inspire at least one other Woman. I was good at academics and wanted to continue as much as possible. Physics was the subject I enjoyed the most, so I continued my journey in physics, eventually earning a PhD in astrophysics and becoming a scientist.

### How did you get into astrochemistry research?

I took a special course in Astrophysics in the final year of my Masters in Physics. I was so impressed with the course that I decided to pursue a PhD in astronomy. I also wanted to pursue it outside of my home country, India, to broaden my horizons, so I began applying for PhD positions in Astronomy in Canada. Prof. Els Peeters and Jan Cami offered me



a PhD position to study the causes of variations in cosmic PAH emission. I was drawn to the research project and began my PhD under their supervision. During my PhD, I had the opportunity to work with Xander Tielens on theoretical modelling of PAH emission, which introduced me to a different area of PAH research.

## **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?**

After finishing my PhD in Astronomy, I decided to pursue a postdoc and got the opportunity to work with incredible JWST data. It was a great experience learning the intricacies of data obtained from a new telescope. As much as I enjoy astronomy, I also wanted to be closer to my family in Canada and to be more financially independent, something I thought I wouldn't be able to achieve if I continued in academia. So, I left academia and entered the finance industry. However, I would like to be involved with astronomy and research, and hopefully, I can find the right balance between my new career and astronomy soon.

## **What are, in your opinion, the present forefronts of astrochemistry research?**

PAHs are present almost everywhere in the universe and exhibit spectral variations in response to the changes in the physical conditions of the environments where they reside. This sensitivity on physical conditions combined with their omnipresence makes PAHs an excellent tool for probing the physical conditions of astrophysical regions. However, the necessary empirical relationships between PAH spectral characteristics and physical conditions have not been fully developed yet. One of the most challenging aspects of establishing such relationships is that we do not fully understand the molecular physics behind the PAH emission. A combined effort of observations and theory is required to make progress in this direction. In order to fully understand the physics underlying the PAH emission, I think developing a comprehensive photo-chemical evolution model would be helpful in interpreting the high spectral resolution PAH spectra observed with the James Webb Space Telescope.

## **What was the most important advice somebody gave you?**

The famous quote by Abraham Lincoln, "I walk slowly, but I never walk backward", has had the greatest impact on me. This quote gets me going on the days I'm not feeling motivated to work.

## **How do you balance your professional and personal life?**

When you work as a full-time researcher, the lines between your professional and personal lives can be a bit blurry. So, I never really learnt the art to maintain the balance.

Even in a new career that requires a lot of learning, it is tough to strike a balance. However, I have understood that spending some time doing things that nourish your mental health is important and will benefit you in the long run, both professionally and personally.

## **What do you do outside of work?**

My family and friends are my stress relievers. So, when I'm not working, I spend most of my time with them. I also enjoy painting, reading, and going for hikes.

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

I am probably not the ideal candidate to answer this question because I am no longer in academia. However, based on what I've observed, I can provide some suggestions. Network as much as possible, be confident in yourself and your work, and seek out new opportunities. It's always helpful to talk to young faculty members in your department because they have been down that path before you and, most importantly, persevere. Finding a full-time job may appear challenging, but I believe that if you persevere, you will eventually succeed.



# Abstracts

## Fragmentation channels of non-fullerene cationic carbon clusters

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The unimolecular fragmentation channels of highly excited small cationic carbon clusters have been measured with a time-of-flight mass spectrometer after photofragmentation. The dominant channel is loss of the neutral trimer, for all  $C_N^+ N = 10-27$  clusters except for  $N = 11, 12$  which decay by monomer emission, and  $C_{25}^+$  which shows competing loss of  $C_2$  and  $C_3$ . The results permit to quantify the role of the rotational entropy in the competition between monomer and trimer decays with the help of energies calculated with density functional theory.

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# Wetting of a Hydrophobic Surface: Far-IR Action Spectroscopy and Dynamics of Microhydrated Naphthalene

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The interaction of water and polycyclic aromatic hydrocarbons is of fundamental importance in areas as diverse as materials science or atmospheric and interstellar chemistry. The interplay between hydrogen bonding and dipole- $\pi$  interactions results in subtle dynamics that are challenging to describe from first principles. Here, we employ far-IR action vibrational spectroscopy with the infrared free-electron laser FELIX to investigate naphthalene with one to three water molecules. We observe diffuse bands associated with intermolecular vibrational modes that serve as direct probes of the loose binding of water to the naphthalene surface. These signatures are poorly reproduced by static DFT or Møller–Plesset computations. Instead, a rationalization is achieved through Born-Oppenheimer Molecular Dynamics simulations, revealing an active mobility of water over the surface, even at low temperatures. Therefore, our work provides direct insights into the wetting interactions associated with shallow potential energy surfaces, while simultaneously demonstrating a solid experimental-computational framework for their investigation.

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# JWST: Deuterated PAHs, PAH-nitriles, and PAH Overtone and Combination Bands I: Program Description and First Look

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A first look is taken at the NIRSpec 1-5  $\mu\text{m}$  observations from *JWST* program 1591 that targets 7 objects along the low-mass stellar life cycle with PAH emission. Spectra extracted from a 1".5 radius sized circular aperture are explored, showing a wealth of features, including the 3  $\mu\text{m}$  PAH complex, the PAH-continuum, and atomic and molecular emission lines from H I, He, H<sub>2</sub>, and other species. CO<sub>2</sub>- and H<sub>2</sub>O-ice absorption and CO emission is also seen. Focusing on the bright-PDR position in M17, the PAH CH stretch falls at 3.29  $\mu\text{m}$  (FWHM = 0.04  $\mu\text{m}$ ). Signs of its 1.68  $\mu\text{m}$  overtone are confused by line emission in all targets. Multi-component decomposition reveals a possible aliphatic deuterated PAH feature centered at 4.65  $\mu\text{m}$  (FWHM = 0.02  $\mu\text{m}$ ), giving  $[D/H]_{\text{alip.}} = 31 \pm 12.7\%$ . However, there is little sign of its aromatic counterpart between 4.36-4.43  $\mu\text{m}$ . There is also little sign of PAH-nitrile emission between 4.34-4.39  $\mu\text{m}$ . A PAH continuum rises from  $\sim 1$  to 3.2  $\mu\text{m}$ , after which it jumps by about a factor of 2.5 at 3.6  $\mu\text{m}$ , with bumps at 3.8, 4.04, and 4.34  $\mu\text{m}$  adding structure. The CO<sub>2</sub> absorption band in M17 is matched with 10:1 H<sub>2</sub>O:CO<sub>2</sub> ice at 10 K. The  $v = 0$  pure rotational molecular hydrogen population diagram reveals  $>2200$  K UV-pumped gas. The hydrogen Pfund series runs from levels 10 to  $>30$ . Considering  $Br\alpha/Br\beta = 0.381 \pm 0.01966$  and Case B recombination results in  $A_V \simeq 8$ . CO emission in IRAS21282+5050 originates from 258 K gas. In-depth spectral-spatial analysis of all features and targets are planned for a series of forthcoming papers.

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# New light on the imbroglia surrounding the $C_8H_6^+$ isomers formed from ionized azulene and naphthalene using ion-molecule reactions

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Most polycyclic aromatic hydrocarbons (PAHs) can isomerize with internal energies near to or below the dissociation threshold. The  $C_{10}H_8^+$  group of ions, made up of the naphthalene (**Naph**<sup>+</sup>) and the azulene (**Azu**<sup>+</sup>) radical cations, is a prototypical example.  $C_8H_6^+$  isomers are important species in the growth kinetics and formation of complex organic molecules, and more generally fragments from larger PAHs, yet information about  $C_8H_6^+$  structures is scarce and contradictory. Here, ion-molecule reactions were carried out and the tunable photoionization chemical monitoring technique was used to probe the  $C_8H_6^+$  isomers formed upon  $C_2H_2$ -loss from **Naph**<sup>+</sup> and **Azu**<sup>+</sup>. The experimental findings were interpreted with the support of *ab initio* and kinetics calculations. To facilitate the interpretation of these data, chemical reactivity starting from phenylacetylene (**PA**) was studied. It was found that most of the  $C_8H_6^+$  ions formed from  $C_{10}H_8$ , in a timescale of 40  $\mu$ s, are **PA**<sup>+</sup> in the vicinity of the dissociation threshold. No evidence of the pentalene radical cation (**PE**<sup>+</sup>) was observed and explanations to reconcile previous results are presented.

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# Spectroscopy of $C_{60}^+$ and $C_{120}^+$ in the mid-infrared

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Infrared spectra of  $C_{60}^+$  and  $C_{120}^+$ , obtained via helium messenger spectroscopy, are reported. For  $C_{60}^+$ , new absorption features have been found just above the discrete vibrational spectrum of the ion. The absorption profile, which is broad and contains little structure, is assigned to one or more electronic absorption transitions and is in good agreement with predictions from time-dependent density functional theory. It seems likely that the transitions observed correspond to excitation from the  $^2A_{1u}$  electronic ground state to one or both of the low-lying  $^2E_{1u}$  and  $^2E_{2u}$  electronic states previously identified as dark states of  $C_{60}^+$ . These states presumably become optically bright through vibronic coupling, and specifically the Jahn-Teller effect. In the case of  $C_{120}^+$ , the simplest positively charged oligomer of  $C_{60}$ , we present the first vibrational spectrum of this ion. Through comparison with theory, the vibrational features are best explained by a peanut-shaped structure for  $C_{120}^+$ , maintained by covalent bonding between the two  $C_{60}$  units. We have also discovered electronic transitions for  $C_{120}^+$  which, similar to  $C_{60}^+$ , lie just above the vibrational spectrum.

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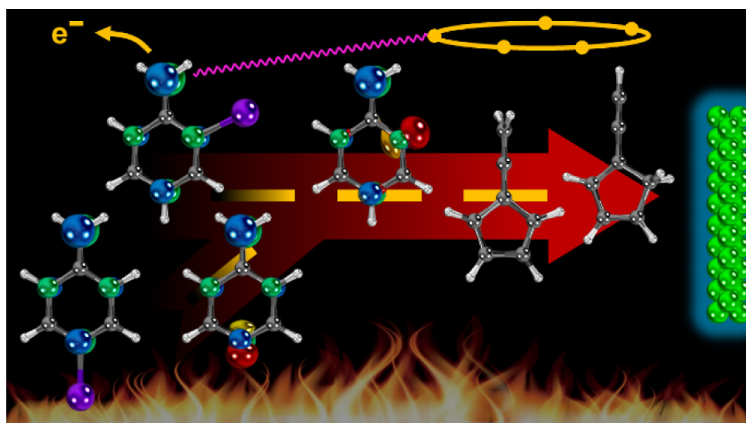
# Thermal Decomposition of 2- and 4-Iodobenzyl Iodide Yields Fulvenallene and Ethynylcyclopentadienes: A Joint Threshold Photoelectron and Matrix Isolation Spectroscopic Study

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The thermal decomposition of 2- and 4-iodobenzyl iodide at high temperatures was investigated by mass-selective threshold photoelectron spectroscopy (ms-TPES) in the gas phase, as well as by matrix isolation infrared spectroscopy in cryogenic matrices. Scission of the benzylic C–I bond in the precursors at 850 K affords 2- and 4-iodobenzyl radicals (*ortho*- and *para*-IC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub><sup>•</sup>), respectively, in high yields. The adiabatic ionization energies of *ortho*-IC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub><sup>•</sup> to the  $\tilde{X}^+(^1A')$  and  $\tilde{a}^+(^3A')$  cation states were determined to be 7.31±0.01 and 8.78±0.01 eV, whereas those of *para*-IC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub><sup>•</sup> were measured to be 7.17±0.01 eV for  $\tilde{X}^+(^1A_1)$  and 8.98±0.01 eV for  $\tilde{a}^+(^3A_1)$ . Vibrational frequencies of the ring breathing mode were measured to be 560±80 and 240±80 cm<sup>-1</sup> for the  $\tilde{X}^+(^1A')$  and  $\tilde{a}^+(^3A')$  cation states of *ortho*-IC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub><sup>•</sup>, respectively. At higher temperatures, subsequent aryl C–I cleavage takes place to form  $\alpha,2$ - and  $\alpha,4$ -didehydrotoluene diradicals, which rapidly undergo ring contraction to a stable product, fulvenallene. Nevertheless, the most intense vibrational bands of the elusive  $\alpha,2$ - and  $\alpha,4$ -didehydrotoluene diradicals were observed in the Ar matrices. In addition, high-energy and astrochemically relevant C<sub>7</sub>H<sub>6</sub> isomers 1-, 2-, and 5-ethynylcyclopentadiene are observed at even higher pyrolysis temperatures along with fulvenallene. Complementary quantum chemical computations on the C<sub>7</sub>H<sub>6</sub> potential energy surface predict a feasible reaction cascade at high temperatures from the diradicals to fulvenallene, supporting the experimental observations in both the gas phase and cryogenic matrices.



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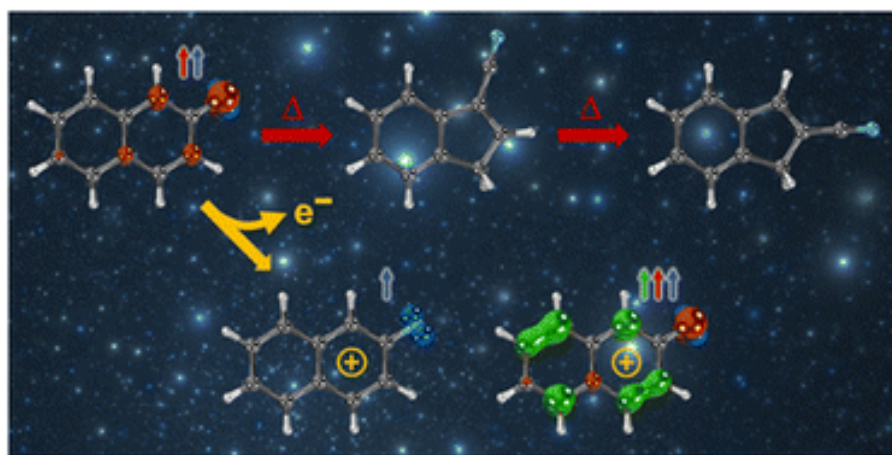
# Photoelectron spectroscopic study of 2-naphthyl nitrene and its thermal rearrangement to cyanoindenes

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2-Cyanoindene has recently been identified in the interstellar medium, however current models cannot fully account for its formation pathways. Herein, we identify and characterize 2-naphthyl nitrene, which is prone to rearrange to 2- and 3-cyanoindene, in the gas phase using photoion mass-selective threshold photoelectron spectroscopy (ms-TPES). The adiabatic ionization energies (AIE) of triplet nitrene ( $^3A''$ ) to the radical cation in its lowest-energy doublet  $\tilde{X}^+(^2A')$  and quartet  $\tilde{a}^+(^4A')$  electronic states were determined to be  $7.72 \pm 0.02$  and  $8.64 \pm 0.02$  eV, respectively, leading to a doublet-quartet energy splitting ( $\Delta E_{D-Q}$ ) of 0.92 eV (88.8 kJ mol<sup>-1</sup>). A ring-contraction mechanism yields 3-cyanoindene, which is selectively formed under mild pyrolysis conditions (800 K), while the lowest-energy isomer, 2-cyanoindene, is also observed under harsh pyrolysis conditions at 1100 K. The isomer-selective assignment was rationalized by Franck-Condon spectral modeling and by measuring the AIEs at  $8.64 \pm 0.02$  and  $8.70 \pm 0.02$  eV for 2- and 3- cyanoindene, respectively, in good agreement with quantum chemical calculations.



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# PDRs4All III: JWST's NIR spectroscopic view of the Orion Bar

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JWST has taken the sharpest and most sensitive infrared (IR) spectral imaging observations ever of the Orion Bar photodissociation region (PDR), which is part of the nearest massive star-forming region the Orion Nebula, and often considered to be the “prototypical” strongly illuminated PDR. We investigate the impact of radiative feedback from massive stars on their natal cloud and focus on the transition from the H II region to the atomic PDR (crossing the ionisation front (IF)), and the subsequent transition to the molecular PDR (crossing the dissociation front (DF)). Given the prevalence of PDRs in the interstellar medium and their dominant contribution to IR radiation, understanding the response of the PDR gas to far-ultraviolet (FUV) photons and the associated physical and chemical processes is fundamental to our understanding of star- and planet formation and for the interpretation of any unresolved PDR as seen by JWST.

We use high-resolution near-IR integral field spectroscopic data from NIRSpec on JWST to observe the Orion Bar PDR as part of the PDRs4All JWST Early Release Science Program. We construct a  $3'' \times 25''$  spatio-spectral mosaic covering  $0.97\text{--}5.27\ \mu\text{m}$  at a spectral resolution  $R$  of  $\sim 2700$  and an angular resolution of  $0.075\text{--}0.173''$ . To study the properties of key regions captured in this mosaic, we extract five template spectra in apertures centered on the three H<sub>2</sub> dissociation fronts, the atomic PDR, and the H II region. This wealth of detailed spatial-spectral information is analysed in terms of variations in the physical conditions—incident UV field, density, and temperature—of the PDR gas.

The NIRSpec data reveal a forest of lines including, but not limited to, He I, H I, and C I recombination lines, ionic lines (e.g., Fe III, Fe II), O I and N I fluorescence lines, Aromatic Infrared Bands (AIBs including aromatic CH, aliphatic CH, and their CD counterparts), CO<sub>2</sub> ice, pure rotational and ro-vibrational lines from H<sub>2</sub>, and ro-vibrational lines HD, CO, and CH<sup>+</sup>, most of them detected for the first time towards a PDR. Their spatial distribution resolves the H and He ionisation structure in the Huygens region, gives insight into the geometry of the Bar, and confirms the large-scale stratification of PDRs. In addition, we observe numerous smaller scale structures whose typical size decreases with distance from  $\theta^1$  Ori C and IR lines from C I, if solely arising from radiative recombination and cascade, reveal very high gas temperatures (a few 1000 K) consistent with the hot irradiated surface of small-scale dense clumps deep inside the PDR. The morphology of the Bar, in particular, the H<sub>2</sub> lines reveals multiple, prominent filaments which exhibit different characteristics. This leaves the impression of a “terraced” transition from the predominantly atomic surface region to the CO-rich molecular zone deeper in. We attribute the different characteristics of the H<sub>2</sub> filaments to their varying depth into the PDR and, in some cases, not reaching the C<sup>+</sup>/C/CO transition.

These observations thus reveal what local conditions are required to drive the physical and chemical processes needed to explain the different characteristics of the DFs and the photochemical evolution of the AIB carriers. This study showcases the discovery space created by JWST to further our understanding of the impact radiation from young stars has on their natal molecular cloud and proto-planetary disk, which touches on star- and planet formation as well as galaxy evolution. E-mail: [epeeters@uwo.ca](mailto:epeeters@uwo.ca)

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# PDRs4All IV. An Embarrassment of Riches: Aromatic Infrared Bands in the Orion Bar

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Mid-infrared observations of photodissociation regions (PDRs) are dominated by strong emission features called aromatic infrared bands (AIBs). The most prominent AIBs are found at 3.3, 6.2, 7.7, 8.6, and 11.2  $\mu\text{m}$ . The most sensitive, highest-resolution infrared spectral imaging data ever taken of the prototypical PDR, the Orion Bar, have been captured by *JWST*. These high-quality data allow for an unprecedentedly detailed view of AIBs.

We provide an inventory of the AIBs found in the Orion Bar, along with mid-IR template spectra from five distinct regions in the Bar: the molecular PDR (i.e. the three H<sub>2</sub> dissociation fronts), the atomic PDR, and the HII region. We used *JWST* NIRSpec IFU and MIRI MRS observations of the Orion Bar from the *JWST* Early Release Science Program, PDRs4All (ID: 1288). We extracted five template spectra to represent the morphology and environment of the Orion Bar PDR. We investigated and characterised the AIBs in these template spectra. We describe the variations among them here.

The superb sensitivity and the spectral and spatial resolution of these *JWST* observations reveal many details of the AIB emission and enable an improved characterization of their detailed profile shapes and sub-components. The Orion Bar spectra are dominated by the well-known AIBs at 3.3, 6.2, 7.7, 8.6, 11.2, and 12.7  $\mu\text{m}$  with well-defined profiles. In addition, the spectra display a wealth of weaker features and sub-components. The widths of many AIBs show clear and systematic variations, being narrowest in the atomic PDR template, but showing a clear broadening in the HII region template while the broadest bands are found in the three dissociation front templates. In addition, the relative strengths of AIB (sub-)components vary among the template spectra as well. All AIB profiles are characteristic of class A sources as designated by Peeters et al. (2002), except for the 11.2  $\mu\text{m}$  AIB profile deep in the molecular zone, which belongs to class B<sub>11.2</sub>. Furthermore, the observations show that the sub-components that contribute to the 5.75, 7.7, and 11.2  $\mu\text{m}$  AIBs become much weaker in the PDR surface layers. We attribute this to the presence of small, more labile carriers in the deeper PDR layers that are photolysed away in the harsh radiation field near the surface. The 3.3/11.2 AIB intensity ratio decreases by about 40% between the dissociation fronts and the HII region, indicating a shift in the polycyclic aromatic hydrocarbon (PAH) size distribution to larger PAHs in the PDR surface layers, also likely due to the effects of photochemistry. The observed broadening of the bands in the molecular PDR is consistent with an enhanced importance of smaller PAHs since smaller PAHs attain a higher internal excitation energy at a fixed photon energy.

Spectral-imaging observations of the Orion Bar using *JWST* yield key insights into the

photochemical evolution of PAHs, such as the evolution responsible for the shift of 11.2  $\mu\text{m}$  AIB emission from class B<sub>11.2</sub> in the molecular PDR to class A<sub>11.2</sub> in the PDR surface layers. This photochemical evolution is driven by the increased importance of FUV processing in the PDR surface layers, resulting in a “weeding out” of the weakest links of the PAH family in these layers. For now, these *JWST* observations are consistent with a model in which the underlying PAH family is composed of a few species: the so-called ‘grandPAHs’.

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# PDRs4All VI: Probing the Photochemical Evolution of PAHs in the Orion Bar Using Machine Learning Techniques

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Extraordinary observations of the Orion Bar by *JWST* have shown, for the first time, the incredible richness of PAH emission bands and their variation on very small scales. These variations are the result of photochemical evolution of the PAH carrier.

We aim to probe the photochemical evolution of PAHs across the key zones of the ideal photodissociation region (PDR) that is the Orion Bar using unsupervised machine learning.

We use *JWST* NIRSpec IFU and MIRI MRS observations of the Orion Bar from the *JWST* Early Release Science Program PDRs4All (ID: 1288). We lever bisecting k-means clustering to generate highly detailed spatial maps of the spectral variability in the 3.2 – 3.6, 5.95 – 6.6, 7.25 – 8.95, and 10.9 – 11.63  $\mu\text{m}$  wavelength regions. We analyse and describe the variations in the cluster profiles and connect them to the conditions of the physical locations from which they arise. We interpret the origin of the observed variations with respect to the following key zones: the H II region, the atomic PDR zone, and the layers of the molecular PDR zone stratified by the first, second, and third dissociation fronts (DF 1, DF 2, and DF 3, respectively).

Observed PAH emission exhibits spectral variation that is highly dependent on spatial

position in the PDR. We find the  $8.6 \mu\text{m}$  band to behave differently than all other bands which vary systematically with one another. Notably, we find uniform variation in the  $3.4 - 3.6 \mu\text{m}$  bands and  $3.4/3.3$  intensity ratio. We attribute the carrier of the  $3.4 - 3.6 \mu\text{m}$  bands to a single side group attached to very similarly sized PAHs. Further, cluster profiles reveal a transition between characteristic profiles classes of the  $11.2 \mu\text{m}$  feature from the atomic to the molecular PDR zones. We find the carriers of each of the profile classes to be independent, and reason the latter to be PAH clusters existing solely deep in the molecular PDR. Clustering also reveals a connection between the  $11.2$  and  $6.2 \mu\text{m}$  bands; and that clusters generated from variation in the  $10.9 - 11.63 \mu\text{m}$  region can be used to recover those in the  $5.95 - 6.6 \mu\text{m}$  region.

Clustering is a powerful and comprehensive tool for characterising PAH spectral variability on both spatial and spectral scales. For individual bands as well as global spectral behaviours, we find ultraviolet-processing to be the most important driver of the evolution of PAHs and their spectral signatures in the Orion Bar PDR.

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# Meetings

## Workshop on Astrochemistry (Workshop de Astroquímica)

Universidade Federal do Rio de Janeiro, CCMN, Ilha do Fundão  
Rio de Janeiro, Brazil

04-05 July, 2024

<https://sites.google.com/fat.uerj.br/workshop-astroquimica/>

Save the date: on 4 and 5 July 2024, the Federal University of Rio de Janeiro (UFRJ) in Brazil will hold a Workshop on Astrochemistry. It will be a two-day meeting with invited talks, oral communications, and poster presentations.

The meeting will bring together the Astrochemistry community from Rio de Janeiro and other Brazilian States. It will be an event to show the work being developed in Astrochemistry, share expertise, and promote collaborations. The meeting focuses on the Brazilian Astrochemistry community and all those interested in contributing to this area of knowledge. Everyone is welcome: undergraduate students, post-graduates, and researchers.

Registrations will begin on 2 February 2024, and the deadline for contribution submissions will be announced soon.

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### AstroPAH Newsletter

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