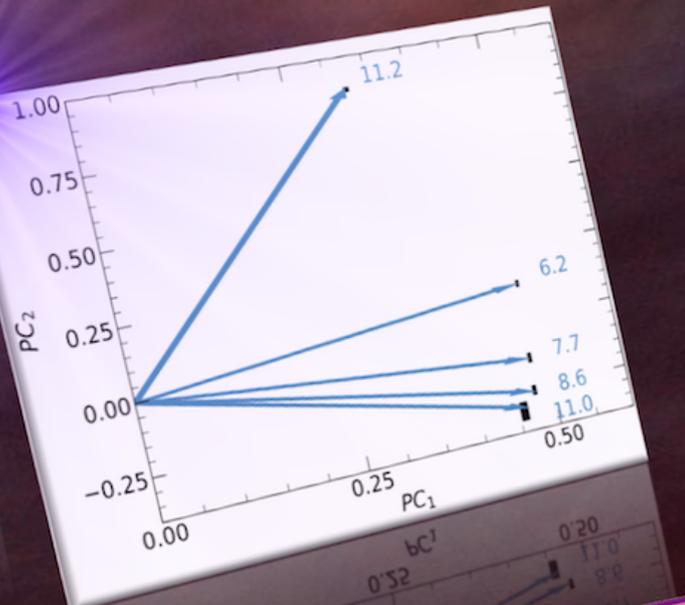
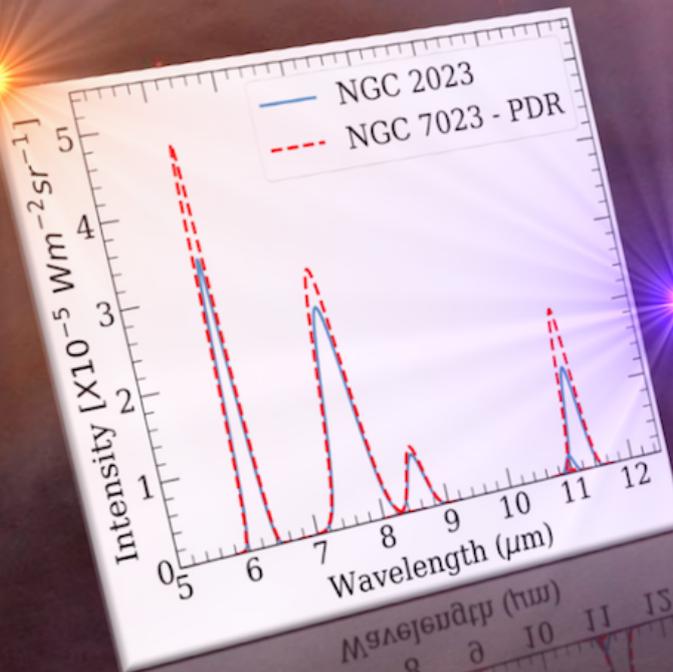


# AstropAH

A Newsletter on Astronomical PAHs

Issue 85 • February 2022



**Principal component analysis  
of PAHs emission in NGC 7023**

# Editorial

## Dear Colleagues,

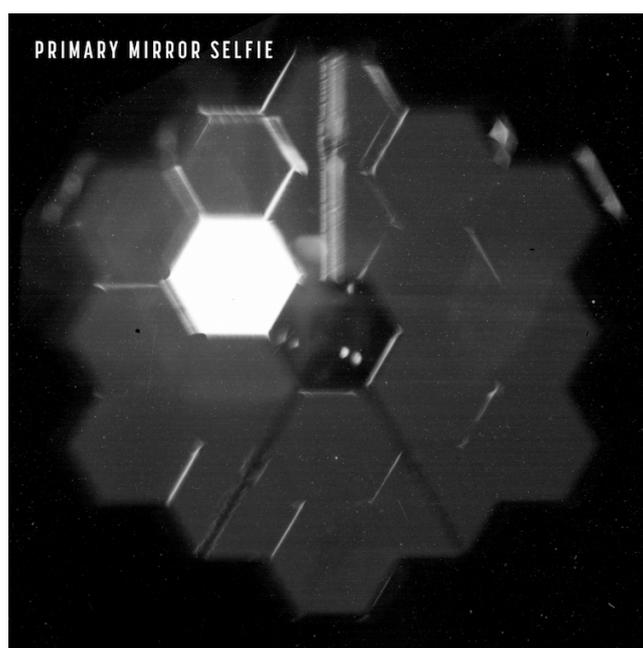
Welcome to our first 2022 AstroPAH! We are back from our January hiatus, and we hope all of you are healthy and doing well!

We are very happy to introduce you to our new editor, Dr. Rijutha Jaganathan! Rijutha joins us from the Center for Interstellar Catalysis at Aarhus University in Denmark. As per our tradition, our interview with Rijutha features in this month's In Focus! Welcome, Rijutha!

Our Picture of the Month relates to a recent study by Sidhu et al. (2022) on a principal component analysis of polycyclic aromatic hydrocarbons emission in NGC 7023. Make sure you check out our abstract section to learn more about it!

We have a plethora of new publications to share with you! Be sure to check them out; they cover a wide array of PAH characteristics in molecular clouds, gas phase synthesis of benzene, and the mysterious benzvalyne.

We also could not resist sharing with you the first "JWST selfie", taken by the NIRCam instrument! This image was taken by a lens inside NIRCam to properly verify the primary mirror segment alignment. JWST is currently going through its Step 2 segment alignment and cooldown portion of the mission. Most recently, JWST completed its [segment image identification](#) which captured the light of an isolated star, where 18 shifted copies of the same star were acquired. This step enables the further important fine-tuning of the telescope!



**Figure 1** – JWST primary mirror selfie. Credit: NASA

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 or other ideas, feel free to use our [email](#).

**The Editorial Team**

**Next issue: 24 March 2022.  
Submission deadline: 11 March 2022.**

# AstroPAH Newsletter

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## PAH Picture of the Month

A principal component analysis of PAHs emission in NGC 7023 by [Sidhu et al. \(2022\)](#). The graph on the left shows a characteristic PAH spectrum of  $PC_1$  in the PDR cavity. The biplots on the right show the projection of the standardized flux variables in the  $PC_1$ - $PC_2$  plane in NGC 7023.

**Credits:** [Sidhu et al. \(2022\)](#). Background image credit: NGC 7023 image by [NASA/ESA](#).

## An Interview with Rijutha Jaganathan

Dr. Rijutha Jaganathan is currently a postdoctoral researcher at the Center for Interstellar Catalysis (InterCat) at Aarhus University in Denmark. She completed her Bachelor's and Master's degrees in Physics in her home city - Bangalore, India. After that, she spent a couple of months as a visiting student at the Tata Institute of Fundamental Research (TIFR), Mumbai, India, during which she became interested in the interdisciplinary field of Astrochemistry. To take that interest forward, she moved to Denmark for her PhD. She did her doctoral research in Professor Liv Hornekær's group under the Horizon2020 Marie Skłodowska-Curie ITN EUROPAH project.



### Can you tell us how you got into PAH-related research, and your current research project?

While looking for astrochemistry-related PhD positions in Europe, I came across the advertisement for a laboratory astrophysics project at Aarhus University. It seemed like a great combination of astronomy and laboratory work and I applied for it. I joined the Surface Dynamics group in September 2017 wherein I used surface science techniques to study the interaction of a variety of polycyclic aromatic hydrocarbons (PAHs) with hydrogen atoms leading to small molecule formation. I was especially interested in the effect of the shape, functionalization and size of the PAHs on their interaction with H atoms. Being a part of the EUROPAH ITN opened up collaborations with other research groups from across Europe. In addition to a theory collaboration with Prof. Xander Tielens' group at Leiden University, I spent some time at the FELIX Laboratory with Prof. Jos Oomens' group obtaining gas phase IR spectra of the PAHs I had studied at Aarhus.

In the interstellar medium, PAHs with nitrogen substitution (similar to the nucleobases in our DNA) or oxygen functionalisation (similar to the molecules that make up membranes) could provide clues to the origins of life on earth and possibly elsewhere. The interaction of PAHs with other constituents of the interstellar medium – atoms, molecules, and radiation, will likely contribute to the rich chemistry of the Universe. Using a combination of surface

science techniques, I am interested in investigating the role of surface reactions in interstellar chemistry especially focusing on pathways that lead to formation of prebiotic molecules.

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

I have been interested in science communication for the last few years and have dabbled in various aspects of it. As a part of AstroPAH, I am keen to find and highlight the interesting work being done in this field along with the people behind it.

## **Which open question in Laboratory Astrophysics would you like to see answered in the near future?**

I am looking forward to work that will investigate the role of PAHs in setting the stage for the molecular building blocks of life to form in space.

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

The pandemic has definitely had a negative impact on the quality and the quantity of my research in the last two years. Lockdowns meant restricted access to the labs and hence delay in getting the required data, travel restrictions meant that beam times at facilities and collaborations had to be put on hold. The lack of in-person conferences meant that discussions with peers were either virtual or non-existent and that it took longer to get feedback on latest results.

## **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?**

I enjoy the multidisciplinary aspect of the field. It can be challenging in terms of communicating ideas, understanding jargon, the data management and the data analysis. However, these same challenges push me out of my comfort zone and hence broaden my horizon. Both during my PhD and now during my postdoc, collaborations have been an integral part – be it with theoretical chemists or with other laboratory astrophysics groups. They have also happened effortlessly due to the nature of the field. Not only have I acquired a wider variety of skill set than I expected to but also made new friends and explored new places because of these collaborations.

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

That it is the journey and not the destination that matters.

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

I am still on the path of finding a balance between the two. It helps that in Denmark, there's a strong culture of enabling work-life balance. There are days on which work takes priority and some others on which personal life takes priority. I am learning to not feel guilty about either.

## What do you do outside of work?

When I am not in the lab or staring at the computer screen, I am cooking, reading or on the hunt for good cake. I also document these adventures on my blog <https://avial7.wordpress.com/blog/>.



# Abstracts

## Machine-learning correlation between infrared bands of PAHs

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Supervised machine learning models are trained with various molecular descriptors to predict infrared emission spectra of interstellar polycyclic aromatic hydrocarbons. We demonstrate that a feature importance analysis based on the random forest algorithm can be utilized to explore the physical correlation between emission features. Astronomical correlations between infrared bands are analyzed as examples of demonstration by finding the common molecular fragments responsible for different bands, which improves the current understanding of the long-observed correlations. We propose a way to quantify the band correlation by measuring the similarity of the feature importance arrays of different bands, via which a correlation map is obtained for emissions in the out-of-plane bending region. Moreover, a comparison between the predictions using different combinations of descriptors underscores the strong prediction power of the extended-connectivity molecular fingerprint, and shows that the combinations of multiple descriptors of other types in general lead to improved predictivity.

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The Astrophysical Journal, 922, 101 (2021)

<https://doi.org/10.3847/1538-4357/ac2c78>

# Gas-phase formation of interstellar pyrimidine nucleobases

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Cytosine, thymine and uracil are three pyrimidine nucleobases that are fundamental units of the genetic code in RNA and DNA. In searching the extraterrestrial origins of the fundamental building blocks of life, previous studies have reported formation routes of nucleobases in interstellar ice analogues. The present work explores the possibility that nucleobases could form from small molecules through gas-phase reactions in the interstellar medium (ISM). Based on quantum chemical calculations, we try to identify the specific interstellar environments that could be favorable to the formation of the nucleobases, with respect to the previously reported detection of relevant reactants.

We report synthetic routes from partially dehydrogenated formamide and vinyl cyanide. The most energetically favorable pathway to the formation of 1H-pyrimidin-2-one, a direct precursor of nucleobases, was found in a molecule-radical reaction with an energy barrier of 19.3 kcal/mol. Such an energy barrier roughly corresponds to a reaction rate coefficient of  $10^{-11}$  cm<sup>3</sup>/s at 180 K, indicating a thermal feasibility in hot molecular cores or in the inner part of the protoplanetary disks. Moreover, the computed pathways suggest that prior H migration in the reactants could be the key rate-determining process for the nucleobase synthesis.

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Astronomy & Astrophysics 656, A84 (2021)

<https://doi.org/10.1051/0004-6361/202140744>

# F12-TZ-cCR: A Methodology for Faster and Still Highly-Accurate Quartic Force Fields

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The F12-TZ-cCR quartic force field (QFF) methodology, defined here as CCSD(T)-F12b/cc-pCVTZ-F12 with further corrections for relativity, is introduced as a cheaper and even more accurate alternative to more costly composite QFF methods like those containing complete basis set extrapolations within canonical coupled cluster theory. F12-TZ-cCR QFFs produce  $B_0$  and  $C_0$  vibrationally averaged principal rotational constants within 7.5 MHz of gas-phase experimental values for tetra-atomic and larger molecules, offering higher accuracy in these constants than the previous composite methods. Further, F12-TZ-cCR offers an order of magnitude decrease in the computational cost of highly-accurate QFF methodologies accompanying this increase in accuracy. An additional order of magnitude in cost reduction is achieved in the F12-DZ-cCR method, while also matching the accuracy of the traditional composite method's  $B_0$  and  $C_0$  constants. Finally, F12-DZ and F12-TZ are benchmarked on the same test set, revealing that both methods can provide anharmonic vibrational frequencies that are comparable in accuracy to all three of the more expensive methodologies, although their rotational constants lag behind. Hence, the present work demonstrates that highly-accurate theoretical rovibrational spectral data can be obtained for a fraction of the cost of conventional QFF methodologies, extending the applicability of QFFs to larger molecules.

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<https://pubs.acs.org/doi/10.1021/acs.jpca.1c08355>

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# A Principal Component Analysis of polycyclic aromatic hydrocarbon emission in NGC 7023

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We carried out a principal component analysis (PCA) of the fluxes of five polycyclic aromatic hydrocarbon (PAH) bands at 6.2, 7.7, 8.6, 11.0, and 11.2  $\mu\text{m}$  in the reflection nebula NGC 7023 comprising of the photodissociation region (PDR) and a cavity. We find that only two principal components (PCs) are required to explain the majority of the observed variance in PAH fluxes (98%). The first PC ( $PC_1$ ), which is the primary driver of the variance, represents the total PAH emission. The second PC ( $PC_2$ ) is related to the ionization state of PAHs across the nebula. This is consistent with the results of a similar analysis of the PAH emission in NGC 2023. The biplots and the correlations of PCs with the various PAH ratios show that there are two subsets of ionic bands with the 6.2 and 7.7  $\mu\text{m}$  bands forming one subset and the 8.6 and 11.0  $\mu\text{m}$  bands the other. However, the distinction between these subsets is only present in the PDR. We have also carried out a separate PCA analysis of the PAH fluxes, this time only considering variations in the cavity. This shows that in the cavity,  $PC_2$  is not related to the charge state of PAHs, but possibly to structural molecular changes.

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Accepted for publication in Monthly Notices of the Royal Astronomical Society

<https://arxiv.org/abs/2201.07172>

# The spatially resolved PAH characteristics in the Whirlpool Galaxy (M51a)

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We present a detailed study on the spatially resolved polycyclic aromatic hydrocarbon (PAH) emission properties in the (circum)nuclear region (NR) and extranuclear regions (ENRs) of M51a using *Spitzer*-IRS observations. Correlations among PAH intensity ratios are examined with respect to each other, local physical parameters, galactocentric distance ( $R_g$ ), and very small grain (VSG) emission. Additional comparison is performed with the mid-infrared emission features in the HII regions of M33 and M83. The NR exhibits the strongest correlation among the PAH intensity ratios, whereas ENRs are showing increased scatter attributed to ISM emission. Overall, the radiation field hardness has a higher impact on PAH emission than metallicity, with the latter regulating PAH variance as a function of  $R_g$ . Specifically, the variance of PAH emission with respect to the different physical parameters suggests a higher rate of small/medium PAH processing compared to large PAHs and a higher ratio of small-to-large PAHs formed with increasing galactocentric distance. We find similarities between the 7.7  $\mu\text{m}$  carriers in M51a's NR and M83's HII regions, the 8.6  $\mu\text{m}$  carriers in M51a's NR and M33 HII regions, and both types of carriers between M51a's ENRs, M33's, and M83's HII regions. We have identified a positive correlation between PAH/VSG and the PAH intensity ratios. We conclude that the relative abundance of PAHs and VSG is not solely driven by the hardness of the radiation field.

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Monthly Notices of the Royal Astronomical Society (2022)

<https://arxiv.org/abs/2201.11713>

# Infrared Spectroscopy and Photochemistry of Anthracoronene in Cosmic Water Ice

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We present a laboratory study of the polycyclic aromatic hydrocarbon (PAH) anthracoronene (AntCor, C<sub>36</sub>H<sub>18</sub>) in simulated interstellar ices in order to determine its possible contribution to the broad infrared absorption bands in the 5–8 μm wavelength interval. The Fourier transform infrared (FTIR) spectrum of AntCor, codeposited with water ice, was collected. The FTIR spectrum of the sample irradiated with ultraviolet photons was also collected. Unirradiated and UV-irradiated AntCor embedded in water ice have not been studied before; therefore, the molecule's band positions and intensities were compared to published data on AntCor in an argon matrix and theoretical calculations (DFT), as well as the published results of its parent molecules, coronene and anthracene, in water ice. The experimental band strengths for unirradiated AntCor exhibit variability as a function of PAH:H<sub>2</sub>O concentration, with two distinct groupings of band intensities. AntCor clustering occurs for all concentrations and has a significant effect on PAH degradation rates and photoproduct variability. Near-IR spectra of irradiated AntCor samples show that AntCor<sup>+</sup> production increases as the concentration of AntCor in water ice decreases. Photoproduct bands are assigned to AntCor<sup>+</sup>, cationic alcohols, protonated AntCor, and ketones. We report the rate constants of the photoproduct production for the 1:1280 AntCor:H<sub>2</sub>O concentration. CO<sub>2</sub> production from AntCor is much less than what was previously reported for Ant and Cor and exhibits two distinct regimes as a function of AntCor:H<sub>2</sub>O concentration. The contribution of AntCor photoproducts to astronomical spectra can be estimated by comparison with the observed intensities in the 7.4–8.0 μm range

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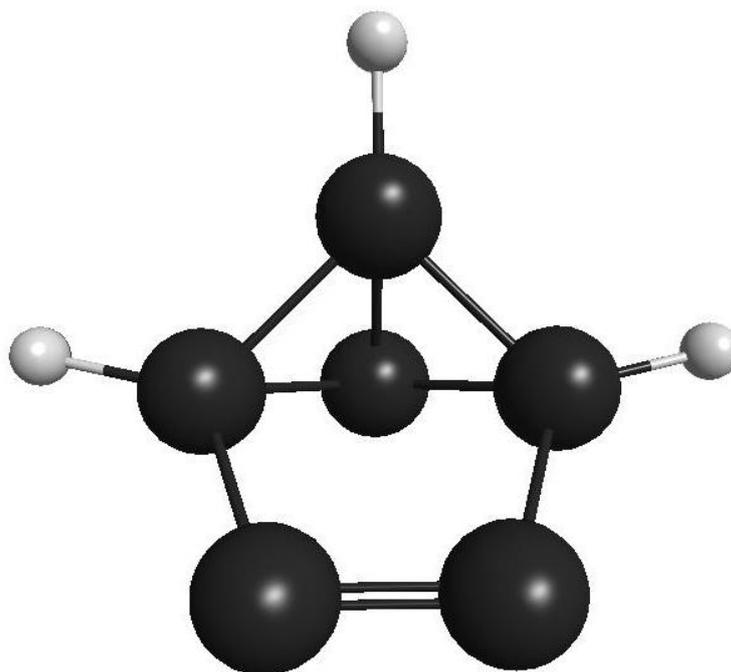
# Benzvalyne: Real or Imaginary?

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Benzvalyne, a benzene-based structure shown in Figure 2, is a molecule of particular interest as an isomerization product of o-benzyne, recently discovered in the Taurus Molecular Cloud (TMC-1). Benzvalyne, however, is not characterized in the literature. At the MCSCF, MP2, CCSD, CCSDT-1b, and CCSDT-2 levels of theory, the structure is designated as a  $C_{2v}$  minimum. Yet, conventional levels of theory, CCSD(T), CCSD(T)-F12, and CCSDT-1a, reveal a single imaginary frequency. Consequently, the increased electron correlation for the CCSDT-1b and CCSDT-2 methods strongly infer that benzvalyne is a verifiable, highly strained, minimum. At the CCSD(T) level, the strain energy is markedly high at  $158.6 \text{ kcal}\cdot\text{mol}^{-1}$ , with  $92 \text{ kcal}\cdot\text{mol}^{-1}$  resulting from the triple bond region of the molecule. Calculated harmonic vibrational frequencies reveal two hindered rotations of the  $C\equiv C$  group. The important chemistry of this molecule may be a result of how this diatomic portion dissociates from the bicyclobutane moiety. Evaluation of the vibrational harmonic frequencies and the calculated dipole moment (2.6 D) of benzvalyne could lead to detection of this molecule in TMC-1, as well.



**Figure 2** – Optimized Structure of Benzvalyne.

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The Journal of Chemical Physics, **156**:024302 (2022)

<https://aip.scitation.org/doi/10.1063/5.0077033>

# Infrared Spectroscopy of Jet-cooled “GrandPAH” in the 3–100 $\mu\text{m}$ Region

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Although large polycyclic aromatic hydrocarbons (PAHs) are likely to be responsible for IR emission of gaseous and dusty regions, their neutral experimental high-resolution gas-phase IR spectra needed to construct accurate astronomical models—have so far remained out of reach because of their nonvolatility. Applying laser desorption to overcome this problem, we report here the first IR spectra of the jet-cooled large PAHs coronene ( $\text{C}_{24}\text{H}_{12}$ ), peropyrene ( $\text{C}_{26}\text{H}_{14}$ ), ovalene ( $\text{C}_{32}\text{H}_{14}$ ), and hexa(peri)benzocoronene ( $\text{C}_{42}\text{H}_{18}$ ) in the 3–100  $\mu\text{m}$  region. Apart from providing experimental spectra that can be compared directly to astronomical data, such IR spectra are crucial for assessing the accuracy of theoretically predicted spectra used to interpret interstellar IR emission. Here we use the experimental spectra to evaluate the performance of conventional calculations using the harmonic approximation, as well as calculations with an anharmonic (GVPT2) treatment. The harmonic prediction agrees well with the experiment between 100 and 1000  $\text{cm}^{-1}$  (100 and 10  $\mu\text{m}$ ) but shows significant shortcomings in the combination band (1600–2000  $\text{cm}^{-1}$ , 6.25–5  $\mu\text{m}$ ) and CH-stretch (2950–3150  $\text{cm}^{-1}$ , 3.4–3.17  $\mu\text{m}$ ) regions. Especially the CH-stretch region is known to be dominated by the effects of anharmonicity, and we find that large PAHs are no exception. However, for the CH out-of-plane region (667–1000  $\text{cm}^{-1}$ , 15–10  $\mu\text{m}$ ) the anharmonic treatment that significantly improves the predicted spectra for small PAHs leads to large and unrealistic frequency shifts, and intensity changes for large PAHs, thereby rendering the default results unreliable. A detailed analysis of the results of the anharmonic treatment suggests a possible route for improvement, although the underlying cause for the large deviations remains a challenge for theory.

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The Astrophysical Journal, **923**:238 (2021)

<https://doi.org/10.3847/1538-4357/ac2f9d>

# Theoretical study of infrared spectra of interstellar PAH molecules with N, NH & NH<sub>2</sub> incorporation

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This work presents theoretical calculations of infrared spectra of nitrogen (N)-containing polycyclic aromatic hydrocarbon (PAH) molecules with incorporation of N, NH and NH<sub>2</sub> using density functional theory (DFT). The properties of their vibrational modes in 2–15 μm are investigated in relation to the Unidentified Infrared (UIR) bands. It is found that neutral PAHs, when incorporated with NH<sub>2</sub> and N (at inner positions), produce intense infrared bands at 6.2, 7.7 and 8.6 μm that have been normally attributed to ionized PAHs so far. The present results suggest that strong bands at 6.2 and 11.2 μm can arise from the same charge state of some N-containing PAHs, arguing that there might be some N-abundant astronomical regions where the 6.2 to 11.2 μm band ratio is not a direct indicator of PAHs' ionization. PAHs with NH<sub>2</sub> and N inside the carbon structure show the UIR band features characteristic to star-forming regions as well as reflection nebulae (Class A), whereas PAHs with N at the periphery have similar spectra to the UIR bands seen in planetary nebulae and post-AGB stars (Class B). The presence of N atom at the periphery of a PAH may attract H or H<sup>+</sup> to form N-H and N-H<sub>2</sub> bonds, exhibiting features near 2.9–3.0 μm, which are not yet observationally detected. The absence of such features in the observations constrains the contribution of NH and NH<sub>2</sub> substituted PAHs that could be better tested with concentrated observations in this range. However, PAHs with N without H either at the periphery or inside the carbon structure do not have the abundance constraint due to the absence of 2.9–3.0 μm features and are relevant in terms of positions of the UIR bands. Extensive theoretical and experimental studies are required to obtain deeper insight.

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Publications of the Astronomical Society of Japan, Accepted (2021)

<https://doi.org/10.1093/pasj/psab116>

<https://arxiv.org/pdf/2112.14453.pdf>

# The Mystery of Unidentified Infrared Emission Bands

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A family of unidentified infrared emission (UIE) bands has been observed throughout the Universe. The current observed spectral properties of the UIE bands are summarized. These properties are discussed in the frameworks of different models of the chemical carriers of these bands. The UIE carriers represent a large reservoir of carbon in the Universe, and play a significant role in the physical and chemical processes in the interstellar medium and galactic environment. A correct identification of the carrier of the UIE bands is needed to use these bands as probes of galactic evolution.

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Astrophysics and Space Science, **367**:16 (2022)

<https://link.springer.com/article/10.1007/s10509-022-04045-6>

# Formation of phenylacetylene and benzocyclobutadiene in the *ortho*-benzyne + acetylene reaction

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*Ortho*-benzyne is a potentially important precursor for polycyclic aromatic hydrocarbon formation, but much is still unknown about its chemistry. In this work, we report on a combined experimental and theoretical study of the *o*-benzyne + acetylene reaction and employ double imaging threshold photoelectron photoion coincidence spectroscopy to investigate the reaction products with isomer specificity. Based on photoion mass-selected threshold photoelectron spectra, Franck–Condon simulations, and ionization cross section calculations, we conclude that phenylacetylene and benzocyclobutadiene (**PA** : **BCBdiene**) are formed at a non-equilibrium ratio of 2 : 1, respectively, in a pyrolysis microreactor at a temperature of 1050 K and a pressure of  $\sim 20$  mbar. The  $C_8H_6$  potential energy surface (PES) is explored to rationalize the formation of the reaction products. Previously unidentified pathways have been found by considering the open-shell singlet (OSS) character of various  $C_8H_6$  reactive intermediates. Based on the PES data, a kinetic model is constructed to estimate equilibrium abundances of the two products. New insights into the reaction mechanism – with a focus on the OSS intermediates – and the products formed in the *o*-benzyne + acetylene reaction provide a greater level of understanding of the *o*-benzyne reactivity during the formation of aromatic hydrocarbons in combustion environments as well as in outflows of carbon-rich stars.

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# The 6.2 $\mu\text{m}$ PAH Feature and the Role of Nitrogen: Revisited

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This study revisits the role of nitrogen inclusion in PAHs (PANHs) on their infrared spectral properties. We present spectra of pure PAHs, PANHs, and protonated PANHs, computed using density functional theory and basis sets that treat polarization. We investigate trends in peak position and relative intensities as a function of nitrogen position, charge, and geometry. We use *Spitzer*-IRS spectral map data of the northwest photodissociation region of NGC 7023 and a database-fitting approach, using exclusively the PA(N)H spectra computed in this paper, to assess their infrared contribution to the cosmic PAH emission. We find that, by including the treatment of polarization, pure PAH cations can account for the class A 6.2  $\mu\text{m}$  PAH emission, with the 6.2  $\mu\text{m}$  band position being dependent on the molecular geometry. PANH cations are required to reproduce the most blueshifted 6.2  $\mu\text{m}$  bands observed in class A sources, albeit PANH cations come with strong 11.0  $\mu\text{m}$  emission. Blind database-fits demonstrate that the restriction imposed by the 11.0  $\mu\text{m}$  emission in the astronomical spectra limits the contribution of PANH cations and the fits have to use neutral PANHs to avoid inflating the 11.0  $\mu\text{m}$  feature even further. By assuming that all the 11.0  $\mu\text{m}$  emission is due to PANHs, we derive an upper limit for the contribution of PANH cations to the astronomical 6.2  $\mu\text{m}$  PAH band of  $\sim 12\%$ . The fits further show hydrogenated PANHs significantly contributing in NGC 7023's more benign region, supporting the view that shielded environments could sustain protonated PA(N)Hs.

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# Gas-phase synthesis of benzene via the propargyl radical self-reaction

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Polycyclic aromatic hydrocarbons (PAHs) have been invoked in fundamental molecular mass growth processes in our galaxy. We provide compelling evidence of the formation of the very first ringed aromatic and building block of PAHs — benzene — via the self-recombination of two resonantly stabilized propargyl ( $C_3H_3$ ) radicals in dilute environments using isomer-selective synchrotron-based mass spectrometry coupled to theoretical calculations. Along with benzene, three other structural isomers (1,5-hexadiyne, fulvene, and 2-ethynyl-1,3-butadiene) and o-benzyne are detected, and their branching ratios are quantified experimentally and verified with the aid of computational fluid dynamics and kinetic simulations. These results uncover molecular growth pathways not only in interstellar, circumstellar, and solar systems environments but also in combustion systems, which help us gain a better understanding of the hydrocarbon chemistry of our universe.

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# A molecular beam and computational study on the barrierless gas phase formation of (iso)quinoline in low temperature extraterrestrial environments

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Despite remarkable progress toward the understanding of the formation pathways leading to polycyclic aromatic hydrocarbons (PAHs) in combustion systems and in deep space, the complex reaction pathways leading to nitrogen-substituted PAHs (NPAHs) at low temperatures of molecular clouds and hydrocarbon-rich, nitrogen-containing atmospheres of planets and their moons like Titan have remained largely obscure. Here, we demonstrate through laboratory experiments and computations that the simplest prototype of NPAHs — quinoline and isoquinoline (C<sub>9</sub>H<sub>7</sub>N) — can be synthesized via rapid and de-facto barrier-less reactions involving o-, m- and p-pyridinyl radicals (C<sub>5</sub>H<sub>4</sub>N<sup>•</sup>) with vinylacetylene (C<sub>4</sub>H<sub>4</sub>) under low-temperature conditions.

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# Formation of Benzene and Naphthalene through Cyclopentadienyl-Mediated Radical-Radical Reactions

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Resonantly stabilized free radicals (RSFRs) have been contemplated as fundamental molecular building blocks and reactive intermediates in molecular mass growth processes leading to polycyclic aromatic hydrocarbons (PAHs) and carbonaceous nanoparticles on Earth and in deep space. By combining molecular beams and computational fluid dynamics simulations, we provide compelling evidence on the formation of benzene via the cyclopentadienyl-methyl reaction and of naphthalene through the cyclopentadienyl self-reaction, respectively. These systems offer benchmarks for the conversion of a five-membered ring to the  $6\pi$ -aromatic (benzene) and the generation of the simplest  $10\pi$ -PAH (naphthalene) at elevated temperatures. These results uncover molecular mass growth processes from the “bottom up” via RSFRs in high temperature circumstellar environments and combustion systems expanding our fundamental knowledge of the organic, hydrocarbon chemistry in our universe.

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# Excited state photochemically driven surface formation of benzene from acetylene ices on Pluto and in the outer solar system

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NASA's New Horizons mission unveiled a diverse landscape of Pluto's surface with massive regions being neutral in color, while others like Cthulhu Macula range from golden-yellow to reddish comprising up to half of Pluto's carbon budget. Here, we demonstrate in laboratory experiments merged with electronic structure calculations that the photolysis of solid acetylene — the most abundant precipitate on Pluto's surface — by low energy ultraviolet photons efficiently synthesizes benzene and polycyclic aromatic hydrocarbons via excited state photochemistry thus providing critical molecular building blocks for the colored surface material. Since low energy photons deliver doses to Pluto's surface exceeding those from cosmic rays by six orders of magnitude, these processes may significantly contribute to the coloration of Pluto's surface and of hydrocarbon-covered surfaces of Solar System bodies such as Triton in general. This discovery critically enhances our perception of the distribution of aromatic molecules and carbon throughout our Solar System.

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# On the radical behavior of large polycyclic aromatic hydrocarbons in soot formation and oxidation

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The mechanism of evolution of polycyclic aromatic hydrocarbons (PAHs) into carbonaceous particles in combustion, atmosphere, and interstellar space has been the subject of intense debate. Recently, there has been emerging evidence supporting resonantly-stabilized radicals as key players in PAH growth. In this work, we build on this hypothesis and propose that, beyond a critical size, PAH reactivity can be assimilated to that of radicals. We found that odd-C-numbered PAHs embedding 5-membered rings rapidly lose a hydrogen atom to form resonantly-stabilized radicals in combustion conditions, while even-C-numbered PAHs react as open-shell rather than closed-shell molecules independently of temperature, as usually assumed. Acenes were used as molecular models of large even-C-numbered PAHs. The construction of a kinetic model including these findings allows to interpret experimental soot oxidation data otherwise irreconcilable with existing chemical kinetic mechanisms.

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# Unconventional excited-state dynamics in the concerted benzyl (C<sub>7</sub>H<sub>7</sub>) radical self-reaction to anthracene (C<sub>14</sub>H<sub>10</sub>)

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Polycyclic aromatic hydrocarbons (PAHs) are prevalent in deep space and on Earth as products in combustion processes bearing direct relevance to energy efficiency and environmental remediation. Reactions between hydrocarbon radicals in particular have been invoked as critical molecular mass growth processes toward cyclization leading to these PAHs. However, the mechanism of the formation of PAHs through radical-radical reactions are largely elusive. Here, we report on a combined computational and experimental study of the benzyl (C<sub>7</sub>H<sub>7</sub>) radical self-reaction to phenanthrene and anthracene (C<sub>14</sub>H<sub>10</sub>) through unconventional, isomer-selective excited state dynamics. Whereas phenanthrene formation is initiated via a barrierless recombination of two benzyl radicals on the singlet ground state surface, formation of anthracene commences through an exotic transition state on the excited state triplet surface through cycloaddition. Our findings challenge conventional wisdom that PAH formation via radical-radical reactions solely operates on electronic ground state surfaces and open up a previously overlooked avenue for a more “rapid” synthesis of aromatic, multi-ringed structures via excited state dynamics in the gas phase.

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# Polarizability in Astrochemical Studies of Complex Carbon-Based Compounds

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This Review summarizes the grounds and applications of polarizability to the astrochemical studies on carbon-based compounds, including polycyclic aromatic hydrocarbons and fullerenes. Polarizability is useful for the analysis of physicochemical processes (interactions with positrons, molecular collisions, quenching, and dielectric screening) and chemical reactions. The idea of a combined use of minimum-polarizability and minimum-energy principles for searching for novel candidates for interstellar/circumstellar detection is considered. Insights into the astrochemistry of fullerenes and helicenes coming from their polarizability are discussed.

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# Experimental and Theoretical Constraints on Amino Acid Formation from PAHs in Asteroidal Settings

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Amino acids and polycyclic aromatic hydrocarbons (PAHs) belong to the range of organic compounds detected in meteorites. In this study, we tested empirically and theoretically if PAHs are precursors for amino acids in carbonaceous chondrites, as previously suggested. We conducted experiments to synthesize amino acids from fluoranthene (PAH), with ammonium bicarbonate as a source for ammonia and carbon dioxide under mimicked asteroidal conditions. In our thermodynamic calculations, we extended our analysis to additional PAH amino acid combinations. We explored 36 reactions involving the PAHs naphthalene, anthracene, fluoranthene, pyrene, triphenylene, and coronene and the amino acids glycine, alanine, valine, leucine, phenylalanine, and tyrosine. Our experiments do not show the formation of amino acids, whereas our theoretical results hint that PAHs could be precursors of amino acids in carbonaceous chondrites at low temperatures.

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## AstroPAH Newsletter

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