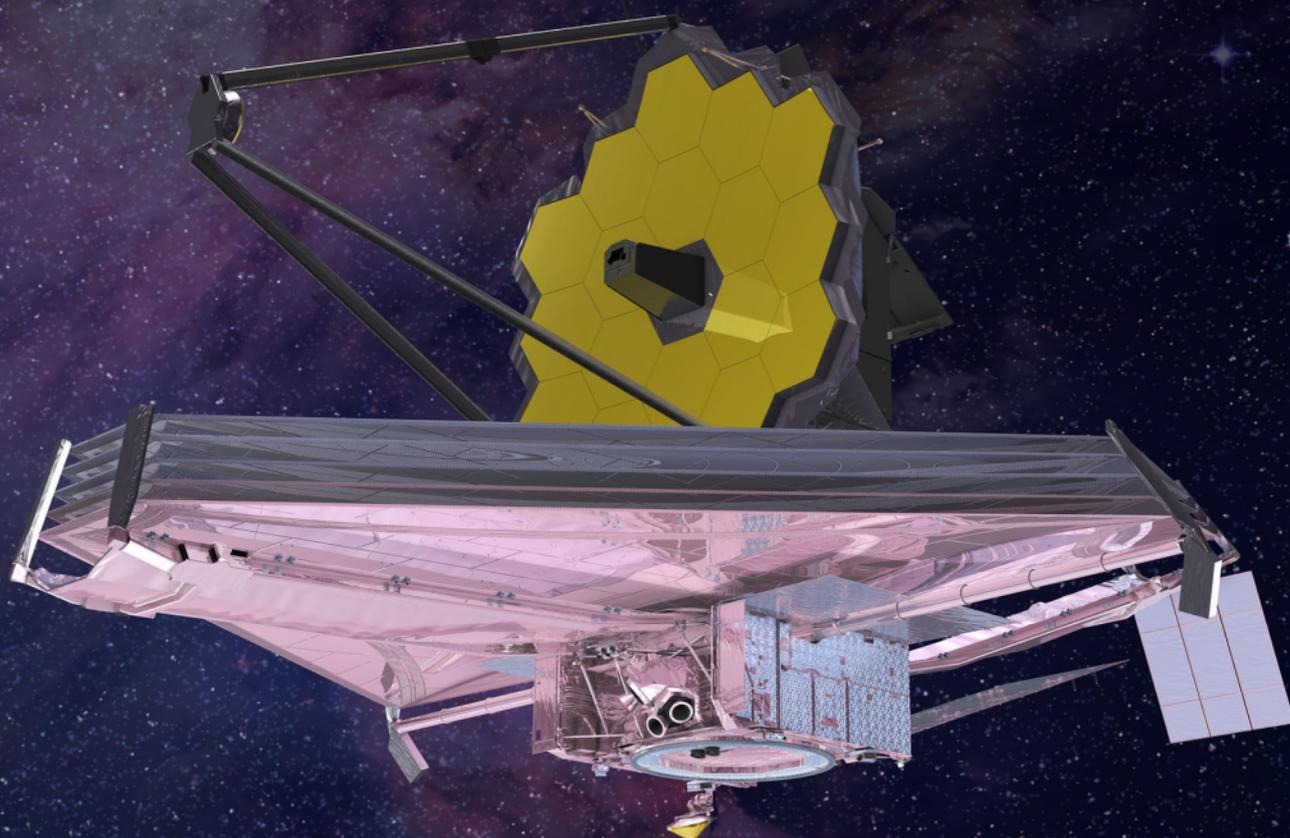


# AstroPAH

A Newsletter on Astronomical PAHs

Issue 73 • November 2020



**Good luck with your  
Cycle 1 JWST Proposals!**



# Editorial

**Dear Colleagues,**

Welcome to our 73<sup>rd</sup> AstroPAH volume! We hope all of you are healthy and doing well.

As you have probably already noticed, this month's cover picture is dedicated to JWST! The Cycle 1 proposal deadline is just around the corner, so what better way to celebrate this exciting mission we are all looking forward to than to have it on our cover!

We are very happy to welcome not one, not two, but **three** new editors to our Editorial Board! Expanding our international reach has always been the spirit of the AstroPAH team, which is why we are very pleased to announce that Dr. Donatella Loru from Deutsches Elektronen-Synchrotron in Germany, Dr. Kin Long Kelvin Lee from the Massachusetts Institute of Technology in the USA and Sandra Wiersma from the Institut de Recherche en Astrophysique et Planétologie in France have joined our team.

We would also like to express our excitement and congratulate one of our editors, Dr. Ella Sciamma-O'Brien, on being the recipient of a NASA Honor Award: the Exceptional Scientific Achievement Medal! Congratulations, Ella!

Our In Focus features an interview with Dr. Xuejuan Yang, a Professor of Astrophysics at Xiangtan University, China, whose research focuses on the structural properties of PAHs. Be sure to read it to find out about her exciting PAH research!

This month we have 12 abstracts featured in our Abstracts section! Check them out!

A new Postdoctoral position in Laboratory Astrochemistry is also listed in this issue. This 2-year position is available at the Center for Astrochemical Studies at the Max Planck Institute for Extraterrestrial Physics in Germany, with a flexible starting date, which could be as early as Spring 2021. Interested applicants should submit their application by December 15, 2020.

We hope you enjoy reading our newsletter, and we thank you for your dedication and interest in AstroPAH! In the meantime, please continue sending us your contributions, and if you wish to contact us, feel free to use our [email](#).

Please be safe and stay healthy.

Enjoy reading our newsletter!

**The Editorial Team**

**Next issue: 17 December 2020.  
Submission deadline: 4 December 2020.**

# AstroPAH Newsletter

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## PAH Picture of the Month

Artistic impression of the James Webb Space Telescope. JWST will observe in mid infrared wavelengths, where PAH bands can be detected. The Cycle 1 Proposal Deadline is 24 November 2020. Good luck with your proposals!

**Credits:** Northrop Grumman.



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## Interview with Xuejuan Yang



Dr. Xuejuan Yang got her PhD in Astrophysics in July 2008 from Beijing Normal University. Then she joined the faculty of Xiangtan University (XTU) and was promoted to professor of astrophysics in 2018. She is serving as the founding director of the Provincial Key Laboratory for Stellar and Interstellar Physics of Hunan Province, China, and an associate dean of School of Physics and Optoelectronics of Xiangtan University. She was trained as an observational astronomer on the X-ray properties of supernova remnants (SNRs) and started to work on PAH astrophysics in December 2012, under the supervision of Prof. Aigen Li as a postdoctoral research scholar. Her research focuses on the structural properties of PAHs, or the carriers of the so-called unidentified infrared emission (UIE) bands, which are ubiquitous and widespread in the universe.

**Our greatest thanks for accepting to do this interview!  
First off, can you tell us how you got into PAH-related research?**

I majored in astronomy during my undergraduate study in Beijing Normal University. Following my graduation with BS in astronomy in July 2003, I became a graduate student supervised by Prof. Fangjun Lu of the Institute of High Energy Physics of Chinese Academy of Sciences. My dissertation was on the X-ray emission properties of young SNRs. After I got my PhD in July 2008, I joined the faculty of XTU. When Prof. Aigen Li of the University of Missouri visited XTU in the summer of 2012, I became very interested in the stability of dust and PAHs in SNRs. Prof. Li kindly invited me to work with him in the University of Missouri as a postdoctoral research scholar. My adventure in PAHs started when I arrived in Columbia, a college town in Missouri, USA in December 2012. We first worked on the first-principle density functional theory calculations of PAHs to explore the chemical structures of the UIE carriers. Such calculations on PAHs with aliphatic side groups were not quite systematic at that time, and they are of importance to understand the aliphaticity of the UIE carriers. This kind of research was completely new and very different from my previous research. At the beginning, it was quite challenging, but also very exciting. On the other hand, this helped

me to fit in the XTU Physics program, where there are about 20 faculty members working on first-principle studies on condensed matter led by Prof. Jianxin Zhong, while there was only one astronomer besides me. During my stay in Missouri, Prof. Rainer Glaser from the Department of Chemistry of the University of Missouri, and Prof. Jianxin Zhong of XTU were always valuable sources of advice and support. In August 2013, we published our first paper on PAHs which thoroughly explored the aliphaticity of the UIE carriers. I very much enjoyed the field of PAH astrophysics, particularly its inter-disciplinary nature.

## Can you tell us about your latest research project?

My latest research is on the deuteration of PAHs. Deuterium (D) is one of the light elements created in the big bang. As the Galaxy evolves, the D/H abundance in the interstellar medium (ISM) decreases from its primordial value due to “astration”. However, the observed gas-phase D/H abundances of some interstellar sightlines are substantially lower than the expected reduction by astration. The missing D could have been depleted onto PAH molecules which are ubiquitous and abundant in interstellar regions. To quantitatively explore the hypothesis of PAHs as a possible reservoir of interstellar D, we are studying quantum-chemically the IR vibrational spectra of deuterated PAHs (and their cations) of various sizes. This also allows us to quantitatively constrain the degree of deuteration of PAHs in the interstellar medium. As JWST will be launched soon, we hope our study will be helpful for preparing and (in the future) interpreting JWST observations.

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

I would very much like to know experimentally how PAHs get deuterated in the interstellar medium; also, how PAHs are formed and evolve in the ISM, and how PAHs are related to other carbon species like hydrogenated amorphous carbon solids, graphene, carbon nanotube and fullerenes. No doubt that we all look forward to the identification of specific PAH molecules in the ISM. They are not easily identified from the infrared spectra. Machine-learning might be helpful. Such a method has been successfully used to predict the IR spectra of PAHs (Kovács et al. 2020, ApJ, 902, 100). I believe it will not only be a supplement to DFT calculations, but also a powerful tool for analyzing the observational spectra.

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

Doing the right thing at the right time”.

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

My job includes teaching, research, and administration. Teaching and administration parts break up time, which is not research-friendly. I have a 6-year-old boy, and I don't want to be absent from his life as he grows up. So it is not easy. I try to do time management better and priority setting more effectively. Say no to less important things. I think trying best to gather time is also very important, especially for doing research. I divide each year into several bulks so that in a relatively long period I can concentrate on one thing. For example,

my management job requires lots of time in the spring, so I schedule my teaching mainly in the spring as well, and leave summer, fall and winter free from teaching and concentrate more on research. I save at least half a day for family gathering together, going to park, shopping or having dinner at restaurants. This refreshes me, and makes me feel much more motivated to work. I play volleyball twice a week, that makes me more energetic. Also I am very lucky that I join a well-collaborative work group, and have a very supportive family. Last, one needs to admit that nothing is perfect. Just do the right thing at the right time, and do our best.



# Abstracts

## Gas-Phase Spectroscopic Characterization of Neutral and Ionic Polycyclic Aromatic Phosphorus Heterocycles (PAPHs)

Ricardo R. Oliveira<sup>1</sup>, Germán Molpeceres<sup>2</sup>, Felipe Fantuzzi<sup>3,4</sup>, Heidy M. Qutián-Lara<sup>5</sup>, Heloisa M. Boechat-Roberty<sup>5</sup> and Johannes Kästner<sup>2</sup>

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Polycyclic aromatic hydrocarbons (PAHs) constitute an essential family of compounds in interstellar (ISM) and circumstellar (CSM) media. Recently, formation routes for the corresponding polycyclic aromatic phosphorus heterocycles (PAPHs) in astrophysical environments have been proposed. In order to contribute to a better understanding of the phosphorus chemistry in the ISM, infrared (IR) spectra and selected properties of PAPHs were computed at the DFT level for neutral, cationic and anionic species. Our results reveal that several protonated PAPHs do not have planar backbones, and all species have permanent dipole moments between 2 D and 4 D. Closed-shell PAPHs have similar ionization potentials compared to the parent PAHs, below the Lyman threshold limit. In addition, all PAPHs show positive electron affinities higher than those of PAHs. Protonation preferably occurs on the heteroatom but with lower proton affinities than those of the corresponding nitrogen analogs (PANHs). In general, neutral species have similar IR spectra profile with the most intense bands around  $800\text{ cm}^{-1}$  ( $12.5\ \mu\text{m}$ ) related to C–H wagging. Charge and protonation affect the IR spectra mainly by decreasing the intensities of these modes and increasing the ones between  $1000\text{ cm}^{-1}$  ( $10.0\ \mu\text{m}$ ) and  $1800\text{ cm}^{-1}$  ( $5.6\ \mu\text{m}$ ). The P–H stretching appears in a different spectral region, between  $2300\text{ cm}^{-1}$  ( $4.3\ \mu\text{m}$ ) and  $2700\text{ cm}^{-1}$  ( $3.7\ \mu\text{m}$ ). Our results are discussed in the context of distinct sources where PAHs and phosphorus are detected. PAPHs, in particular the coronene derivatives, can contribute to the Unidentified Infrared Emission (UIR) band at  $6.2\ \mu\text{m}$ .

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MNRAS, accepted (2020)

<https://doi.org/10.1093/mnras/staa3460>

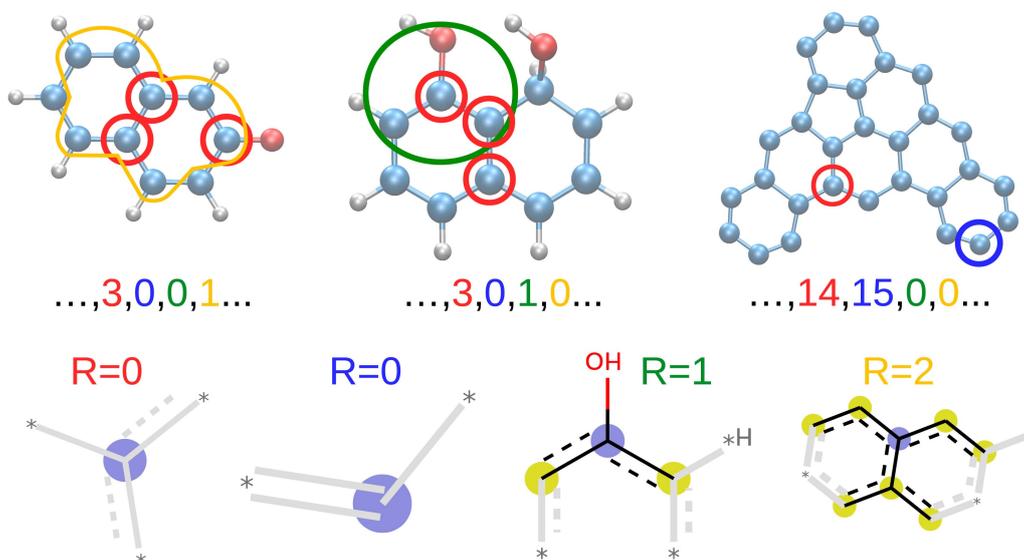
# Machine-learning prediction of infrared spectra of interstellar PAHs

Péter Kovács<sup>1</sup>, Xiaosi Zhu<sup>2</sup>, Jesús Carrete<sup>1</sup>, Georg K. H. Madsen<sup>1</sup> and Zhao Wang<sup>2</sup>

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We design and train a neural network (NN) model to efficiently predict the infrared spectra of interstellar polycyclic aromatic hydrocarbons with a computational cost many orders of magnitude lower than what a first-principles calculation would demand. The input to the NN is based on the Morgan fingerprints extracted from the skeletal formulas of the molecules and does not require precise geometrical information such as interatomic distances. The model shows excellent predictive skill for out-of-sample inputs, making it suitable for improving the mixture models currently used for understanding the chemical composition and evolution of the interstellar medium. We also identify the constraints to its applicability caused by the limited diversity of the training data and estimate the prediction errors using an ensemble of NNs trained on subsets of the data. With help from other machine-learning methods like random forests, we dissect the role of different chemical features in this prediction. The power of these topological descriptors is demonstrated by the limited effect of including detailed geometrical information in the form of Coulomb matrix eigenvalues.



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ApJ 902, 100 (2020)

<https://iopscience.iop.org/article/10.3847/1538-4357/abb5b6>

# Unimolecular fragmentation and radiative cooling of isolated PAH ions: A quantitative study

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Time-resolved spontaneous and laser-induced unimolecular fragmentation of perylene cations ( $C_{20}H_{12}^+$ ) has been measured on timescales up to 2 s in a cryogenic electrostatic ion beam storage ring. We elaborate a quantitative model which includes fragmentation in competition with radiative cooling *via* both vibrational and electronic (recurrent fluorescence) de-excitation. Excellent agreement with experimental results is found when sequential fragmentation of daughter ions co-stored with the parent perylene ions is included in the model. Based on comparison of the model to experiment, we constrain the oscillator strength of the  $D_1 \rightarrow D_0$  emissive electronic transition in perylene ( $f^{RF} = 0.055 \pm 0.011$ ), as well as the absolute absorption cross section of the  $D_5 \leftarrow D_0$  excitation transition ( $\sigma_{abs} > 670$  Mb). The former transition is responsible for the laser-induced and recurrent fluorescence of perylene and the latter is the most prominent in the absorption spectrum. The vibrational cooling rate is found to be consistent with the Simple Harmonic Cascade approximation. Quantitative experimental benchmarks of unimolecular processes in Polycyclic Aromatic Hydrocarbon ions like perylene are important for refining astrochemical models.

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J. Chem. Phys. 153, 154303 (2020)

<https://doi.org/10.1063/5.0027773>

## Gas-Phase Formation of Fulvenallene ( $C_7H_6$ ) via the Jahn-Teller Distorted Tropylium ( $C_7H_7$ ) Radical Intermediate under Single-Collision Conditions

Chao He<sup>1</sup>, Aaron M. Thomas<sup>1</sup>, Galiya R. Galimova<sup>2</sup>, Alexander N. Morozov<sup>2</sup>, Alexander M. Mebel<sup>2</sup>, Ralf I. Kaiser<sup>1</sup>

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The fulvenallene molecule ( $C_7H_6$ ) has been synthesized via the elementary gas-phase reaction of the methylidyne radical (CH) with the benzene molecule ( $C_6H_6$ ) on the doublet  $C_7H_7$  surface under single collision conditions. The barrier-less route to the cyclic fulvenallene molecule involves the addition of the methylidyne

radical to the  $\pi$ -electron density of benzene leading eventually to a Jahn–Teller distorted tropyli ( $C_7H_7$ ) radical intermediate and exotic ring opening–ring contraction sequences terminated by atomic hydrogen elimination. The methylidyne-benzene system represents a benchmark to probe the outcome of the elementary reaction of the simplest hydrocarbon radical—methylidyne—with the prototype of a closed-shell aromatic molecule—benzene—yielding nonbenzenoid fulvenallene. Combined with electronic structure and statistical calculations, this bimolecular reaction sheds light on the unusual reaction dynamics of Hückel aromatic systems and remarkable (polycyclic) reaction intermediates, which cannot be studied via classical organic, synthetic methods, thus opening up a versatile path to access this previously largely obscure class of fulvenallenes.

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<https://pubs.acs.org/doi/full/10.1021/jacs.9b13269>

## A Unified Mechanism on the Formation of Acenes, Helicenes, and Phenacenes in the Gas Phase

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A unified low-temperature reaction mechanism on the formation of acenes, phenacenes, and helicenes—polycyclic aromatic hydrocarbons (PAHs) that are distinct via the linear, zigzag, and *ortho*-condensed arrangements of fused benzene rings—is revealed. This mechanism is mediated through a barrierless, vinylacetylene mediated gas-phase chemistry utilizing tetracene, [4]phenacene, and [4]helicene as benchmarks contesting established ideas that molecular mass growth processes to PAHs transpire at elevated temperatures. This mechanism opens up an isomer-selective route to aromatic structures involving submerged reaction barriers, resonantly stabilized free-radical intermediates, and systematic ring annulation potentially yielding molecular wires along with racemic mixtures of helicenes in deep space. Connecting helicene templates to the Origins of Life ultimately changes our hypothesis on interstellar carbon chemistry.

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<https://onlinelibrary.wiley.com/doi/abs/10.1002/anie.201913037>

# A Free-Radical Prompted Barrierless Gas-Phase Synthesis of Pentacene

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A representative, low-temperature gas-phase reaction mechanism synthesizing polyacenes via ring annulation exemplified by the formation of pentacene (C<sub>22</sub>H<sub>14</sub>) along with its benzo[a]tetracene isomer (C<sub>22</sub>H<sub>14</sub>) is unraveled by probing the elementary reaction of the 2-tetracenyl radical (C<sub>18</sub>H<sub>11</sub>·) with vinylacetylene (C<sub>4</sub>H<sub>4</sub>). The pathway to pentacene—a prototype polyacene and a fundamental molecular building block in graphenes, fullerenes, and carbon nanotubes—is facilitated by a barrierless, vinylacetylene mediated gas-phase process thus disputing conventional hypotheses that synthesis of polycyclic aromatic hydrocarbons (PAHs) solely proceeds at elevated temperatures. This low-temperature pathway can launch isomer-selective routes to aromatic structures through submerged reaction barriers, resonantly stabilized free-radical intermediates, and methodical ring annulation in deep space eventually changing our perception about the chemistry of carbon in our universe.

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<https://onlinelibrary.wiley.com/doi/full/10.1002/anie.202003402>

## Gas phase formation of phenalene via 10 $\pi$ -aromatic, resonantly stabilized free radical intermediates

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For the last few decades, the Hydrogen-Abstraction/αCetylene-Addition (HACA) mechanism has been fundamental in aiding our understanding of the source of polycyclic aromatic hydrocarbons (PAHs) in combustion processes and in circumstellar envelopes of

carbon rich stars. However, the reaction mechanisms driving high temperature molecular mass growth beyond triphenylene ( $C_{18}H_{12}$ ) along with the link between PAHs and graphene-type nanostructures as identified in carbonaceous meteorites such as in Murchison and Allende has remained elusive. By exploring the reaction of the 1-naphthyl radical ( $C_{10}H_7$ ) with methylacetylene ( $CH_3CCH$ ) and allene ( $H_2CCCH_2$ ) under conditions prevalent in carbon-rich circumstellar environments and combustion systems, we provide compelling evidence on a facile formation of 1H-phenalene ( $C_{13}H_{10}$ ) – the central molecular building block of graphene-type nanostructures. Beyond PAHs, molecular mass growth processes from 1H-phenalene via ring-annulation through C3 molecular building blocks may ultimately lead to two-dimensional structures such as graphene nano flakes and after condensation of multiple layers to graphitized carbon. These fundamental reaction mechanisms are of crucial significance to facilitate an understanding of the origin and chemical evolution of carbon in our Galaxy.

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Phys. Chem. Chem. Phys. 22, 15381-15388 (2020)

<https://pubs.rsc.org/en/content/articlelanding/2020/cp/d0cp02216k#!divAbstract>

## Gas phase formation of cyclopentanaphthalene (benzindene) isomers via reactions of 5- and 6-indenyl radicals with vinylacetylene

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The tricyclic polycyclic aromatic hydrocarbons (PAHs) 3H-cyclopenta[a]naphthalene ( $C_{13}H_{10}$ ), 1H-cyclopenta[b]naphthalene ( $C_{13}H_{10}$ ) and 1H-cyclopenta[a]naphthalene ( $C_{13}H_{10}$ ) along with their indene-based bicyclic isomers (E)-5-(but-1-en-3-yn-1-yl)-1H-indene, (E)-6-(but-1-en-3-yn-1-yl)-1H-indene, 5-(but-3-ene-1-yn-1-yl)-1H-indene, and 6-(but-3-ene-1-yn-1-yl)-1H-indene were formed via a “directed synthesis” in a high-temperature chemical micro reactor at the temperature of  $1300 \pm 10$  K through the reactions of the 5- and 6-indenyl radicals ( $C_9H_7$ ) with vinylacetylene ( $C_4H_4$ ). The isomer distributions were probed utilizing tunable vacuum ultraviolet light by recording the photoionization efficiency curves at mass-to-charge of  $m/z = 166$  ( $C_{13}H_{10}$ ) and  $167$  ( $^{13}C_{12}H_{10}$ ) of the products in a supersonic molecular beam. The underlying reaction mechanisms involve the initial formation of van-der-Waals complexes followed by addition of the 5- and 6-indenyl radicals to vinylacetylene via submerged barriers, followed by isomerization (hydrogen shifts, ring closures), and

termination via atomic hydrogen elimination accompanied by aromatization. All the barriers involved in the formation of 3H-cyclopenta[a]naphthalene, 1H-cyclopenta[b]naphthalene and 1H-cyclopenta[a]naphthalene are submerged with respect to the reactants indicating that the mechanisms are in fact barrierless, potentially forming PAHs via the hydrogen abstraction – vinylacetylene addition (HAVA) pathway in the cold molecular clouds such as Taurus Molecular Cloud-1 (TMC-1) at temperatures as low as 10 K.

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Phys. Chem. Chem. Phys. 22, 22493-22500 (2020)

<https://pubs.rsc.org/en/content/articlelanding/2020/cp/d0cp03846f#fn1>

## **Intrinsic absorption profile and radiative cooling rate of a PAH cation revealed by action spectroscopy in the cryogenic electrostatic storage ring DESIREE**

**Mark H. Stockett, Mikael Björkhage, Henrik Cederquist, Henning T. Schmidt & Zettergren Henning**

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The multi-photon photodissociation (MPD) action spectrum of the coronene cation ( $C_{24}H_{12}^+$ ) has been measured as a function of storage time up to 60 s in the cryogenic electrostatic storage ring DESIREE. These measurements reveal not only the intrinsic absorption profile of isolated coronene cations, but also the rate at which hot-band absorptions are quenched by radiative cooling. The cooling rate is interpreted using a Simple Harmonic Cascade model of infrared vibrational emission.

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Proc. Int. Astron. Union 15, 127131 (2019)

<http://dx.doi.org/10.1017/S1743921319007130>

## **Detection of PAH and nbL features in planetary nebulae NGC 7027 and BD +30° 3639 with TIRCAM2 instrument on 3.6 m DOT**

**Rahul Kumar Anand<sup>1</sup>, Shantanu Rastogi<sup>1</sup>, Brijesh Kumar<sup>2</sup>, Arpan Ghosh<sup>2</sup>, Saurabh Sharma<sup>2</sup>, D. K. Ojha<sup>3</sup> S. K. Ghosh<sup>3</sup>**

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High resolution infrared imaging observations of the young planetary nebulae (PNe) NGC 7027 and BD +30° 3639, taken with the newly installed TIFR near infrared camera-

II (TIRCAM2) on 3.6 m Devasthal optical telescope (DOT), ARIES, Nainital, are being reported. The images are acquired in J, H, K, polycyclic aromatic hydrocarbon (PAH) and narrow-band L (nbL) filters. The observations show emission from warm dust and PAHs in the circumstellar shells. The imaging of the two objects is among the first observations in PAH and nbL bands using TIRCAM2 on DOT. The NGC 7027 images in all bands show similar elliptical morphology with  $\sim 6''.7$  and  $\sim 4''.5$  semi-major and semi-minor axes. Considering size up to 10% of peak value the nebula extends up to  $8''$  from the central star revealing a multipolar evolution. The relatively cooler BD +30° 3639 shows a rectangular-ring shaped nebula. In J and H bands it shows an angular diameter of  $\sim 8''$ , while a smaller  $\sim 6''.9$  size is observed in K, PAH and nbL bands. The  $3.28 \mu\text{m}$  emission indicates presence of PAHs at about 6000 and 5000 AU from the central stars in NGC 7027 and BD +30° 3639 respectively. Analysis suggests domination of neutral PAHs in BD +30° 3639, while in NGC 7027 there is higher ionization and more processed PAH population.

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## Formation, Destruction and Identification of Complex Organic Molecules (COMs) in Circumstellar Environments

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The universe is rich in chemical and molecular complexity. To date, more than 200 molecules have been detected in interstellar and circumstellar regions including protostellar objects and planetary nebulae (PNe), with more than 60 observed in extragalactic objects. Studies on the mechanisms of formation, destruction of molecules, as well as the identification of molecules in observational spectra, are fundamental for the understanding of chemistry in astrophysical environments. In this work, experimental and observational techniques were used for the chemical description of different astrophysical objects in which complex organic molecules (COMs) and polycyclic aromatic hydrocarbons (PAHs) are present. Experimentally, the formation and destruction of molecules derived from benzene ( $\text{C}_6\text{H}_6$ ), the basic unit of PAHs, were studied through the interaction of photons in the X-ray range with molecules in the gas phase employing time-of-flight mass spectrometry (MS-TOF), thus simulating the processes that occur in the PNe photodissociation regions (PDRs). We analyzed the following molecules:  $\text{C}_6\text{H}_6$ , naphthalene ( $\text{C}_{10}\text{H}_8$ ), biphenyl ( $\text{C}_{12}\text{H}_{10}$ ) and cyclohexane ( $\text{C}_6\text{H}_{12}$ ), the latter being the basic unit of super-hydrogenated PAHs ( $\text{H}_n$ -PAHs). Additionally, we studied the protonation and deprotonation effects of benzene rings of these molecules in the condensed phase by the Electron Stimulated Ion Desorption technique (ESID) of astrophysical ice analogs. The ice was prepared from pure samples of  $\text{C}_6\text{H}_6$ ,

$C_6H_{12}$  and chlorobenzene ( $C_6H_5Cl$ ), as well as from a phenol solution ( $C_6H_5OH$ ). For  $C_6H_{12}$  in gas phase, the results show a greater tendency to dissociate it compared to benzene, associated with the reduction of the carbon backbone binding energy after hydrogenation. On the other hand, the photoabsorption cross section of benzene at energies close to the inner shell resonance (C1s) is larger than the one of cyclohexane, which ultimately leads to a higher efficiency of dissociation for the aromatic molecule. The results suggest that a similar effect is experienced by PAHs in X-ray rich environments, such as the NGC 7027 PDR, so that their hydrogenation may act as a protective mechanism as a consequence of decreasing the photoabsorption cross section. For the biphenyl molecule, the major mono- ( $A^+$ ) and double ( $A^{2+}$ ) charged fragments formed by dissociative photoionization at the energies of 275 and 310 eV were identified. Also its ionic production percentages (PIYs) were determined. From these values, the biphenyl half-life times were estimated in four PNe in which PAHs emissions are present: NGC 7027, BD+30°3639, NGC 5315 and NGC 40. In the condensed phase experiments, we observe hydrogenation of aromatic rings due to interaction with electrons in the keV range, as well as a competitive route for deprotonation of these molecules. These results suggest possible pathways of PAH formation with aliphatic fragments, as well as  $H_n$ -PAHs, on the frozen surface of dust grains in cold regions of the circumstellar environment. In the observational part of this work, a survey analysis of the molecular composition of the Class 0 protostellar object IRAS 4A was performed from data obtained by the IRAM 30m radiotelescope. Ninety-two molecular species were identified and cataloged with 1456 rotational frequencies, including narrow and wide profiles, by analyzing the molecular content of IRAS 4A. The results show that IRAS 4A is dominated by simple molecules containing carbon, nitrogen, oxygen, sulfur and silicon. We also identified COMs such as  $CH_3OH$ ,  $CH_3CHO$  and  $CH_3COCH_3$ , the most abundant ones containing oxygen in the structure. Based on our results, we could identify three excitation temperature components, associated with different regions of the source, and estimate the column density of each molecule with respect to  $H_2$ , both in the protostellar envelope and in the bipolar jet associated with the protostar.

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PhD Thesis Download: <http://objdig.ufrj.br/14/teses/898208.pdf>

## Interstellar Extinction and Elemental Abundances

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Elements in the interstellar medium (ISM) exist in the form of gas or dust. The interstellar extinction and elemental abundances provide crucial constraints on the composition, size and quantity of interstellar dust. Most of the extinction modeling efforts have assumed the total (gas and dust) abundances of the dust-forming elements—known as the “interstellar abundances”, “interstellar reference abundances”, or “cosmic abundances”—to be solar and

the gas-phase abundances to be environmentally independent. However, it remains unclear if the solar abundances are an appropriate representation of the interstellar abundances. Meanwhile, the gas-phase abundances are known to exhibit appreciable variations with local environments. Here we explore the viability of the abundances of B stars, the solar and protosolar abundances, and the protosolar abundances augmented by Galactic chemical enrichment (GCE) as an appropriate representation of the interstellar abundances by quantitatively examining the extinction and abundances of ten interstellar sightlines for which both the extinction curves and the gas-phase abundances of all the major dust-forming elements (i.e., C, O, Mg, Si and Fe) have been observationally determined. Instead of assuming a specific dust model and then fitting the observed extinction curves, for each sightline we apply the model-independent Kramers-Kronig relation, which relates the wavelength-integrated extinction to the total dust volume, to place a lower limit on the dust depletion. This, together with the observationally-derived gas-phase abundances, allows us to rule out the B-star, solar, and protosolar abundances as the interstellar reference standard and support the GCE-augmented protosolar abundances as a viable representation of the interstellar abundances.

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# Announcements

Max-Planck-Institut für extraterrestrische Physik

Max Planck Institute for Extraterrestrial Physics



## Postdoctoral position in Laboratory Astrochemistry 27/2020

The Max Planck Institute for Extraterrestrial Physics (MPE) in Garching (Bavaria/Germany) is a world-leading institute in space- and ground-based experimental astrophysics, with leading roles in a number of large astronomical projects.

The Center for Astrochemical Studies (CAS; <http://www.mpe.mpg.de/CAS>) at the MPE, invites applications for one Postdoctoral position in laboratory astrochemistry. CAS hosts experimentalists, observers and theoreticians who study together the chemical and physical evolution of star- and planet-forming regions, from the parent clouds to protoplanetary disks, with links to exoplanets and our Solar System. Researchers with experience in laboratory astrophysics, in particular ion traps, are encouraged to apply. Two CAS ion traps have been recently built to measure: (i) the rate coefficients of astrochemically relevant ion-molecule reactions and (ii) physical and chemical properties of interstellar dust analogue nanoparticles.

The flexible starting date could be as early as Spring 2021, for 2 years guaranteed with the possibility of extension to up to five years. Applicants should have a PhD in physics or related field before starting.

Salaries will be paid at German civil service rates (TVöD-Bund) depending on postdoctoral experience.

Applicants should submit their documents (in English, and in PDF form) online (Link), including a CV, a list of publications, and a brief (max. 1 page) description of research interests, by December 15th, 2020.

Later applications may also be considered in case the post is not filled until January 15th, 2021.

The name of three referees who can provide letters of recommendation should be included in the application; they will be contacted by the selection committee in case the applicant is short-listed.

Prospective applicants can contact Prof. Paola Caselli for further information ([caselli@mpe.mpg.de](mailto:caselli@mpe.mpg.de)).

The Max Planck Society is committed to increasing the number of individuals with disabilities in its workforce and therefore encourages applications from such qualified individuals.

Furthermore, the Max Planck Society seeks to increase the number of women in those areas where they are underrepresented and therefore explicitly encourages women to apply.

## AstroPAH Newsletter

<http://astropah-news.strw.leidenuniv.nl>

[astropah@strw.leidenuniv.nl](mailto:astropah@strw.leidenuniv.nl)

Next issue: 17 December 2020

Submission deadline: 4 December 2020