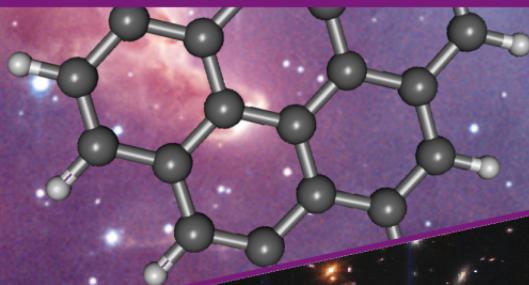


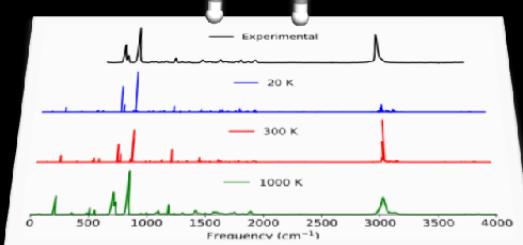
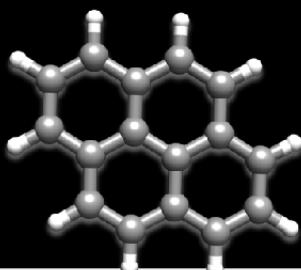
# AstroPAH

A Newsletter on Astronomical PAHs

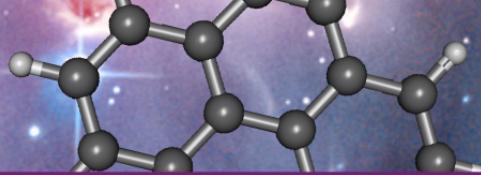


Issue 93 • November 2022

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**Dr. Timothy J. Lee**  
1959-2022



# Editorial

**Dear Colleagues,**

Welcome to our 93<sup>rd</sup> AstroPAH volume. We hope all of you are healthy and doing well.

Sadly, Dr. Timothy Lee (NASA/Ames) recently passed away. We remember him and his legacy as part of our Picture of the Month and with a tribute on page 4.

We would like to thank Dr. Felipe Fantuzzi for contributing a very exciting *In Focus* on interstellar PAHs and quantum chemistry.

Many thanks to all of you for so many abstracts contributions this month. Check out our *Abstracts* section for papers on NPAHs, interstellar H<sub>2</sub> formation, and galactic PAH emission.

Mark your calendars for the next PAH workshop that will be held in the Summer of 2025 at the University of Western Ontario, London, Ontario, Canada.

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

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

**The Editorial Team**

**Next issue: 15 December 2022.  
Submission deadline: 3 December 2022.**

# AstroPAH Newsletter

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## PAH Picture of the Month

In memory of Dr. Timothy J. Lee (1959-2022).

**Credits:** Picture of Tim Lee kindly provided by A. Tielens and C. Mackie. Experimental and simulated infrared spectra of pyrene by T. Chen et al.. Background image: [Galaxy cluster SMACS J0723.3-7327](#) by JWST, credits to NASA, ESA, CSA, and STScI



## Tribute to Tim Lee

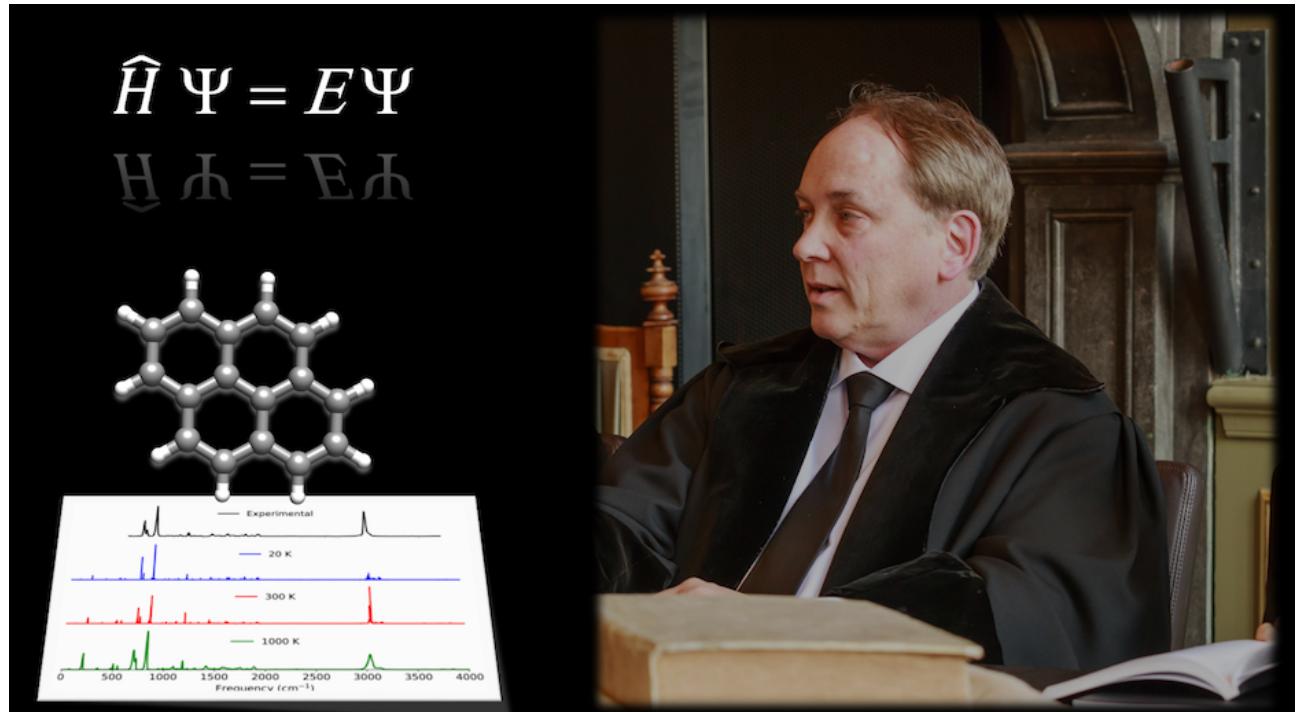
Our colleague, Dr. Timothy J. Lee recently passed away earlier this month. He was a leading quantum chemist and instrumental in pushing for the study of PAH anharmonicity. Tim was also very active in establishing line lists for their use in stellar and exoplanetary atmosphere modeling and in identifying and quantifying chemical reaction routes of astrophysical relevance. All of his studies are directly linked to and validated by experimental studies. Moreover, they are in clear support of NASA missions.

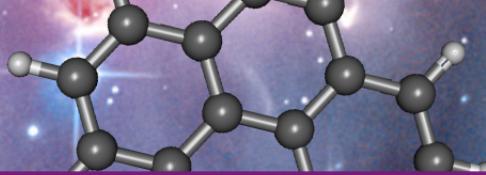
Tim had a very rich career at NASA Ames Research Center for 33 years, and among those, served as the Division Chief of the Space Science and Astrobiology Division for 10 years. He received two NASA Exceptional Scientific Achievement Medals (1998 and 2011) as well as a Dirac Medal from the World Association of Theoretical and Computational Chemists in 1988. His involvement in the field was also illustrated by him being an elected Fellow of the American Physical Society and of the American Association for the Advancement of Science.

Tim was also an excellent teacher and mentor of students and postdocs. An outstanding and influential colleague and friend, we will miss him dearly.

An online memorial can be visited following this link:

<https://everloved.com/life-of/timothy-lee/?flow=201>





# In FOCUS

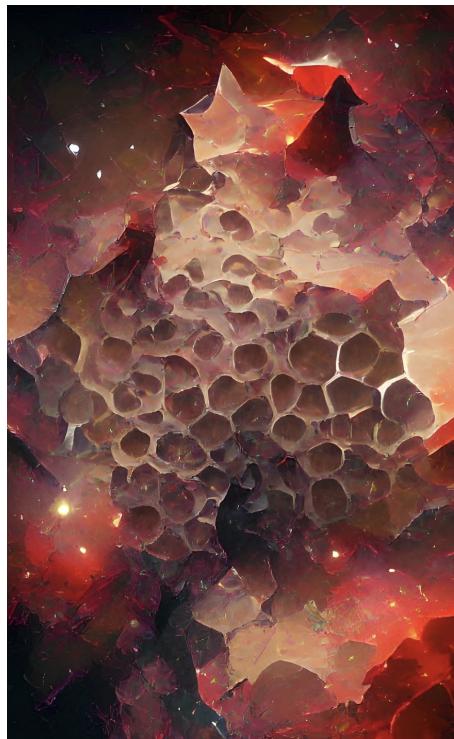
## AstroPAHs through the Lens of Computational Chemistry

by Felipe Fantuzzi

### Introduction

The last few years have witnessed fascinating accomplishments and breakthroughs in our understanding of polycyclic aromatic hydrocarbons (PAHs) in astronomical environments (Figure 1). Indeed, PAHs constitute one of the most important classes of molecules in both the interstellar (ISM) and circumstellar (CSM) media. Around 10–15% of the interstellar carbon matter is attributed to such molecular archetypes. Amongst their numerous astrophysical roles, PAHs can work as temperature and charge-state regulators of the ISM. Furthermore, PAHs are considered key substrates in surface reactions, and are particularly relevant for the formation of molecular hydrogen ( $H_2$ ) (Oliveira et al., 2020).

From a structural point of view, PAHs can be categorised into two major groups, namely i) planar and ii) bowl-shaped PAHs. The first class contains the better known PAHs, such as naphthalene, anthracene and higher acenes, pyrene, coronene, and hexabenzocoronene, amongst several others. In turn, some important representatives of the second class of PAHs are corannulene, diindenochrysene, hemifullerene, and circumtrindene. These systems are characterised by the presence of at least one five-membered ring, which is responsible for folding the PAH skeleton into a curved structure. Such pentagonal rings also make up the molecular structure of buckminsterfullerene  $C_{60}$ , which is another very important carbon-based molecule of astronomical relevance. The overall structure of PAHs, including their size and curvature, drastically affects their electronic properties and reactivity. Therefore, a solid underpinning of how the geometrical features of PAHs are influenced by physical properties, such as molecular charge and spin states, as well as the presence of atomic doping and/or structural defects, is crucial for a thorough understanding of the role of PAHs in different fields, including medicinal chemistry, materials science, and astrochemistry (Fernández, 2020).



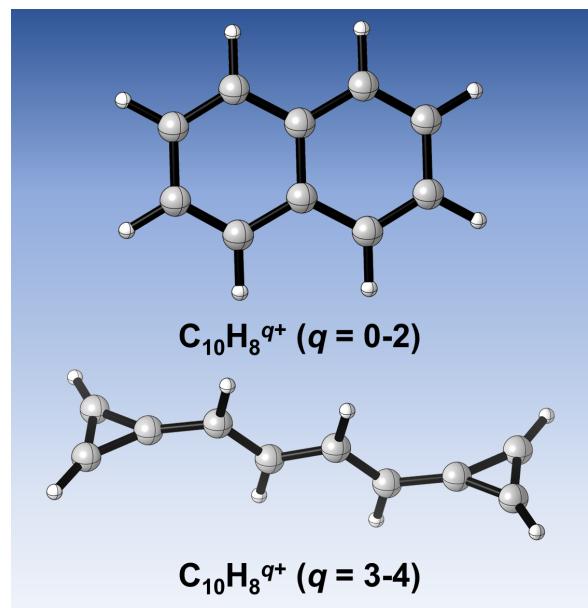
**Figure 1 – PAHs in astrophysical environments: an artistic interpretation.**

In order to provide relevant information regarding the electronic structure, bonding situation, and spectroscopic properties of interstellar molecules, our group has specialised in developing and applying distinct computational tools based on Density Functional Theory (DFT) and Wave Function Theory (WFT). The aforementioned properties are strongly dependent on the molecular structure of the system, which is ultimately defined by the relative position of the various atomic nuclei composing the molecule in its equilibrium geometry. However, for a given stoichiometry, different stable atomic arrangements can usually be found, each giving rise to a unique molecular isomer with distinct electronic, spectroscopic, and thermochemical characteristics. Furthermore, the equilibrium structures and the relative energy between distinct isomers can be drastically influenced by the charge state. A typical example is benzene ( $C_6H_6$ ), whose global minimum energy structure at the neutral charge state is characterised by a six-membered planar carbon ring with  $D_{6h}$  point-group symmetry, while its doubly charged analogue features a pentagonal-pyramidal  $C_5H_5$  ring with an additional CH motif pointing perpendicularly relative to the pentagonal base (Fantuzzi et al., 2017). As part of our systematic investigation of the structure and stability of multiply charged molecular ions, herein we highlight some of our recent findings related to mono-, di-, tri-, and tetracations produced by the photo-ionisation of astrophysically relevant PAHs and their monocyclic prototypes.

## The $C_{10}H_8^{q+}$ Family

Naphthalene ( $C_{10}H_8$ ) is the simplest PAH, composed of two fused benzene rings. The recent detection of two nitrile-functionalised ( $-CN$ ) anthracene isomers in Taurus Molecular Cloud 1 (TMC-1) by McGuire et al. (2021) inspired us to undertake a systematic computational investigation into the influence of the charge state on the structure and stability of neutral, singly, and multiply charged naphthalene and their  $C_{10}H_8^{q+}$  isomers (Santos et al., 2022). The most stable systems with  $q = 0 - 2$  are predominantly composed of fused rings (Figure 2). However, for higher charge states, this profile changes appreciably, with open chains dominating the low-energy structures of  $C_{10}H_8^{4+}$ . The neutral charge state is clearly highly stabilised by aromaticity. For higher charge states, and especially for  $q = 3$ , the population of isomers with electronic energies slightly higher than that of the global minimum increases significantly. Thus, isomerisation reactions should be more frequent and consequently play a more important role in higher charge states. For  $q = 4$ , charge repulsion leads to destabilisation of structures with fused five-, six-, and seven-membered rings, while cyclopropenyl aromatic rings and open-chain CH motifs are preferred as they allow a better charge separation.

We also evaluated the spectroscopic properties of the most stable  $C_{10}H_8^{q+}$  structures in

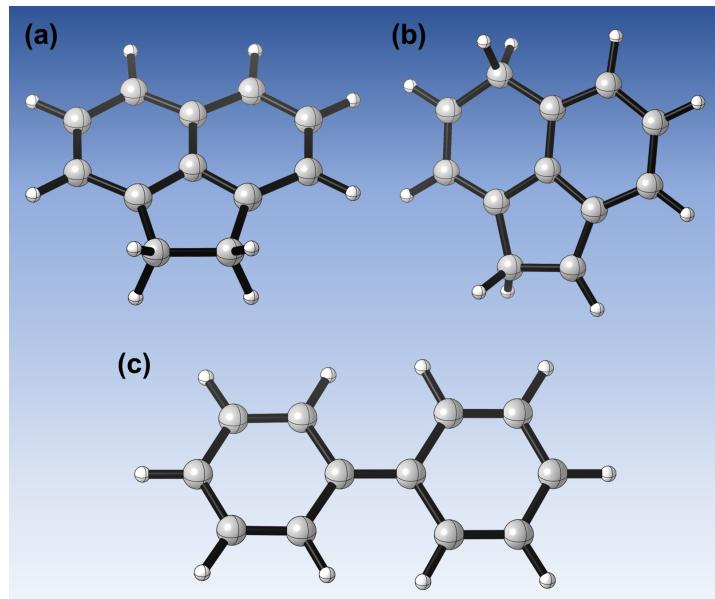


**Figure 2 – Global minimum energy structures of  $C_{10}H_8^{q+}$  ( $q = 0 - 4$ ).**

the infrared (IR) region, in order to support the interpretation of astronomical observations. We simulated both harmonic and non-harmonic IR spectra, and derived scaling factors according to PAHdb guidelines (Bauschlicher Jr. et al., 2018) based on the experimentally measured bands of neutral, single, and doubly charged global minima. In general, the scaled-harmonic spectra were reasonably close to the available experimental results. Comparatively, the anharmonic spectrum of neutral naphthalene was appreciably less accurate than the scaled-harmonic equivalent. For higher charge states, however, the anharmonic corrections became increasingly important, eventually yielding a more accurate spectrum than the scaled-harmonic approach for the dication species. Yet, all the spectra obtained by us were satisfactorily close to the experiments and hence both approaches appear suitable to assist astronomical observations.

## The $\text{C}_{12}\text{H}_{10}^{q+}$ Family

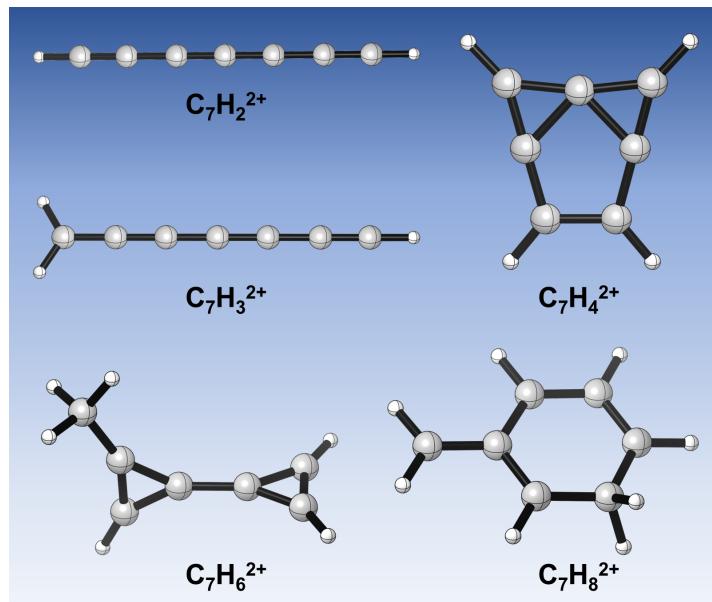
Biphenyl ( $\text{C}_{12}\text{H}_{10}$ ) is an aromatic molecule composed of two phenyl ( $\text{C}_6\text{H}_5$ ) radicals connected through a C–C sigma bond. Although  $\text{C}_{12}\text{H}_{10}$  was not detected in the ISM so far, the system is believed to work as an important building block for the formation of larger PAHs through a hydrogen-abstraction/acetylene-addition (HACA) mechanism (Yang et al., 2017). With respect to  $\text{C}_{12}\text{H}_{10}^{q+}$  molecular ions, the monocationic  $\text{C}_{12}\text{H}_{10}^+$  species is the second most prominent ion produced by the interaction of biphenyl with soft X-rays, according to recent experiments (Quitián-Lara et al., 2020). The  $\text{C}_{12}\text{H}_{10}^+$  global minimum energy geometry is associated with the singly-charged acenaphthene molecule (Figure 3), which is characterised by a  $\text{C}_2$ -bridged naphthalene structure. This geometry is ca. 20 kcal mol<sup>-1</sup> more stable than the biphenyl-like structure. Similarly, the biphenyl-like structure of  $\text{C}_{12}\text{H}_{10}^{2+}$  lies more than 30 kcal mol<sup>-1</sup> above the global minimum energy of the system, which is again composed of an acenaphthene carbon backbone, but with a distinct hydrogen arrangement compared to that of the singly charged  $\text{C}_{12}\text{H}_{10}^+$ . The high energy of the dicationic biphenyl-like structure can be attributed to the steric repulsion of the hydrogen atoms in *ortho* position as a consequence of the reduction of the torsional angle between the rings to almost 0° and the significant shortening of the central C–C bond length.



**Figure 3 – Global minimum energy structures of (a)  $\text{C}_{12}\text{H}_{10}^+$  and (b)  $\text{C}_{12}\text{H}_{10}^{2+}$ . (c) Biphenyl-like structure with reduced torsional angle.**

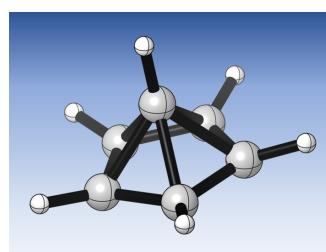
## The $C_7H_n^{2+}$ Family

Toluene ( $C_7H_8$ ) is the simplest alkyl-functionalised benzene derivative, in which a  $CH_3$  group replaces one of the benzene hydrogen atoms. Although  $C_7H_8$  has not been detected so far in the ISM, the system is one of the major constituents of the Murchison and Allende meteorites (Studier et al., 1972) and its protonated  $C_7H_9^+$  counterpart has a spectral signature that matches reasonably with the unidentified interstellar infrared emission band near  $6.2\ \mu m$  (Doublerly et al., 2008). Upon interaction with soft X-ray photons, several doubly charged molecular ions containing seven carbon atoms with considerable abundance were found in the corresponding mass spectra, which motivated our computational investigation of  $C_7H_n^{2+}$  species (Monfredini et al., 2016). Our analysis revealed that, while  $C_7H_2^{2+}$  and  $C_7H_3^{2+}$  present polyyne-like structures, a cyclic structure containing a planar tetracoordinate carbon is one of the possible global minima of  $C_7H_4^{2+}$  (Figure 4). Furthermore, a previously non-reported structure featuring two cyclopropenyl groups connected by a C–C sigma bond was found as the global minimum of  $C_7H_6^{2+}$ . Finally, for the parent dication  $C_7H_8^{2+}$ , the *meta*-protonated benzyl cation was obtained as the most stable structure, highlighting the loss of structural integrity from neutral toluene as previously suggested in the literature (Roithová et al., 2006).



**Figure 4 – Global minimum energy structures of  $C_7H_2^{2+}$ ,  $C_7H_3^{2+}$ ,  $C_7H_4^{2+}$ ,  $C_7H_6^{2+}$  and  $C_7H_8^{2+}$ .**

In a recent work (Wolff et al., 2020), we reported a careful, systematic search of long-lived  $C_6H_n^{2+}$  ( $n = 3 - 6$ ) dications from electron ionisation time-of-flight measurements of distinct benzene derivatives in combination with global minimum energy structure calculations. The benzene-like  $C_6H_6^{2+}$  structure at the triplet state is slightly non-planar, and is  $15.8\text{ kcal mol}^{-1}$  above the pentagonal-pyramidal global minimum energy structure (Figure 5). In turn, the  $C_6H_5^{2+}$  global minimum structure has a twisted cumulenic linear carbon chain attached to a cyclopropenyl ring. The  $C_6H_4^{2+}$  global minimum structure is composed of a dicyclopropenyl dication,  $(C_3H_2)_2^{2+}$ , and agrees with that of Lammertsma and Schleyer (1988). Finally, the global minimum of  $C_6H_3^{2+}$  features a linear carbon chain with cumulene character attached to a terminal cyclopropenyl ring.



**Figure 5 –  $C_6H_6^{2+}$ .**

## What's next?

The investigations highlighted herein showcase the importance of quantum chemistry approaches for the understanding of the geometrical, electronic, and thermochemical properties of multiply charged species of astrochemical interest. In the future, we plan to extend our work to larger PAHs and those exhibiting functional groups and backbone heteroatoms. We hope to contribute to a better understanding of interstellar PAHs, including their role as catalysts for the formation of complex organic molecules and prebiotic compounds.

## Acknowledgements

F. F. acknowledges the excellent support provided by co-workers of the studies featured herein: Heloisa M. Boechat-Roberty, Lucia H. Coutinho, Gerhard Hilgers, Yanna Martins-Franco, Karín Menéndez-Delmestre, Thiago Monfredini, Marco A. C. Nascimento, Ricardo R. Oliveira, Amir Perlin, Heidy M. Quítian-Lara, Fabio de A. Ribeiro, Julia C. Santos, and Wania Wolff. F. F. also thanks the National Laboratory for Scientific Computing (LNCC/MCTI, Brazil) for providing HPC resources of the SDumont supercomputer (<http://sdumont.lncc.br>).

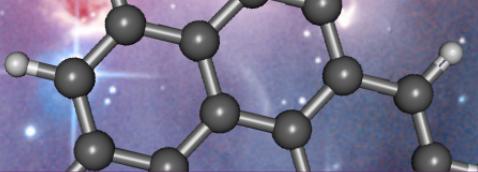


**Dr Felipe Fantuzzi** is a Lecturer in Chemistry at the University of Kent (UK) since December 2021. He obtained his MSc (2013) and PhD (2017) in Chemistry from the Universidade Federal do Rio de Janeiro (Brazil) with Thiago M. Cardozo and Marco A. C. Nascimento. During his post-graduate studies, Felipe investigated the role of quantum interference in chemical bonds using modern valence bond methods and applied density functional theory and wave function-based methods to problems in astrochemistry and materials science. After a post-doctoral stay at the Pacific Northwest National Laboratory (USA) with Simone Raugei in computational electrocatalysis, he moved to Julius-Maximilians-Universität Würzburg (Germany) as an Alexander von Humboldt post-doctoral fellow (2018). He worked with computational main-group chemistry at the Institute for Sustainable Chemistry & Catalysis with Boron (ICB) with Holger Braunschweig and Bernd Engels. He was also a visiting researcher at the University of Wisconsin-Madison (USA) with Frank Weinhold (2019) and the MBN Research Center (Germany) with Andrey V. Solov'yov (2022). The Fantuzzi Group research interests lie in the application and development of modern computational quantum chemistry methods for describing the electronic structure, bonding, reactivity, and excited-state properties of novel main-group and organometallic compounds. Their motivation goes from fundamentals to applications in fields such as small-molecule activation, metal and metal-free catalysis, bioactive and biomimetic compounds, molecular design, materials science, and astrochemistry.

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# Abstracts

## Rotational spectra of interstellar N- and CN-PAHs: pyrene and coronene

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The detection of benzonitrile ( $C_6H_5CN$ ), 1- and 2-cyano-naphthalene ( $C_{10}H_7CN$ ) in the cold, dark molecular cloud TMC-1 at centimetre (cm) wavelengths has opened up prospects for the detection of other N- and CN-containing polycyclic aromatic hydrocarbons (PAHs). In this light, the pure rotational spectra of N-pyrene ( $C_{15}H_9N$ ), CN-pyrene ( $C_{15}H_9CN$ ), N-coronene ( $C_{23}H_{11}N$ ) and CN-coronene ( $C_{23}H_{11}CN$ ) are reported here for the first time. The B3LYP/6-311+G(d,p) level of theory, in the Density Functional Theory (DFT) calculations, achieves the best performance for calculating the spectroscopic parameters and simulating the rotational spectra. The large permanent dipole moment of CN-PAHs makes them the most suitable PAH species for detection in the interstellar medium. Additionally, pyrene's smaller partition function makes CN-pyrene a prime candidate to be discovered in cold, dark molecular clouds such as the TMC-1. The present work sets a benchmark for theoretical rotational spectra of N- and CN-containing PAHs and may act as a guide for laboratory experiments and observational searches.

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<https://doi.org/10.1093/mnras/stac3157>

<https://arxiv.org/submit/4574133/view>

# Gas-phase synthesis of racemic helicenes and their potential role in the enantiomeric enrichment of sugars and amino acids in meteorites

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The molecular origins of homochirality on Earth is not understood well, particularly how enantiomerically enriched molecules of astrobiological significance like sugars and amino acids might have been synthesized on icy grains in space preceding their delivery to Earth. Polycyclic aromatic hydrocarbons (PAHs) identified in carbonaceous chondrites could have been processed in molecular clouds by circularly polarized light prior to the depletion of enantiomerically enriched helicenes onto carbonaceous grains resulting in chiral islands. However, the fundamental low temperature reaction mechanisms leading to racemic helicenes are still unknown. Here, by exploiting synchrotron based molecular beam photoionization mass spectrometry combined with electronic structure calculations, we provide compelling testimony on barrierless, low temperature pathways leading to racemates of [5] and [6]helicene. Astrochemical modeling advocates that gas-phase reactions in molecular clouds lead to racemates of helicenes suggesting a pathway for future astronomical observation and providing a fundamental understanding for the origin of homochirality on early Earth.

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[http://uhmreactiondynamics.org/publication\\_papers/p545.pdf](http://uhmreactiondynamics.org/publication_papers/p545.pdf)

# A CRYSTAL-based parameterization of carbon atom dynamic polarizabilities to compute optical properties of curved carbonaceous nanostructures

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A better estimation of the absorption cross-section of dust particles in the UV-visible part of the spectrum is needed to better characterize their contribution to the radiative forcing of the Earth atmosphere. Among the methods used for this purpose, the Atomic Point Dipole Interaction model has the distinctive advantage of being sensitive to the atomistic geometry of the particle and to the chemical functions it contains. However this requires an adequate parameterization of the atomic polarizabilities for all the atomic species forming the particle, over the UV-visible spectrum. In this paper, we illustrate how new methodological improvements based on quantum chemistry, allow taking into account the curvature of the carbon network in the parametrization of the carbon atomic polarizabilities, using the C<sub>60</sub> molecule to fit the adequate set of parameters. We thus show how this leads to significant differences in the computed curves of the absorption cross-section of pure carbonaceous nanoparticles as a function of the frequency, with respect to calculations performed using parameters issued from graphite. We thus believe that the values of the carbon atomic polarizability determined here can actually serve for the determination of the optical properties of carbonaceous structures of atmospheric or interstellar interest such as fullerenes and their derivatives, as well as soot or small carbonaceous grains, on the basis of their atomistic details, through the PDI method. This would represent a nice, and hopefully more precise, alternative to the usual DDA or T-matrix approaches which usually neglect those levels of description.

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# Polyaromatic Hydrocarbons with an Imperfect Aromatic System as Catalysts of Interstellar H<sub>2</sub> Formation

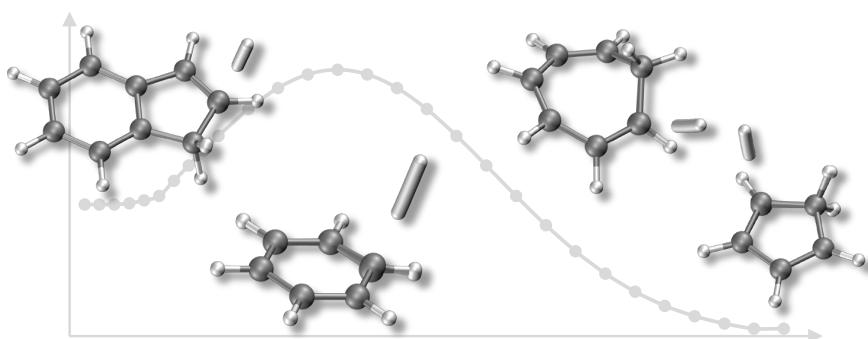
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Although H<sub>2</sub> is the simplest and the most abundant molecule in the Universe, its formation in the interstellar medium, especially in the photodissociation regions is far from being fully understood. According to suggestions, the formation of H<sub>2</sub> is catalyzed by polyaromatic hydrocarbons (PAHs) on the surface of interstellar grains. In the present study we have investigated the catalytic effect of small PAHs with an imperfect aromatic system. Quantum chemical computations were performed for the H-atom-abstraction and H-atom-addition reactions of benzene, cyclopentadiene, cycloheptatriene, indene, and 1H-phenalene. Heights of reaction barriers and tunnelling reaction rate constants were computed with density functional theory using the MPWB1K functional. For each molecule, the reaction path and the rate constants were determined at 50 K using ring-polymer instanton theory, and the temperature dependence of the rate constants was investigated for cyclopentadiene and cycloheptatriene. The computational results reveal that defects in the aromatic system compared to benzene can increase the rate of the catalytic H<sub>2</sub> formation at 50 K.

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# Tracing PAH Emission in $\lambda$ -Orionis Using COBE/DIRBE Data

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We use archival COBE/DIRBE data to construct a map of polycyclic aromatic hydrocarbon (PAH) emission in the  $\lambda$ -Orionis region. The presence of the 3.3  $\mu\text{m}$  PAH feature within the DIRBE 3.5  $\mu\text{m}$  band and the corresponding lack of significant PAH spectral features in the adjacent DIRBE bands (1.25, 2.2, and 4.9  $\mu\text{m}$ ) enable estimation of the PAH contribution to the 3.5  $\mu\text{m}$  data. Having the shortest wavelength of known PAH features, the 3.3  $\mu\text{m}$  feature probes the smallest PAHs, which are also the leading candidates for carriers of anomalous microwave emission (AME). We use this map to investigate the association between the AME and the emission from PAH molecules. We find that the spatial correlation in  $\lambda$ -Orionis is higher between AME and far-infrared dust emission (as represented by the DIRBE 240  $\mu\text{m}$  map) than it is between our PAH map and AME. This finding, in agreement with previous studies using PAH features at longer wavelengths, is in tension with the hypothesis that AME is due to spinning PAHs. However, the expected correlation between mid-infrared and microwave emission could potentially be degraded by different sensitivities of each emission mechanism to local environmental conditions even if PAHs are the carriers of both.

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# Efficiency of the top-down PAH-to-fullerene conversion in UV irradiated environments

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Polycyclic aromatic hydrocarbons (PAHs) and fullerenes play a major role in the physics and chemistry of the interstellar medium. Based on a number of recent experimental and theoretical investigations we developed a model in which PAHs are subject to photo-dissociation (carbon and hydrogen loss) and hydrogenation. We take into account that dehydrogenated PAHs may fold into closed structures – fullerenes. Fullerenes, in their turn, can be also hydrogenated, becoming fulleranes, and photo-dissociated, losing carbon and hydrogen atoms. The carbon loss leads to shrinking of fullerene cages to smaller ones. We calculate the abundance of PAHs and fullerenes of different sizes and hydrogenation level depending on external conditions: the gas temperature, intensity of radiation field, number density of hydrogen atoms, carbon atoms, and electrons. We highlight the conditions, which are favourable for fullerene formation from PAHs, and we conclude that this mechanism works not only in H-poor environment but also at modest values of hydrogen density up to  $10^4 \text{ cm}^{-3}$ . We found that fulleranes can be formed in the ISM, although the fraction of carbon atoms locked in them can be maximum around  $10^{-9}$ . We applied our model to two photo-dissociation regions, Orion Bar and NGC 7023. We compare our estimates of the fullerene abundance and synthetic band intensities in these objects with the observations and conclude that our model gives good results for the closest surroundings of ionising stars. We also demonstrate that additional fullerene formation channels should operate along with UV-induced formation to explain abundance of fullerenes far from UV sources.

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<https://academic.oup.com/mnras/article-abstract/517/3/3732/6760012?redirectedFrom=fulltext>

<https://arxiv.org/abs/2210.11156>

# A high angular resolution view of the PAH emission in Seyfert galaxies using JWST/MRS data

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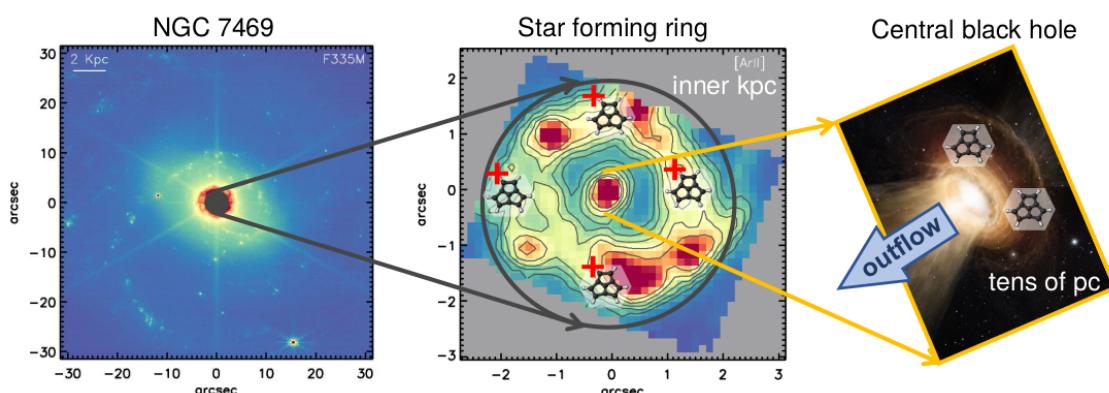
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Polycyclic aromatic hydrocarbons (PAHs) are carbon-based molecules that are ubiquitous in a variety of astrophysical objects and environments. In this work we use JWST/MIRI MRS spectroscopy of three Seyferts to compare their nuclear PAH emission with that of star-forming (SF) regions. This study represents the first of its kind to use sub-arcsecond angular resolution data of local luminous Seyferts ( $L_{\text{bol}} 10^{44.46}$  erg/s) with a wide wavelength coverage (4.9-28.1  $\mu\text{m}$ ). We present an analysis of their nuclear PAH properties by comparing the observed ratios with PAH diagnostic model grids derived from theoretical spectra. Our results show that a suite of PAH features is present in the innermost parts of luminous Seyfert galaxies ( $\sim 0.45$  arcsec at 12  $\mu\text{m}$ ; in the inner  $\sim 142$ -245 pc). We find that the nuclear regions of active galactic nuclei (AGN) lie at different positions of the PAH diagnostic diagrams, whereas the SF regions are concentrated around the average values of SF galaxies. In particular, we find that the nuclear PAH emission mainly originates in neutral PAHs. In contrast, PAH emission originating in the SF regions favours ionised PAH grains. The observed PAH ratios in the nuclear region of the AGN-dominated galaxy NGC 6552 indicate the presence of larger PAH molecules compared with those of the SF regions. Therefore, our results provide evidence that the AGN have a significant impact on the ionisation state (and probably the size) of the PAH grains on scales of  $\sim 142$ -245 pc.



Left panel: JWST/F335M image of NGC 7469, one of the active galaxies used in this work (Garcia-Bernete et al. 2022). Central panel: Zoomed-in view of the central region of the galaxy using JWST/MRS observations. Right panel: artist's impression of a black hole (credit: ESO/ M. Kornmesser).

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[https://www.aanda.org/articles/aa/full\\_html/2022/10/aa44806-22/aa44806-22.html](https://www.aanda.org/articles/aa/full_html/2022/10/aa44806-22/aa44806-22.html)

<https://arxiv.org/abs/2208.11620>

# Astrochemical model to study the abundances of branched carbon-chain molecules in a hot molecular core with realistic binding energies

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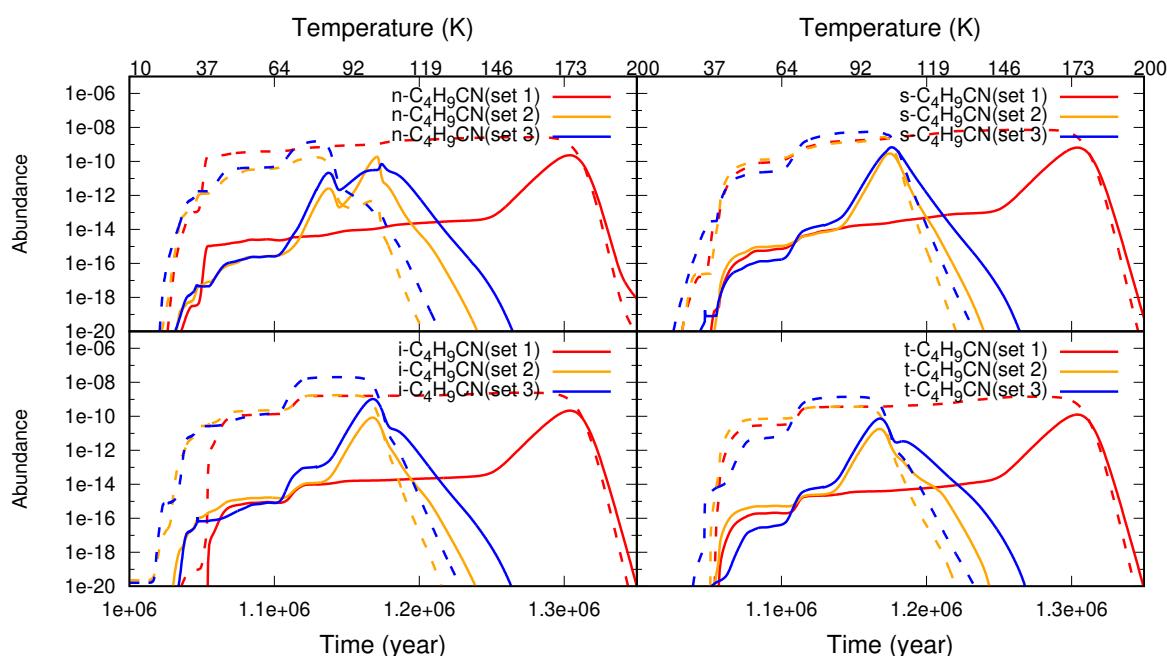
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*Time evolution of  $n\text{-C}_4\text{H}_9\text{CN}$ ,  $i\text{-C}_4\text{H}_9\text{CN}$ ,  $s\text{-C}_4\text{H}_9\text{CN}$ , and  $t\text{-C}_4\text{H}_9\text{CN}$  during the warm-up phase for various BE sets. Set 1 is constructed with the old BE values. Set 2 is constructed with the same BE values used in set 1 except for the branched-chain and some related species considered here. Set 3 contains the same BE of the branched-chain species as set 2, but for the others, the most updated values are used from the Kinetic Database for Astrochemistry. Solid curves represent the gas-phase abundance, whereas the dashed curves represent the abundance of ice-phase species.*

Straight-chain (normal-propyl cyanide,  $n\text{-C}_3\text{H}_7\text{CN}$ ) and branched-chain (iso-propyl cyanide,  $i\text{-C}_3\text{H}_7\text{CN}$ ) alkyl cyanides are recently identified in the massive star-forming regions (Sgr B2(N) and Orion). These branched-chain molecules indicate that the key amino acids (side-chain structures) may also be present in a similar region. The process by which this branching could propagate towards the higher-order (butyl cyanide,  $\text{C}_4\text{H}_9\text{CN}$ ) is an active field of research. Since the grain catalysis process could have formed a major portion of these species, considering a realistic set of binding energies are indeed essential. We employ quantum chemical calculations to estimate the binding energy of these species considering water as a substrate because water is the principal constituent of this interstellar

ice. We find significantly lower binding energy values for these species than were previously used. It is noticed that the use of realistic binding energy values can significantly change the abundance of these species. The branching is more favorable for the higher-order alkyl cyanides with the new binding energies. With the inclusion of our new binding energy values and one essential destruction reaction ( $i\text{-C}_3\text{H}_7\text{CN} + \text{H} \longrightarrow \text{CH}_3\text{C}(\text{CH}_3)\text{CN} + \text{H}_2$ ), having an activation barrier of 947 K), abundances of  $t\text{-C}_4\text{H}_9\text{CH}$  dramatically increased.

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# Adsorption of Helium and Hydrogen on Triphenylene and 1,3,5-Triphenylbenzene

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The adsorption of helium or hydrogen on cationic triphenylene (TPL, C<sub>18</sub>H<sub>12</sub>), a planar polycyclic aromatic hydrocarbon (PAH) molecule, and of helium on cationic 1,3,5-triphenylbenzene (TPB, C<sub>24</sub>H<sub>18</sub>), a propeller-shaped PAH, is studied by a combination of high-resolution mass spectrometry and classical and quantum computational methods. Mass spectra indicate that He<sub>n</sub>TPB<sup>+</sup> complexes are particularly stable if n = 2 or 6, in good agreement with the quantum calculations which show that for these sizes the helium atoms are strongly localized on either side of the central carbon ring for n = 2 and on either side of the three outer rings for n = 6. Theory suggests that He<sub>14</sub>TPL<sup>+</sup> is also particularly stable, with the helium atoms strongly localized on either side of the central and outer rings plus the vacancies between the outer rings. For He<sub>n</sub>TPB<sup>+</sup> the mass spectra hint at enhanced stability for n = 2, 4 and, possibly, 11. Here the agreement with theory is less satisfactory, probably because TPB<sup>+</sup> is a highly fluxional molecule. In the global energy minimum, the phenyl groups are rotated in the same direction but when the zero-point harmonic correction is included, a structure with one phenyl group being rotated opposite to the other two becomes lower in energy. The energy barrier between the two isomers is very small, and TPB<sup>+</sup> could be in a mixture of symmetric and antisymmetric states, or possibly even vibrationally delocalized.

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# Solvation of Large Polycyclic Aromatic Hydrocarbons in Helium: Cationic and Anionic Hexabenzocoronene

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The adsorption of helium on charged hexabenzocoronene (Hbc,  $C_{42}H_{18}$ ), a planar polycyclic aromatic hydrocarbon (PAH) molecule of  $D_{6h}$  symmetry, is investigated by a combination of high-resolution mass spectrometry and classical and quantum computational methods. The ion abundance of  $He_nHbc^+$  complexes versus size n features prominent local anomalies at  $n = 14, 38, 68, 82$ , and a weak one at 26, indicating that for these “magic” sizes the helium evaporation energies are relatively large. Surprisingly, mass spectra of anionic  $He_nHbc^-$  complexes feature a different set of anomalies, namely at  $n = 14, 26, 60$ , and 62, suggesting that the preferred arrangement of the adsorbate atoms depends on the charge of the substrate. The results of our quantum calculations show that the adsorbate layer grows by successive filling of concentric rings that surround the central benzene ring which is occupied by one helium atom each on either side of the substrate. The helium atoms are fairly localized in filled rings and they approximately preserve the  $D_{6h}$  symmetry of the substrate, but helium atoms in partially filled rings are rather delocalized. The first three rings contain 6 atoms each; they account for magic numbers at  $n = 14, 26$ , and 38. The size of the first ring shrinks as atoms are filled into the second ring, and the position of atoms in the second ring changes from hollow sites to bridge sites as atoms are filled into the third ring. Beyond  $n = 38$ , however, the arrangement of helium atoms in the first three rings remains essentially frozen. Presumably, another ring is filled at  $n = 68$  for cations and  $n = 62$  for anions. The calculated structures and energies do not account for the difference between charge states, although they agree with the measurements for the cations and show that the first solvation shell of  $Hbc^\pm$  is complete at  $n = 68$ . Beyond that size the adsorbate layer becomes three-dimensional, and the circular arrangement of helium changes to hexagonal.

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# The kinetic energy of PAH dication and trication dissociation determined by recoil-frame covariance map imaging

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We investigated the dissociation of dications and trications of three polycyclic aromatic hydrocarbons (PAHs), fluorene, phenanthrene, and pyrene. PAHs are a family of molecules ubiquitous in space and involved in much of the chemistry of the interstellar medium. In our experiments, ions are formed by interaction with 30.3 nm extreme ultraviolet (XUV) photons, and their velocity map images are recorded using a PImMS2 multi-mass imaging sensor. Application of recoil-frame covariance analysis allows the total kinetic energy release (TKER) associated with multiple fragmentation channels to be determined to high precision, ranging 1.94–2.60 eV and 2.95–5.29 eV for the dications and trications, respectively. Experimental measurements are supported by Born–Oppenheimer molecular dynamics (BOMD) simulations.

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<https://pubs.rsc.org/en/content/articlelanding/2022/cp/d2cp02252d>

# PDRs4All: A JWST Early Release Science Program on Radiative Feedback from Massive Stars

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Massive stars disrupt their natal molecular cloud material through radiative and mechanical feedback processes. These processes have profound effects on the evolution of interstellar matter in our Galaxy and throughout the universe, from the era of vigorous star formation at redshifts of 1–3 to the present day. The dominant feedback processes can be probed by observations of the Photo-Dissociation Regions (PDRs) where the far-ultraviolet photons of massive stars create warm regions of gas and dust in the neutral atomic and molecular gas. PDR emission provides a unique tool to study in detail the physical and chemical processes that are relevant for most of the mass in inter- and circumstellar media including diffuse clouds, proto-planetary disks, and molecular cloud surfaces, globules, planetary nebulae, and star-forming regions. PDR emission dominates the infrared (IR) spectra of star-forming galaxies. Most of the Galactic and extragalactic observations obtained with the James Webb Space Telescope (JWST) will therefore arise in PDR emission. In this paper we present an Early Release Science program using the MIRI, NIRSpec, and NIRCam instruments dedicated to the observations of an emblematic and nearby PDR: the Orion Bar. These early JWST observations will provide template data sets designed to identify key PDR characteristics in JWST observations. These data will serve to benchmark PDR models and extend them into the JWST era. We also present the Science-Enabling products that we will provide to the community. These template data sets and Science-Enabling products will

guide the preparation of future proposals on star-forming regions in our Galaxy and beyond and will facilitate data analysis and interpretation of forthcoming JWST observations.

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<https://iopscience.iop.org/article/10.1088/1538-3873/ac604c>

# Theoretical Spectra and Energetics for *c*-C<sub>3</sub>HC<sub>2</sub>H, *l*-C<sub>5</sub>H<sub>2</sub>, and Bipyrasidal D<sub>3h</sub> C<sub>5</sub>H<sub>2</sub>

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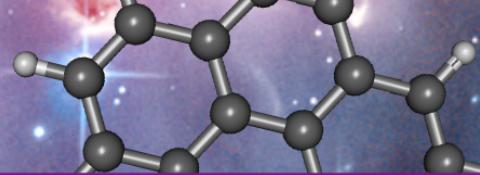
The recent astronomical detection of *c*-C<sub>3</sub>HC<sub>2</sub>H and *l*-C<sub>5</sub>H<sub>2</sub> has led to increased interest in C<sub>5</sub>H<sub>2</sub> isomers and their relative stability. The present work provides the first complete list of anharmonic vibrational spectral data with infrared intensities for three such isomers as well as including the first set of rotational data for the bipyrasidal C<sub>5</sub>H<sub>2</sub> isomer allowing for these molecules to serve as potential tracers of interstellar carbon. All three isomers have fundamental vibrational frequencies with at least one notably intense fundamental frequency. The *l*-C<sub>5</sub>H<sub>2</sub> isomer has, by far, the highest intensities out of the three isomers at 2076.3 cm<sup>-1</sup> (738 km mol<sup>-1</sup>) and 1887.5 cm<sup>-1</sup> (182 km mol<sup>-1</sup>). The *c*-C<sub>3</sub>HC<sub>2</sub>H isomer has one intense peak at 3460.6 cm<sup>-1</sup> (84 km mol<sup>-1</sup>), and the bipyrasidal C<sub>5</sub>H<sub>2</sub> isomer has one intense peak at 489.3 cm<sup>-1</sup> (78 km mol<sup>-1</sup>). The relative intensities highlight that while *l*-C<sub>5</sub>H<sub>2</sub> is not the lowest energy isomer, its notable intensities should make it more detectable in the infrared than the lower *c*-C<sub>3</sub>HC<sub>2</sub>H form. The bipyrasidal isomer is firmly established here to lie 44.98 kcal mol<sup>-1</sup> above the cyclic form. The explicitly correlated coupled cluster rovibrational spectral data presented herein should assist with future laboratory studies of these C<sub>5</sub>H<sub>2</sub> isomers and aid in detection in astronomical environments especially through the newly operational James Webb Space Telescope.

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# meetings

## 1st COST NanoSpace Joint Scientific Meeting 1st Announcement

Ljubljana, Slovenia  
9–11 February, 2023

<https://research.iac.es/proyecto/nanospace/pages/events/1st-cost-nanospace-joint-scientific-meeting/1st-announcement.php>

### General Action Scope:

The main aim and objective of the COST Action NanoSpace ("Carbon molecular nanostructures in space"; CA21126) is to advance the fundamental understanding of the physics and chemistry of cosmic carbon nanomaterials (nanocarbons; nC) and their relevance in non-terrestrial environments by promoting the interdisciplinary combination of state-of-the-art astronomical, laboratory, and theoretical studies, among others.

The main scientific challenges are the following:

- What nanocarbon species are present in space and how can we identify them?
- What are the chemical pathways that lead to their formation and destruction?
- What is the role of nanocarbon species in non-terrestrial environments? This is in cosmic and in prebiotic chemistry (astrobiology) and in astrophysics.

In order to attack the scientific challenge, NanoSpace proposes an interdisciplinary approach, combining the expertise from a wide range of disciplines like observational astronomy, laboratory astrophysics, astrobiology, theoretical chemistry, synthetic chemistry, molecular reaction dynamics, material science, spectroscopy, graph theory, and data science (AI, big data). The ambitious interdisciplinary nature of NanoSpace has the advantage that nanocarbons have potential applications in nanotechnology. Researchers and innovators from all these fields are thus welcome to participate both in the meeting and in the Action (see below).

NanoSpace takes advantage of the recent successful operation of the James Webb Space Telescope (JWST), the new facilities that can better mimic the interstellar medium (ISM) on the ground as well as the recent developments in the computational facilities and in laboratory techniques.

The Action is organized in four interdisciplinary Working Groups (WG):

- WG 1: "The Cosmic Inventory of nanocarbons".
- WG 2: "Processing, reactivity and relaxation pathways of nC".
- WG 3: "Role and Importance of nC in Non-Terrestrial Environments".
- WG 4: "Impact, Inclusiveness and Outreach".

### **Specific 1st Action Meeting Scope:**

This is the first COST NanoSpace Joint Scientific Meeting (in person), which will mark the start-up of the Action, knowing each other towards a common understanding of the scientific challenge, starting the interaction, learning, and collaboration and integrating young and ITC researchers. The main scope of this first meeting is thus two-fold:

- To start building a common scientific language.
- To start understanding and accepting the challenge and the limitations of the laboratory, theoretical and astronomical approaches.

**Deadline for registration (free) and abstract submission:** 3rd January 2023

### **Preliminary Program Plan:**

- NanoSpace overview and updates.
- WGs overview (main challenges, aims, and tasks).
- Flash oral presentations by NanoSpace participants/groups (5 min).
- Breaking scientific news oral presentations (10-15 min).
- Invited key Action talks (25-30 min).
- Poster sessions.

### **Organizing committee:**

Dr. Polona Umek, Jozef Stefan Institute, Slovenia

Prof. Denis Arcon, Jozef Stefan Institute, Slovenia

Dr. Nino Basic, University of Primorska, Slovenia

Dr. Domingo Anibal García Hernández, Instituto de Astrofísica de Canarias, Spain

Prof. Eleanor Campbell, University of Edinburgh, Scotland (UK)

Dr. Chris Ewels, CNRS - Institut des Matériaux Jean Rouxel, France

Dr. Dogan Erbahar, Dogus University, Turkey

Dr. Alicja Domracka, CNRS - CIMAP, France

Dr. Cornelia Jäger, MPIA, Germany

**The Action NanoSpace in the COST website:** <https://www.cost.eu/actions/CA21126>

**Apply to join the COST Action NanoSpace:** [Join here!](#)

**Final note:** Please check the meeting website for news and updates about the final list of invited speakers, hotel registration links, etc. More detailed information will be given in the second announcement.

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## AstroPAH Newsletter

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Submission deadline: 3 December 2022