

AstropAH

A Newsletter on Astronomical PAHs

Issue 109 • June 2024

JWST finds abundance of carbon molecules around low-mass star

Artist's Concept



Editorial

Dear Colleagues,

Welcome to our new 109th AstroPAH volume! We hope that you are all healthy and doing well!

Our cover picture features an artist's concept of the protoplanetary disk ISO-Chal 147 referring to observations of this disk, made with JWST using the MIRI instrument. The study revealed the largest number of carbon-containing molecules (13) detected in the disk of a very low-mass star and the first detection of ethane outside of our Solar System.

Our In Focus features an interview with Jerry Kamer who is conducting a PhD at the Laboratory for Astrophysics in Leiden. Jerry tells us how he got into astrochemistry and his research on the photodissociation and fragmentation of PA(N)Hs.

We wish to thank you all for the diverse abstract contributions this month. They cover papers on diamond phases, investigations on metallofullerenes, H-atom-based reactions, and PANHs photoprocessing.

We will see you again in a month, before our annual break in August.

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: 25 July 2024.
Submission deadline: 12 July 2024.**

AstroPAH Newsletter Editorial Board:

Editor-in-Chief

Prof. Alexander Tielens

Leiden University (The Netherlands)

Executive Editors

Dr. Isabel Aleman

University of São Paulo (Brazil)

Dr. Ella Sciamma-O'Brien

NASA Ames Research Center (USA)

Editors

Dr. David Dubois

NASA Ames Research Center
BAER Institute (USA)

Dr. Helgi Rafn Hróðmarsson

Laboratoire Inter-Universitaire
des Systèmes Atmosphériques
(France)

Dr. Donatella Loru

Deutsches Elektronen-Synchrotron
(Germany)

Dr. Julianna Palotás

University of Edinburgh (UK)

Dr. Pavithraa Sundararajan

Leiden University (The Netherlands)

Dr. Sandra Wiersma

Institute de Recherche en
Astrophysique et Planétologie
(France)

Contact us:

astropah@strw.leidenuniv.nl

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

[Click here to Subscribe to AstroPAH](#)

[Click here to Contribute to AstroPAH](#)

Follow us on:



Contents

PAH Picture of the Month	1
Editorial	2
In Focus	4
Recent Papers	7

PAH Picture of the Month

This month's cover features an artist's concept of a protoplanetary disk. Using JWST, a team of astronomers investigated the composition of gas and dust around a young star. [Their study](#) revealed the highest number of carbon molecules detected in such a disk to date.

Credits: NASA-JPL. The image is available [here](#).

In Focus

An interview with Jerry Kamer

Jerry Kamer received his Bachelor in Applied Physics in 2018 at The Hague University of Applied Sciences and subsequently got his Master in Applied Physics, specializing in Quantum Mechanics and Nanoscience, in 2021 at the Delft University of Technology. After his masters, he got a position as a PhD student in the group of Prof. Harold Linnartz at the Laboratory for Astrophysics in Leiden, The Netherlands. Here, he studies the photodissociation and fragmentation of PA(N)Hs using the i-PoP (Instrument for Photodynamics of PAHs) system in close collaboration with Dr. Jordy Bouwman. During his 3 years of being a PhD student, he became a specialist on quadrupole ion trap and time-of-flight mass spectrometry systems.



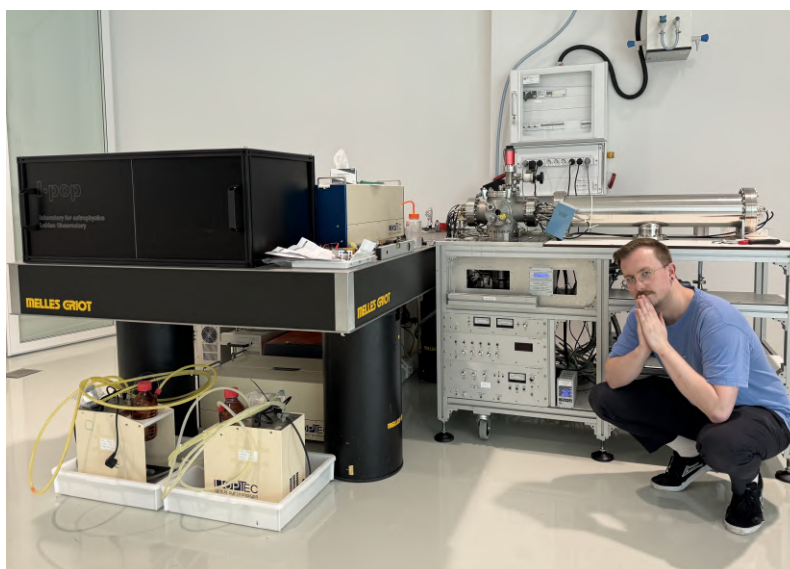
What inspired you to become a scientist?

As a little Jerry I was always busy trying to figure out how stuff works, for example by blatantly asking people and also by simply just trying out things myself. Therefore, I became very interested in nature and physics. I also remember that, as a kid, I wanted to invent something that would help humanity. However, the moment for me that really made me want to become a scientist was during one of my chemistry classes during high school. The teacher showed how two separate clear liquids would become blue when poured in the same beaker. This made me even more curious to nature and physics (and I should also mention chemistry) so I knew becoming a scientist was the path for me!

How did you get into astrochemistry research?

Interestingly enough, I never thought about astrochemistry too much. I graduated high school thinking I wanted to study chemistry, but eventually ended up in applied physics. For my bachelor thesis I had to apply for an internship. On our bulletin board, I saw an advertisement by Dr. Jordy Bouwman for a bachelor student in the group of Prof. Harold Linnartz at the Laboratory for Astrophysics (LfA), at Leiden University. I applied and got accepted to study the photodissociation of polycyclic aromatic hydrocarbons (PAHs) on the i-PoP system. After my bachelor I thought I was done with astrochemistry and did my masters on quantum mechanics and nanoscience. Perhaps it was all the PAHs that I

breathed in during my bachelor project, but during my masters I could hear the i-PoP system whispering my name. After my masters I applied for a PhD position on the i-PoP system and got accepted!



Jerry Kamer in front of the Instrument for Photodynamics of PAHs (i-PoP) housed at the Laboratory for Astrophysics (LfA), Leiden University, The Netherlands

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

My career path is not that long. After finishing my studies and already having made contact with the LfA, it was quite an easy choice to try for a PhD at the LfA. So far I have not faced that many difficulties, and I really hope it stays that way! As for guidance, I think the fun I had and interest I gained during my bachelor project, really made me enthusiastic to do more research at the LfA.

What are your current research goals?

Currently, I'm unravelling the mysteries of nitrogen substituted PAHs (PANHs). This type of molecule has been shown to match very well with the aromatic infrared bands (AIBs). I believe these molecules have been neglected with regards to AIB research and should gain more priority. My goal would be to show the world that these molecules are worth studying, and therewith hopefully convince others to study them.

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

I think there are still many questions that are unanswered, but close to my heart would be the origin of AIBs. So much of the same infrared features in such a vastly different universe is almost unthinkable, yet it is there. I think we do have some very good ideas for the origin of AIBs, but I still think there is much more to discover.

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 always try to be as straight forward and honest as possible. I've noticed that good communication is always in your benefit and that of the other, and thus will benefit your project. Also, I think it is important not to forget that every researcher is (just) a human being.

The thing that I like most about these interactions and collaborations is always the cultural differences. These can really inspire me and I also just like discovering new things I never heard about. For example, I recently ate some delicious Indian *dosa*, which I'd never have eaten if it wasn't for my collaborators.

What was the most important advice somebody gave you?

A dear friend of mine once spoke the wise words: "Life only starts outside of your comfort zone." I try to live by those words as often as possible.

How do you balance your professional and personal life?

When I'm at home, no more work. Although sometimes I need to have meetings with people on the other side of the world, so then a little work is done when I'm at home. But I always try to compensate that by leaving earlier, or arriving later. If I could give a tip for a nice work/life balance: **don't put your work email on your phone!**

What do you do outside of work?

I love to solve puzzles (hence the PhD I guess), so outside of work I love to do bouldering, which is basically puzzling with your entire body, and make crossword puzzles. Also, I occasionally play puzzling music on my fretless bass. When I don't want to puzzle and simply chill out, I play some video games, and I swear that these involve no puzzles.

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

A while back I gave a presentation to master students about how it is to do a PhD. What I noticed is that a lot of them underestimated the amount of luck that is involved in getting a PhD position. There is a certain chance that not all applications will lead to a PhD position and to be honest I think most won't. So, don't be defeated if you've heard "no" a couple of times. It's not because you're not good enough, it's probably because you're just out of luck that day.

To finish off this interview, in this issue of the AstroPAH newsletter two of my works can be found on **page 11 and 13**. So, if you're interested in PANHs, be sure to give it a read!



Abstracts

Diamond phase in space and possibility of its spectroscopic detection

A. A. Shiryaev¹

¹Institute of Physical Chemistry and Electrochemistry RAS, Moscow, Russia

Eventual presence of diamond carbon allotrope in space is discussed in numerous theoretical and experimental studies. The review summarises principal mechanisms of nanodiamond formation and experimental results of spectroscopic and structural investigations of nano- and microdiamonds extracted from meteorites. Size dependence of diamond spectroscopic properties is discussed. Infrared spectroscopy allows detection of C-H bonds on surfaces of hot nanodiamond grains. Spectroscopic observation of nitrogen-related point defects in nanodiamonds is very challenging; moreover, such defects were never observed in nanodiamonds from meteorites. At the same time, photoluminescence and, eventually, absorption, of some impurity-related defects, in particular, of silicon-vacancy (SiV) center, observed in real meteoritic nanodiamonds, opens a possibility of diamond detection in astronomical observations.

E-mail: a.shiryaev@mail.ru

Accepted to Physics Uspekhi

<http://arxiv.org/abs/2405.17584>

Metallofullerenes as potential candidates for the explanation of astrophysical phenomena

Ransel Barzaga^{1,3} and Gao-Lei Hou²

¹Instituto de Astrofísica de Canarias, Spain

²MOE Key Laboratory for Non-Equilibrium Synthesis and Modulation of Condensed Matter, School of Physics, Xian Jiaotong University, China

³Departamento de Astrofísica, Universidad de La Laguna (ULL), Spain

Detection of complex organic species in space has been one of the biggest challenges of the astrophysical community since the beginning of space exploration, with C₆₀-fullerene representing one of the largest molecules so far detected. The presence of small metal-containing organic molecules, like MgNC or CaCN, in space, promoted the idea that C₆₀ may also interact with metals and form metallofullerenes based on the fact that in certain circumstellar and interstellar environments, the ingredients for the formation of metallofullerenes, *i.e.*, metal and fullerenes, are abundant. In this perspective, we summarized the current effort to explore the presence of metallofullerenes in space, which started soon after the discovery of fullerenes about 40 years ago. Several implications of astrophysical phenomena were briefly discussed and shown to be addressable as the possible consequence of metallofullerenes' presence. We highlighted the spectral fingerprints that might be followed to achieve the future detection of cosmic metallofullerenes from a combined effort of laboratory and quantum chemical calculations. These results are expected to gain great importance with the James Webb Space Telescope (JWST), whose capability of unprecedented high sensitivity and high spectral resolution in the far- to mid-infrared range could aid the unequivocal detection of metallofullerenes in space.

E-mail: gaolei.hou@xjtu.edu.cn

Physical Chemistry Chemical Physics, **26**, 13622-13633 (2024)

<https://doi.org/10.1039/D4CP00146J>

Investigating H-atom reactions in small PAHs with imperfect aromaticity: A combined experimental and computational study of indene (C₉H₈) and indane (C₉H₁₀)

Anita Schneiker^{1,2,3}, Sándor Góbi^{1,2}, Gopi Ragupathy^{1,a}, Barbara Keresztes^{1,2,3}, Gábor Bazsó⁴, and György Tarczay^{1,2,5}

¹MTA-ELTE Lendület Laboratory Astrochemistry Research Group, Institute of Chemistry, ELTE Eötvös Loránd University, Budapest, Hungary

²Laboratory of Molecular Spectroscopy, Institute of Chemistry, ELTE Eötvös Loránd University, Budapest, Hungary

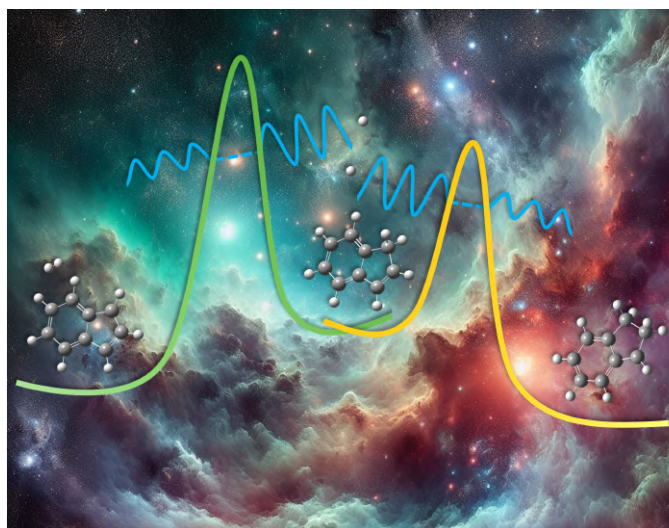
³George Hevesy Doctoral School, ELTE Eötvös Loránd University, Budapest, Hungary

⁴Wigner Research Centre for Physics, Budapest, Hungary

⁵Centre for Astrophysics and Space Science, ELTE Eötvös Loránd University, Budapest, Hungary

^aPresent address: School of Advanced Sciences (SAS), Vellore Institute of Technology, Vellore Campus, Vellore, India

Polycyclic aromatic hydrocarbons (PAHs) are widely recognized as catalysts for interstellar H₂ formation. Extensive exploration into the catalytic potential of various PAHs has encompassed both theoretical investigations and experimental studies. In the present study, we focused on studying the reactivity of an imperfect aromatic molecule, indene (C₉H₈), and its hydrogenated counterpart, indane (C₉H₁₀), as potential catalysts for H₂ formation within the interstellar medium (ISM). The reactions of these molecules with H atoms at 3.1 K were investigated experimentally using the *para*-H₂ matrix isolation technique. Our experimental results demonstrate that both indene and indane are reactive toward H atoms. Indene can participate in H-atom-abstraction and H-atom-addition reactions, whereas indane primarily undergoes H-atom-abstraction reactions. The H-atom-abstraction reaction of indene results in the formation of the 1-indenyl radical (**R1**) (C₉H₇) and H₂ molecule. Simultaneously, an H-atom-addition reaction forms the 1,2-dihydro-indene-3-yl radical (**R2**) (C₉H₉). Experiments also reveal that the H-atom-abstraction reaction of indane also produces the **R2** radical. To the best of our knowledge, this study represents the first reporting of the IR spectra of **R1** and **R2** radicals. The experimental results, combined with theoretical findings, suggest that indane and indene may play a role in the catalytic formation of interstellar H₂. Furthermore, these results imply a quasi-equilibrium between the investigated molecules and the formed radicals via H-atom-addition and H-atom-abstraction reactions.



E-mail: gyorgy.tarczay@ttk.elte.hu

Journal of Chemical Physics, **160**, 214303 (2024)

<https://doi.org/10.1063/5.0209722>

Photoprocessing of cationic triazacoronene: Dissociation characteristics of polycyclic aromatic nitrogen heterocycles in interstellar environments

Domenik Schleier^{1,2}, Jerry Kamer¹, Andy Jiao³, Grégory F. Schneider³, Harold Linnartz¹, and Jordy Bouwman^{4,5,6}

¹Laboratory for Astrophysics, Leiden Observatory, Leiden University, Leiden, The Netherlands.

²Lehrstuhl Technische Thermodynamik, Fakultät für Maschinenbau, Universität Paderborn, Paderborn, Germany.

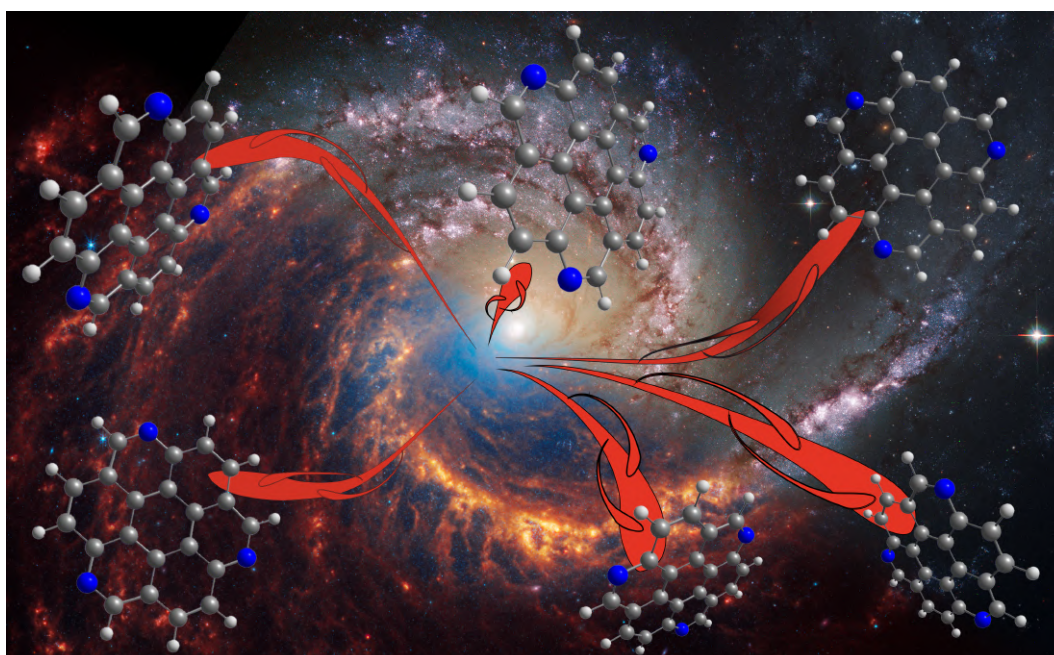
³Leiden Institute of Chemistry, Leiden University, Leiden, The Netherlands.

⁴Laboratory for Atmospheric and Space Physics, University of Colorado, Boulder, CO, USA.

⁵Department of Chemistry, University of Colorado, Boulder, CO, USA.

⁶Institute for Modeling Plasma, Atmospheres and Cosmic Dust (IMPACT), NASA/SSERVI, Boulder, CO, USA.

Polycyclic aromatic nitrogen heterocycles (PANHs) are present in various astronomical environments where they are subjected to intense radiation. Their photodissociation pathways give crucial insights into the cycle of matter in the universe, yet so far only the dissociation characteristics of few PANHs have been investigated. Moreover, most experiments use single photon techniques that only reveal the initial dissociation step, and are thus unsuited to replicate astronomical environments and timescales. In this work, we use the Instrument for the Photodynamics of PAHs (i-PoP) at the Laboratory for Astrophysics to simulate the interstellar photodissociation of a model PANH, cationic triazacoronene (TAC^+ , $\text{C}_{21}\text{H}_9\text{N}_3$). Comparing the observed fragments to similar PAHs such as the isoelectronic coronene can give mechanistic insight into PAH dissociation. For coronene the major dissociation products were found to be C_9H^+ , C_{10}^+ , and C_{11}^+ . In contrast, fragmentation in TAC^+ is initiated by up to three HCN losses often in combination with H- or H_2 losses. At lower masses the fragments show similarities to comparable PAHs like coronene, but for TAC^+ the inclusion of nitrogen atoms into the ionic fragments in the form of e.g. (di)cyanopolynes is also observed. These nitrogen-containing species may be important tracers of regions in interstellar space where interstellar PANHs are being photodissociated.



E-mail: domenik.schleier@uni-paderborn.de, jordy.bouwman@colorado.edu

Physical Chemistry Chemical Physics, **26**, 15547 (2024)

<https://dx.doi.org/10.1039/d4cp01387e>

<https://pubs.rsc.org/en/content/articlepdf/2024/cp/d4cp01387e>

Exploring the scaling factors for infrared modes of PANHs - A case study on cationic 3-Azafluoranthene⁺ and protonated 3-Azafluoranthene

Domenik Schleier^{1,2}, Jerry Kamer¹, J. Martens³, G. Berden³, J. Oomens^{3,4}, and Jordy Bouwman^{5,6,7}

¹Laboratory for Astrophysics, Leiden Observatory, Leiden University, Leiden, The Netherlands.

²Lehrstuhl Technische Thermodynamik, Fakultät für Maschinenbau, Universität Paderborn, Paderborn, Germany

³Institute for Molecules and Materials, FELIX Laboratory, Radboud University, Nijmegen, The Netherlands

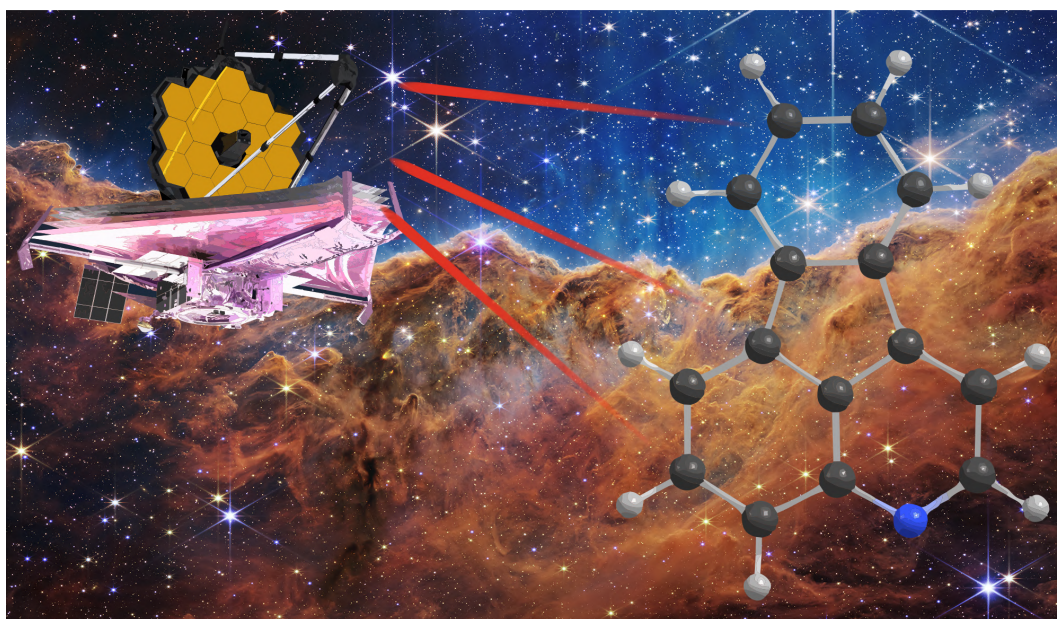
⁴University of Amsterdam, The Netherlands

⁵Laboratory for Atmospheric and Space Physics, University of Colorado, Boulder, CO, USA

⁶Department of Chemistry, University of Colorado, Boulder, CO, USA

⁷Institute for Modeling Plasma, Atmospheres and Cosmic Dust (IMPACT), NASA/SSERVI, Boulder, CO, USA

Infrared (IR) emission bands by interstellar Polycyclic Aromatic Hydrocarbons (PAHs) and Polycyclic Aromatic Nitrogen Heterocycles (PANHs) are observed towards a large variety of interstellar objects and offer detailed insights into the chemistry and physics of the interstellar medium. The analysis of the emission bands, and thus the interpretation of the molecular characteristics of the carriers, heavily relies on the use of density functional theory (DFT) calculated IR spectra. However, there are significant challenges in accurately predicting the experimental IR band positions, particularly for PANH emission vibrational modes around 6 μm . In this work, we present gas-phase mid-infrared (mid-IR) spectra of cationic 3-azafluoranthene (**3AF⁺**) and its hydrogenated congener (**3AFH⁺**) to investigate their experimental IR band positions in relation to DFT calculated bands. The experimental spectra are compared to DFT simulated spectra, where different approaches were followed to correct for anharmonicities. The best agreement is achieved by scaling frequencies of modes with large nitrogen displacements with a different factor. Even though our findings might be limited to a small number of PANH structures, they indicate, that nitrogen atom incorporation needs to be accounted for by carefully adjusting the corresponding scaling factors while computing IR spectra of PANHs on DFT level.



E-mail: domenik.schleier@uni-paderborn.de, jordy.bouwman@colorado.edu

Accepted to ChemPhysChem (2024)

<https://doi.org/10.1002/cphc.202300915>

<https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/cphc.202300915>

AstroPAH Newsletter

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

astropah@strw.leidenuniv.nl

Next issue: 25 July 2024

Submission deadline: 12 July 2024