



AstropAH

A Newsletter on Astronomical PAHs

Issue 84 • December 2021

The James Webb Space Telescope



Editorial

Dear Colleagues,

Welcome to the last AstroPAH of 2021!

As you can see in our cover, we are anxious for the James Webb Space Telescope launch and all the new science it is going to produce.

We are ending this year with very interesting abstracts, announcements of a PhD position in Germany and a call for abstracts for a session at AbSciCon 2022 focused on "Titan as a Prebiotic Laboratory".

Our In Focus this month is a greeting card with our wishes for a great new year to you all!

We welcome your contributions! In addition to abstracts and announcements, you can also propose ideas for In Focus and Picture of the Month. AstroPAH would love to advertise that great project you are conducting! Email us at astropah@strw.leidenuniv.nl.

Thank you for following AstroPAH. We will be back with our next newsletter in February 2022.

The Editorial Team

**Next issue: 17 February 2022.
Submission deadline: 4 February 2022.**

AstroPAH Newsletter

Editorial Board:

Editor-in-Chief

Prof. Alexander Tielens

Leiden Observatory
(The Netherlands)

Executive Editors

Dr. Isabel Aleman

Institute of Physics and Chemistry,
UNIFEI (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

Leiden Observatory
(The Netherlands)

Dr. Donatella Loru

Deutsches Elektronen-Synchrotron
(Germany)

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
Happy New Year!	4
Recent Papers	5
Announcements	10

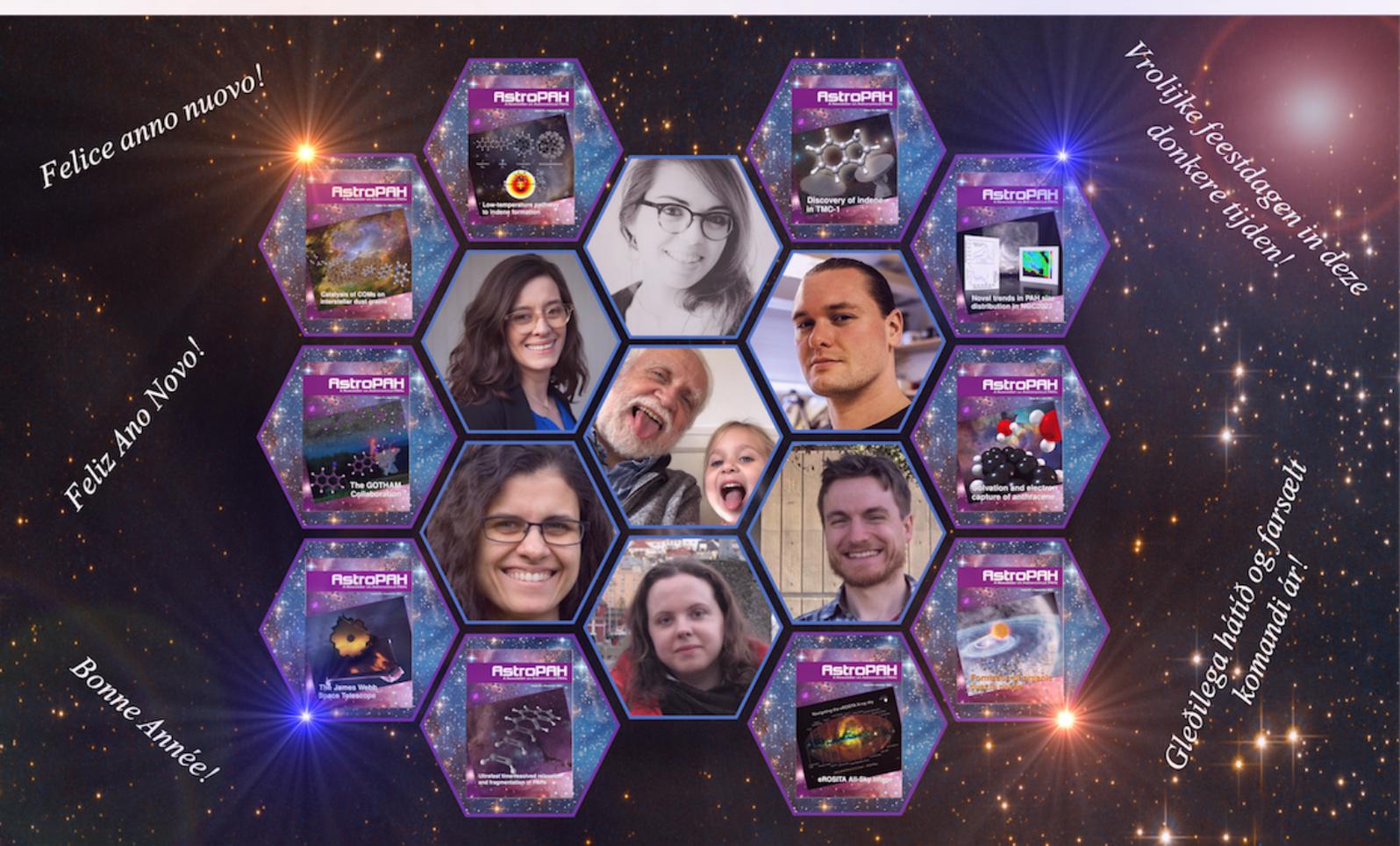
PAH Picture of the Month

Artist conception of the James Webb Space Telescope. Check the countdown to the observatory's launch following [this link](#).

Credits: ✨ Adriana Manrique Gutierrez, NASA Animator.

Happy New Year 2022!

from the AstroPAH Editorial Board



Background picture credit: ESA/Hubble & NASA. Acknowledgements: R. Sahai (Jet Propulsion Laboratory), Serge Meunier
Background hexagons credit: NASA, ESA, and the Hubble Heritage Team (STScI/AURA)-ESA/Hubble Collaboration



Abstracts

The Ionization and Destruction of Polycyclic Aromatic Hydrocarbons in Powerful Quasars

Yanxia Xie¹ and Luis C. Ho^{1,2}

¹Kavli Institute for Astronomy and Astrophysics, Peking University, Beijing, China

²Department of Astronomy, School of Physics, Peking University, Beijing, China

We reanalyze the mid-infrared (5–40 μm) Spitzer spectra of 86 low-redshift ($z < 0.5$) Palomar-Green quasars to investigate the nature of polycyclic aromatic hydrocarbon (PAH) emission and its utility as a star formation rate (SFR) indicator for the host galaxies of luminous active galactic nuclei (AGNs). We decompose the spectra with our recently developed template-fitting technique to measure PAH fluxes and upper limits, which we interpret using mock spectra that simulate the effects of AGN dilution. While luminous quasars can severely dilute and affect the detectability of emission lines, PAHs are intrinsically weak in some sources that are otherwise gas-rich and vigorously forming stars, conclusively demonstrating that powerful AGNs destroy PAH molecules. Comparing PAH-based SFRs with independent SFRs derived from the mid-infrared fine-structure neon lines and the total infrared luminosity reveals that PAHs can trace star formation activity in quasars with bolometric luminosities $\lesssim 10^{46}$ erg s⁻¹, but increasingly underestimate the SFR for more powerful quasars, typically by ~ 0.5 dex. Relative to star-forming galaxies and low-luminosity AGNs, quasars have a comparable PAH 11.3 μm /7.7 μm ratio but characteristically lower ratios of 6.2 μm /7.7 μm , 8.6 μm /7.7 μm , and 11.3 μm /17.0 μm . We suggest that these trends indicate that powerful AGNs preferentially destroy small grains and enhance the PAH ionization fraction.

E-mail: yanxia.xie@pku.edu.cn

The Astrophysical Journal, Accepted (2021)

<https://arxiv.org/abs/2110.09705v1>

Formation and growth mechanisms of polycyclic aromatic hydrocarbons: A mini-review

Edina Reizer^{1,2}, Béla Viskolcz^{1,2} and Béla Fiser^{1,2,3}

¹Institute of Chemistry, University of Miskolc, H-3515, Miskolc, Miskolc-Egyetemváros, Hungary

²Higher Education and Industrial Cooperation Centre, University of Miskolc, H-3515, Miskolc-Egyetemváros, Hungary

³Ferenc Rákóczi II. Transcarpathian Hungarian College of Higher Education, UA, 90200, Beregszász, Transcarpathia, Ukraine

Polycyclic aromatic hydrocarbons (PAHs) are mostly formed during the incomplete combustion of organic materials, but their importance and presence in materials science, and astrochemistry has also been proven. These carcinogenic persistent organic pollutants are essential in the formation of combustion generated particles as well. Due to their significant impact on the environment and human health, to understand the formation and growth of PAHs is essential. Therefore, the most important growth mechanisms are reviewed, and presented here from the past four decades (1981–2021) to initiate discussions from a new perspective. Although, the collected and analyzed observations are derived from both experimental, and computational studies, it is neither a systematic nor a comprehensive review. Nevertheless, the mechanisms were divided into three main categories, acetylene additions (e.g. HACA), vinylacetylene additions (HAVA), and radical reactions, and discussed accordingly.

E-mail: fiser@uni-miskolc.hu

Chemosphere, **132793** (2021)

<https://www.sciencedirect.com/science/article/pii/S0045653521032653>

Radiation-induced closure of the second aromatic ring: Possible way to PAH starting from a styrene-acetylene complex

Mariia A. Lukianova¹ and Vladimir I. Feldman¹

¹Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

The radiation-induced assembling of the naphthalene molecule was first directly observed under X-ray irradiation of the isolated styrene-acetylene complex in a solid krypton matrix at 6 K using FTIR spectroscopy. The observation of naphthalene radical cation in the presence of electron scavenger suggests a cationic pathway of this reaction. This finding makes it possible to propose a new mechanism for the formation of polycyclic aromatic hydrocarbons in astrochemical ices.

E-mail: feldman@rad.chem.msu.ru

Radiation Physics and Chemistry, **191**:109847 (2021)

<https://doi.org/10.1016/j.radphyschem.2021.109847>

Polycyclic Aromatic Hydrocarbons in Seyfert and star-forming galaxies

I. García-Bernete¹, D. Rigopoulou¹, A. Alonso-Herrero², M. Pereira-Santaella³, P.F. Roche¹ and B. Kerkeni^{1,4,5}

¹Department of Physics, University of Oxford, Oxford OX1 3RH, UK

²Centro de Astrobiología, CSIC-INTA, ESAC Campus, E-28692, Villanueva de la Cañada, Madrid, Spain

³Centro de Astrobiología, CSIC-INTA, Crta. de Torrejón a Ajalvir, E-28880 Torrejón de Ardoz, Madrid, Spain

⁴Département de Physique, LPMC, Faculté des Sciences de Tunis, Université de Tunis, Tunis 2092, Tunisia

⁵ISAMM, Université de la Manouba, La Manouba 2010 Tunisia

Polycyclic Aromatic Hydrocarbons (PAHs) are carbon-based molecules resulting from the union of aromatic rings and related species, which are likely responsible for strong infrared emission features. In this work, using a sample of 50 Seyfert galaxies ($D_L < 100$ Mpc) we compare the circumnuclear (inner kpc) PAH emission of AGN to that of a control sample of star-forming galaxies (22 luminous infrared galaxies and 30 H II galaxies), and investigate the differences between central and extended PAH emission. Using Spitzer/InfraRed Spectrograph spectral data of Seyfert and star-forming galaxies and newly developed PAH diagnostic model grids, derived from theoretical spectra, we compare the predicted and observed PAH ratios. We find that star-forming galaxies and AGN-dominated systems are located in different regions of the PAH diagnostic diagrams. This suggests that not only are the size and charge of the PAH molecules different, but also the nature and hardness of the radiation field that excite them. We find tentative evidence that PAH ratios in AGN-dominated systems are consistent with emission from larger PAH molecules ($N_c > 300-400$) as well as neutral species. By subtracting the spectrum of the central source from the total, we compare the PAH emission in the central vs extended region of a small sample of AGN. In contrast to the findings for the central regions of AGN-dominated systems, the PAH ratios measured in the extended regions of both type 1 and type 2 Seyfert galaxies can be explained assuming similar PAH molecular size distribution and ionized fractions of molecules to those seen in central regions of star-forming galaxies ($100 < N_c < 300$).

E-mail: igbernete@gmail.com

Monthly Notices of the Royal Astronomical Society, **509**, 4256-4275 (2022)

<https://doi.org/10.1093/mnras/stab3127>

Measurements of Ortho-to-para Nuclear Spin Conversion of H₂ on Low-temperature Carbonaceous Grain Analogs: Diamond-like Carbon and Graphite

Masashi Tsuge¹, Akira Kouchi¹ and Naoki Watanabe¹

¹Institute of Low Temperature Science, Hokkaido University, Sapporo, Japan

Hydrogen molecules have two nuclear spin isomers: ortho-H₂ and para-H₂. The ortho-to-para ratio (OPR) is known to affect chemical evolution as well as gas dynamics in space. Therefore, understanding the mechanism of OPR variation in astrophysical environments is important. In this work, the nuclear spin conversion (NSC) processes of H₂ molecules on diamond-like carbon and graphite surfaces are investigated experimentally by employing temperature-programmed desorption and resonance-enhanced multiphoton ionization methods. For the diamond-like carbon surface, the NSC time constants were determined at temperatures of 10–18 K and from 3900 ± 800 s at 10 K to 750 ± 40 s at 18 K. Similar NSC time constants and temperature dependence were observed for a graphite surface, indicating that bonding motifs (sp³ or sp² hybridization) have little effect on the NSC rates.

E-mail: tsuge@lowtem.hokudai.ac.jp

The Astrophysical Journal, **923**:71 (2021)

<https://iopscience.iop.org/article/10.3847/1538-4357/ac2a33>

<https://arxiv.org/abs/2109.12734>



Announcements

PhD position in Molecular Physics / Physical Chemistry / Laboratory Astrophysics

Advertised by Prof. Otto Dopfer

A **PhD position (3 years)**, fully funded by the German Science Foundation (DFG), is available in the **laser molecular spectroscopy group** of **Otto Dopfer** at **Technische Universität Berlin, Germany**. This project deals with the laser spectroscopic and quantum chemical characterization of the geometric, electronic, optical and chemical properties of aromatic cluster cations and their microsolvated solvated clusters in the context of intermolecular forces, solvation effects, interstellar chemistry, combustion, and materials science.

Further information about the group and its projects (and recent publications) is available at: https://www.ioap.tu-berlin.de/menue/arbeitsgruppen/ag_dopfer/ A key paper for this particular project is: *Aromatic Charge Resonance Interaction Probed by Infrared Spectroscopy*, K. Chatterjee, Y. Matsumoto, O. Dopfer, *Angew. Chem. Int. Ed.* 58, 3351 (2019), www.doi.org/10.1002/anie.201811432. Interested candidates send their application to Prof. Otto Dopfer (dopfer@physik.tu-berlin.de). Evaluation of the applications will begin January 15, 2022 and continue until the position is filled. Desired starting date is as soon as possible (but negotiable to some extent). Being a European capital, Berlin offers an exciting international scientific and cultural environment.

Deadline: January 15, 2022

E-mail for contact: dopfer@physik.tu-berlin.de

Webpage: https://www.ioap.tu-berlin.de/menue/arbeitsgruppen/ag_dopfer/

AbSciCon 2022 Session

Titan as a Prebiotic Laboratory

Advertised by S. MacKenzie, C. Neish, E. Sciamma-O'Brien

Please consider submitting an abstract to our Titan-focused AbSciCon 2022 session, “**Titan as a Prebiotic Laboratory**”.

From the ionosphere to its rocky core, Titan offers a unique opportunity to explore pathways for prebiotic chemistry. In its N_2 - CH_4 -based atmosphere, photolytic and radiolytic chemistry creates a plethora of organic compounds, including large, complex haze particles. These compounds eventually make their way to the surface where geological processes rework and redistribute Titan’s prebiotic manna. Primordial organic material in the interior may be dissolved in the subsurface ocean and serve as the ultimate source of Titan’s atmospheric methane. Whether either of these realms —atmosphere, surface, interior— interacts with the other through the icy crust remains unknown. As the most organic-rich ocean world in the solar system beyond Earth, Titan represents a compelling world to investigate prebiotic chemistry. This session will explore how investigating Titan’s different realms provides new insight into our understanding of the limits of prebiotic evolution. Results from remote sensing data, laboratory experiments, modeling, ground-based observations are all welcome.

Deadline: January 19, 2022

Webpage: <https://agu.confex.com/agu/abscicon21/prelim.cgi/Session/112042>

AstroPAH Newsletter

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

astropah@strw.leidenuniv.nl

Next issue: 17 February 2022

Submission deadline: 4 February 2022