

AstropAH

A Newsletter on Astronomical PAHs

Issue 105 • February 2024



Prof. Harold V. J. Linnartz
1965 - 2023



Editorial

Dear Colleagues,

Welcome to our 105th volume. Sadly, we recently heard about the passing of Prof. Harold V. J. Linnartz on the night of December 31. Prof. Linnartz inspired all of us one way or another. This is why we have dedicated our Picture of the Month and In Focus to him. He will be missed! Harold's obituary is available [here](#). If you wish, you can leave a message in the online condolence register: [condolence register](#). Feel free to read more about Harold's life in our interview with him from [February 2018](#).

We have an abundance of abstracts for new publications ranging from water formation on carbonaceous dust to JWST observations and X-ray spectroscopy. As always, thank you for your dedication!

Two meeting announcements are featured this month, with the 2nd COST NanoSpace "Carbon molecular nanostructures in space" (free registration + abstract submission deadline March 15th), and the EAS2024 "European Laboratory Astrophysics in the JWST Era" with an early bird registration deadline on February 26th.

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: 21 March 2024.
Submission deadline: 8 March 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	5
Meetings	22

PAH Picture of the Month

In memory of Prof. Harold V. J. Linnartz
(1965-2023).

Tribute to Harold V. J. Linnartz

On New Year's eve, our friend and colleague, Harold Linnartz suddenly passed away at the age of 58. He is survived by his wife, Helga, and his children, Anne and Thomas.

Harold was the head of the Astrophysics Laboratory and also served as the education director of Leiden Observatory. Harold was a leader in the field of molecular astrophysics, specifically in the areas of molecular spectroscopy and its application to the carriers of the Diffuse Interstellar Bands, in the spectroscopy and reactions of low temperature solids as relevant to interstellar ices, and in the photochemistry of PAHs as they speak to the challenges of the AIBs. Harold was an excellent group leader and over his career, Harold supervised the research of some 50 graduate students and postdocs, providing inspiration and advice on their studies and their subsequent careers. We all fondly remember his "paper cakes" that celebrated the acceptance of a scientific paper of which there were many.

Throughout his career, Harold Linnartz focused on unlocking the chemistry of the heavens. As a spectroscopist *pur sang*, shining light on molecules in space was one of his guiding principles. Fathom the behavior of molecules under the extreme conditions of space was another. Harold had many ideas to continue his research in these areas over the coming years, but it is not to be.

We will miss him dearly as a colleague, as a mentor, and, in particular, as a friend.



*Photo: courtesy of Ewine van Dishoeck
(06/2023)*



Abstracts

Experimental H₂O formation on carbonaceous dust grains at temperatures up to 85 K

Francesco Grieco^{1,2}, François Dulieu¹, Ilse De Looze², and Saoud Baouche¹

¹CY Cergy Paris Université, Observatoire de Paris, PSL University, Sorbonne Université, CNRS, LERMA, Cergy, France

²University of Ghent, Department of Physics and Astronomy, Ghent, Belgium

Water represents the main component of the icy mantles on dust grains, it is of extreme importance for the formation of new species and it represents the main component for life. Water is observed both in the gas-phase and frozen in the ISM, where the solid-phase formation route has been proven essential to explain abundances in molecular clouds. So far, experiments have focused on very low temperatures (around 10 K). We present the experimental evidence of solid water formation on coronene, PAH-like surface, for a higher range of temperatures. Water is efficiently formed up to 85 K through the interaction of oxygen and hydrogen atomic beams with a carbonaceous grain analogue. The beams are aimed towards the surface connected to a cryostat exploring temperatures from 10 K to 100 K. The results are obtained with a QMS and analyzed through a temperature-programmed desorption technique. We observe an efficient water formation on coronene from 10 K up to 85 K mimicking the temperature conditions from the dense ISM to translucent regions, where the ice mantle onset is supposed to start. The results show the catalytic nature of coronene and the role of chemisorption processes. The formation of the icy mantles could be happening in less dense and warmer environments, helping explaining oxygen depletion in the ISM. The findings have several applications such as the disappearance of PAHs in translucent regions and the snowlines of protoplanetary disks. We stress on how JWST projects characterizing PAHs can be combined with H₂O observations to study water formation at warm temperatures.

E-mail: Francesco.Grieco@UGent.be

Mon. Not. R. Astron. Soc., **527**(4), 10604–10614 (2024)

<https://doi.org/10.1093/mnras/stad3854>

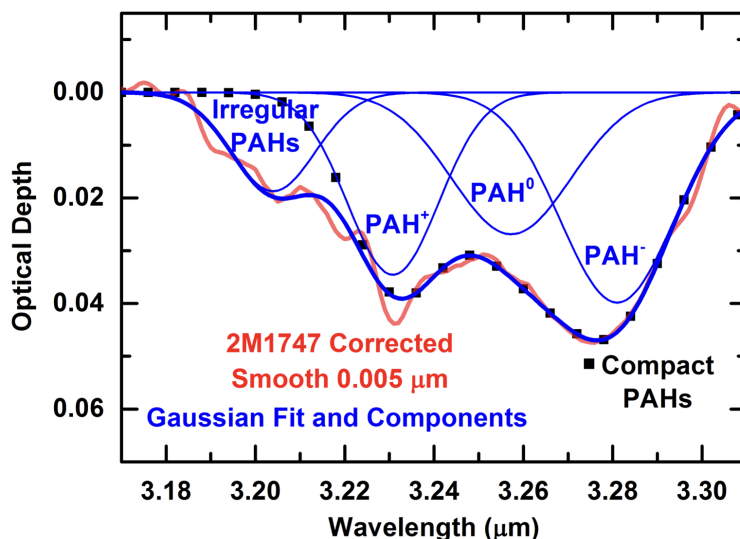
Analysis of the 3.2–3.3 μm Interstellar Absorption Feature on Three Milky Way Sightlines

L. S. Bernstein¹ and T. R. Geballe²

¹63 Forest Glen Ln., Topsham, ME 04086, USA

²Gemini Observatory/NSF's NOIRLab, 670 N. A'ohoku Pl., Hilo, HI 96720 USA

We report new analyses of spectra of the 3.2–3.3 μm absorption feature observed in the diffuse interstellar medium toward three Milky Way sources: 2MASS *J*17470898–829561 (2M1747) and the Quintuplet Cluster, both located in the Galactic center, and Cygnus OB2-12. The 3.2–3.3 μm interval coincides with the CH-stretching region for compact polycyclic aromatic hydrocarbons (PAHs). We focus on the 2M1747 spectrum. Its published optical depth spectrum contains residual telluric transmission features, which arise from the 0.06 difference in mean airmasses between the observations of the source and its telluric standard star. We corrected the published spectrum by adding the airmass residual optical depth spectrum. The corrected spectrum is well fit by a superposition of four Gaussians. The absorption spectra of the other two sources were also fit by four Gaussians, with similar central wavelengths, widths, and relative peak opacities. We associate the three longer wavelength Gaussians covering the 3.2–3.3 μm interval with compact PAHs in positive, neutral, and negative charge states. We identify the shortest wavelength Gaussian, near 3.21 μm , with irregularly-shaped PAHs. Constraints imposed by spectral smoothness on the corrected 2M1747 spectrum, augmented by a PAH cluster formation model for post-asymptotic giant branch stars, suggests that $> 99\%$ of the PAHs in the diffuse interstellar medium reside in small clusters. This study supports the PAH hypothesis, and suggests that a family of primarily compact PAHs with a $\text{C}_{66}\text{H}_{20}$ (circumvalene) parent is consistent with the observed mid- infrared and ultraviolet interstellar absorption spectrum.



Comparison of atmosphere-corrected, smoothed 2M1747 spectrum (red curve) and four-Gaussian fit (thick blue curve). Also displayed are the individual component Gaussians in the fit (thin blue lines). The component Gaussians can be associated with specific PAH symmetry types, compact and irregular, and charge states, cationic, neutral, and anionic as labeled (see Section 3.2 for details). The sum of the compact PAHs is denoted by the thin black curve passing through the filled squares

E-mail: tom.geballe@noirlab.edu

Astrophys. J., accepted

<https://arxiv.org/pdf/2312.03086.pdf>

JWST observations of the Ring Nebula (NGC 6720): I. Imaging of the rings, globules, and arcs

R. Wesson^{1,2}, Mikako Matsuura¹, Albert A. Zijlstra³, Kevin Volk⁴, Patrick J. Kavanagh^{5,6}, Guillermo García-Segura⁷, I. McDonald^{3,8}, Raghvendra Sahai⁹, M. J. Barlow², Nick L. J. Cox¹⁰, Jeronimo Bernard-Salas^{10,11}, Isabel Aleman^{12,13}, Jan Cami^{14,15,16}, Nicholas Clark^{14,15}, Harriet L. Dinerstein¹⁷, K. Justtanont¹⁸, Kyle F. Kaplan¹⁷, A. Manchado^{19,20,21}, Els Peeters^{14,15,16}, Griet C. Van de Steene²², and Peter A. M. van Hoof²²

¹Cardiff Hub for Astrophysics Research and Technology (CHART), School of Physics and Astronomy, Cardiff University, Cardiff, UK

²Department of Physics and Astronomy, University College London, London, United Kingdom

³Jodrell Bank Centre for Astrophysics, Department of Physics & Astronomy, The University of Manchester, Manchester, UK

⁴Space Telescope Science Institute, Baltimore, MD, USA

⁵Department of Experimental Physics, Maynooth University, Maynooth, Co Kildare, Ireland

⁶School of Cosmic Physics, Dublin Institute for Advanced Studies, Dublin, Ireland

⁷Instituto de Astronomía, Universidad Nacional Autónoma de México, Ensenada, Mexico

⁸Department of Physical Sciences, The Open University, Milton Keynes, UK

⁹Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, USA

¹⁰ACRI-ST, Centred'Etudes et de Recherche de Grasse (CERGA), Grasse, France

¹¹INCLASS Common Laboratory, Grasse, France

¹²Department of Computer Science, Institute of Mathematics and Statistics, University of São Paulo, São Paulo, SP, Brazil

¹³Instituto de Física e Química, Universidade Federal de Itajubá, Itajubá, MG, Brazil

¹⁴Department of Physics and Astronomy, University of Western Ontario, London, Ontario, Canada

¹⁵Institute for Earth and Space Exploration, University of Western Ontario, London, Ontario, Canada

¹⁶SETI Institute, Mountain View, CA, USA

¹⁷University of Texas at Austin, Austin, TX, USA

¹⁸Chalmers University of Technology, Onsala Space Observatory, Onsala, Sweden

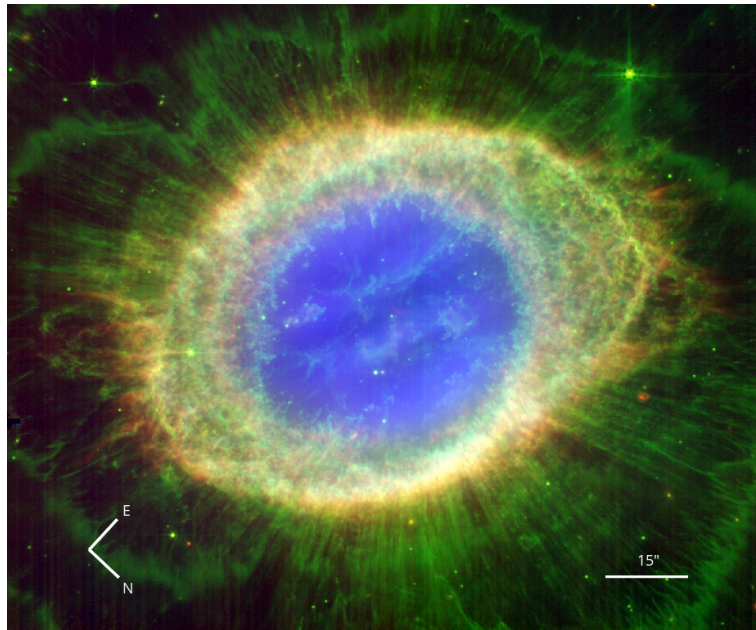
¹⁹Instituto de Astrofísica de Canarias, Tenerife, Spain

²⁰Departamento de Astrofísica, Universidad de La Laguna, Tenerife, Spain

²¹Consejo Superior de Investigaciones Científicas (CSIC), Spain

²²Royal Observatory of Belgium, Brussels, Belgium

We present *JWST* images of the well-known planetary nebula NGC 6720 (the Ring Nebula), covering wavelengths from 1.6 μm to 25 μm . The bright shell is strongly fragmented with some 20 000 dense globules, bright in H_2 , with a characteristic diameter of 0.2 arcsec and density $n_{\text{H}} \sim 10^5\text{--}10^6 \text{ cm}^{-3}$. The shell contains a narrow ring of polycyclic aromatic hydrocarbon (PAH) emission. H_2 is found throughout the shell and also in the halo. H_2 in the halo may be located on the swept-up walls of a biconal polar flow. The central cavity is filled with high ionization gas and shows two linear structures which we suggest are the edges of a biconal flow, seen in projection against the cavity. The central star is located 2 arcsec from the emission centroid of the cavity and shell. Linear features ('spikes') extend outward from the ring, pointing away from the central star. Hydrodynamical simulations reproduce the clumping and possibly the spikes. Around ten low-contrast, regularly spaced concentric arc-like features are present; they suggest orbital modulation by a low-mass companion with a period of about 280 yr. A previously known much wider companion is located at a projected separation of about 15 000 au; we show that it is an M2–M4 dwarf. NGC 6720 is therefore a triple star system. These features, including the multiplicity, are similar to those seen in the Southern Ring Nebula (NGC 3132) and may be a common aspect of such nebulae.



NGC 6720 JWST/MIRI composite (red: F1130W, green: F560W, blue: F2550W)

E-mail: rw@nebulousresearch.org

Mon. Not. R. Astron. Soc., **528**(2), 3392–3416 (2024)

<https://arxiv.org/abs/2308.09027>

The Atacama Cosmology Telescope: Galactic Dust Structure and the Cosmic PAH Background in Cross-correlation with WISE

Rodrigo Córdova Rosado¹, Brandon S. Hensley¹, Susan E. Clark^{2,3},
Adriaan J. Duivenvoorden⁴, Zachary Atkins⁵, Elia Stefano Battistelli⁶,
Steve K. Choi^{7,8}, Jo Dunkley^{5,1}, Carlos Hervías-Caimapo⁹, Zack Li¹⁰,
Thibaut Louis¹¹, Sigurd Naess¹², Lyman A. Page⁵, Bruce Partridge¹³,
Cristóbal Sifón¹⁴, Suzanne T. Staggs⁵, Cristian Vargas⁹, and Edward J.
Wollack¹⁵

¹Department of Astrophysical Sciences, Peyton Hall, Princeton University, Princeton, NJ, USA

²Department of Physics, Stanford University, Stanford, CA, USA

³Kavli Institute for Particle Astrophysics & Cosmology, Stanford University, Stanford, CA, USA

⁴Center for Computational Astrophysics, Flatiron Institute, New York, NY, USA

⁵Joseph Henry Laboratories of Physics, Jadwin Hall, Princeton University, Princeton, NJ, USA

⁶Sapienza University of Rome, Physics Department, Rome, Italy

⁷Department of Physics, Cornell University, Ithaca, NY, USA

⁸Department of Astronomy, Cornell University, Ithaca, NY, USA

⁹Instituto de Astrofísica and Centro de Astro-Ingeniería, Facultad de Física, Pontificia Universidad Católica de Chile, Macul, Santiago, Chile

¹⁰Canadian Institute for Theoretical Astrophysics, University of Toronto, Toronto, ON, Canada

¹¹Université Paris-Saclay, CNRS/IN2P3, IJCLab, Orsay, France

¹²Institute of Theoretical Astrophysics, University of Oslo, Norway

¹³Department of Physics and Astronomy, Haverford College, Haverford, PA, USA

¹⁴Instituto de Física, Pontificia Universidad Católica de Valparaíso, Valparaíso, Chile

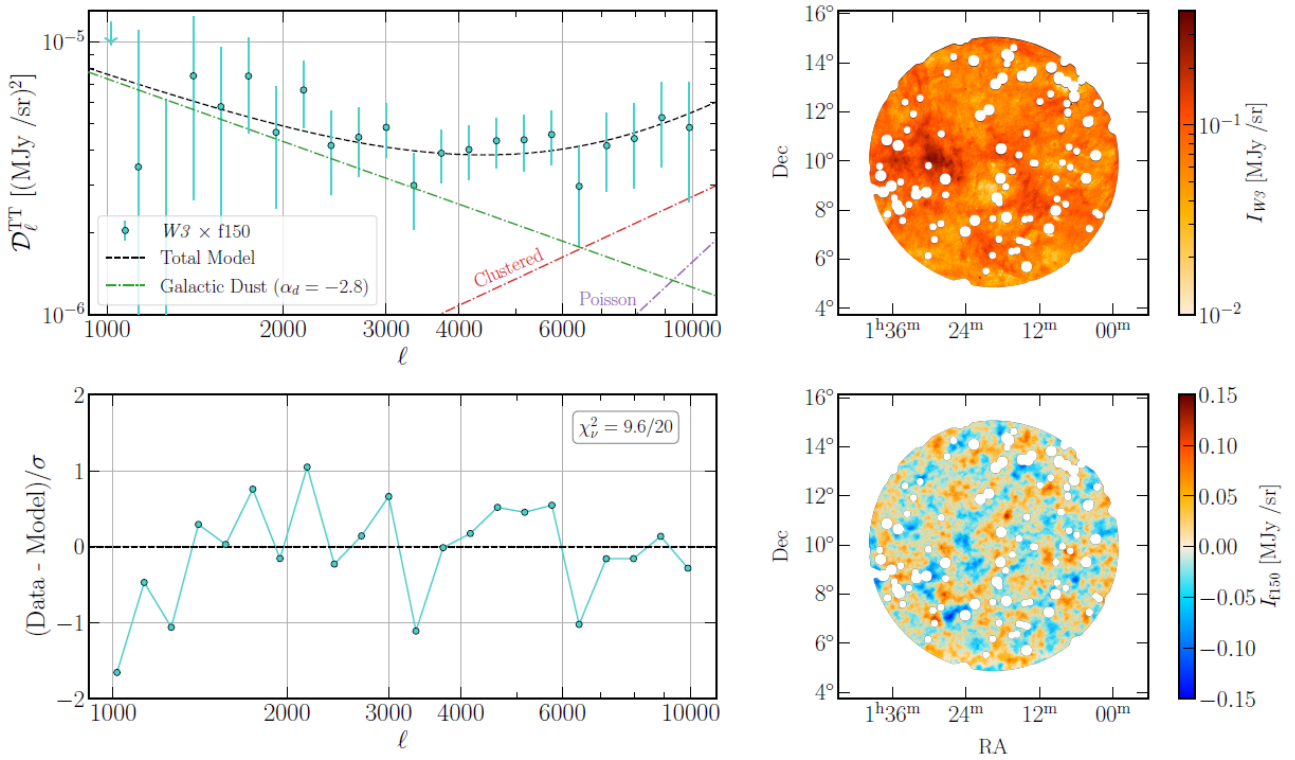
¹⁵NASA/Goddard Space Flight Center, Greenbelt, MD, USA

We present a cross-correlation analysis between 1' resolution total intensity and polarization observations from the Atacama Cosmology Telescope (ACT) at 150 and 220 GHz and 15'' mid-infrared photometry from the Wide-field Infrared Survey Explorer (WISE) over 107 $12.5^\circ \times 12.5^\circ$ patches of sky. We detect a spatially isotropic signal in the WISE \times ACT TT cross power spectrum at 30σ significance that we interpret as the correlation between the cosmic infrared background at ACT frequencies and polycyclic aromatic hydrocarbon (PAH) emission from galaxies in WISE, i.e., the cosmic PAH background. Within the Milky Way, the Galactic dust TT spectra are generally well-described by power laws in ℓ over the range $10^3 < \ell < 10^4$, but there is evidence both for variability in the power law index and for non-power law behavior in some regions. We measure a positive correlation between WISE total intensity and ACT E -mode polarization at $1000 < \ell \lesssim 6000$ at $> 3\sigma$ in each of 35 distinct $\sim 100 \text{ deg}^2$ regions of the sky, suggesting alignment between Galactic density structures and the local magnetic field persists to sub-parsec physical scales in these regions. The distribution of TE amplitudes in this ℓ range across all 107 regions is biased to positive values, while there is no evidence for such a bias in the TB spectra. This work constitutes the highest- ℓ measurements of the Galactic dust TE spectrum to date and indicates that cross-correlation with high-resolution mid-infrared measurements of dust emission is a promising tool for constraining the spatial statistics of dust emission at millimeter wavelengths.

E-mail: rodrigoc@princeton.edu

Astrophys. J., **960**:96 (2024)

<http://doi.org/10.3847/1538-4357/ad05cd>



Example model fit of the WISE W3 \times ACT f150 TT spectrum in a moderately high-latitude region ($l = 134.5^\circ$, $b = -52.2^\circ$; Tile 236). The top left panel shows the measured TT spectrum (blue circles with error bars) where 2σ upper limits are quoted for bandpowers consistent with zero. Also shown is the total fit model (black) with its region-specific best-fit Galactic dust component (green) along with the global best-fit CIB-C (cosmic infrared background - Clustered) and CIB-P (CIB - Poisson) components in red and purple, respectively. The residuals of the fit are presented in the lower left panel. The upper and lower right panels show the WISE and ACT maps of the region, respectively, including the applied mask. The TT spectrum transitions from Galactic emission at low- ℓ to extragalactic emission at high- ℓ and is well-fit by the model.

Mid-infrared spectroscopy of 1-cyanonaphthalene cation for astrochemical consideration

Julianna Palotás¹, Francis C. Daly¹, Thomas E. Douglas-Walker¹, and Ewen K. Campbell¹

¹School of Chemistry, University of Edinburgh, Joseph Black Building, Kings Buildings, Edinburgh, UK

We present the low temperature gas-phase vibrational spectrum of ionised 1-cyanonaphthalene (1-CNN⁺) in the mid-infrared region. Experimentally, 1-CNN⁺ ions are cooled below 10 K in a cryogenic ion trapping apparatus, tagged with He atoms and probed with tuneable radiation. Quantum-chemical calculations are carried out at a density functional theory level. The spectrum is dominated by the CN-stretch at 4.516 μm , with weaker CH modes near 3.2 μm .

E-mail: e.k.campbell@ed.ac.uk

Phys. Chem. Chem. Phys., Advance Article (2024)

<https://doi.org/10.1039/D3CP05784D>

A comparative laboratory study of soft X-ray-induced ionization and fragmentation of five small PAH cations

Yining Huo¹, Mónica K Espinoza Cangahuala¹, Vicente Zamudio-Bayer², Marcelo Goulart¹, Markus Kubin², Martin Timm², J. Tobias Lau^{2,3}, Bernd von Issendorff³, Ronnie Hoekstra^{1,4}, Shirin Faraji¹, and Thomas Schlathölter^{1,5}

¹Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands

²Abteilung für Hochempfindliche Röntgenspektroskopie, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

³Physikalisches Institut, Universität Freiburg, Freiburg, Germany

⁴Advanced Research Center for Nanolithography (ARCNL), Amsterdam, The Netherlands

⁵University College Groningen, University of Groningen, Groningen, The Netherlands

The interaction between polycyclic aromatic hydrocarbon (PAH) radical cations and X-rays predominantly leads to photofragmentation, a process that strongly depends on PAH size and geometry. In our experiments, five prototypical PAHs were exposed to monochromatic soft X-ray photons with energies in the C K-edge regime. As a function of soft X-ray photon energy, photoion yields were obtained by means of time-of-flight mass spectrometry. The resulting near-edge X-ray absorption mass spectra were interpreted using time-dependent density functional theory (TD-DFT) with a short range corrected functional. We found that the carbon backbone of anthracene⁺ (C₁₄H₁₀⁺), pyrene⁺ (C₁₆H₁₀⁺) and coronene⁺ (C₂₄H₁₂⁺) can survive soft X-ray absorption, even though mostly intermediate size fragments are formed. In contrast, for hexahydroperylene⁺ (C₁₆H₁₆⁺) and triphenylene⁺ (C₁₈H₁₂⁺) molecular survival is not observed and the fragmentation pattern is dominated by small fragments. For a given excitation energy, molecular survival evidently does not simply correlate with PAH size but strongly depends on other PAH properties.

E-mail: t.a.schlatholter@rug.nl

Eur. Phys. J. D, **77**:181 (2023)

<https://doi.org/10.1140/epjd/s10053-023-00763-w>

An X-ray spectroscopy study of structural stability of superhydrogenated pyrene derivatives

Yining Huo¹, Mónica K Espinoza Cangahuala¹, Vicente Zamudio-Bayer², Marcelo Goulart¹, Martin Timm², J. Tobias Laur^{2,3}, Bernd von Issendorff³, Ronnie Hoekstra^{1,4}, Shirin Faraji¹ and Thomas Schlathölter^{1,5}

¹Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands

²Abteilung für Hochempfindliche Röntgenspektroskopie, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

³Physikalisches Institut, Universität Freiburg, Freiburg, Germany

⁴Advanced Research Center for Nanolithography (ARCNL), Amsterdam, The Netherlands

⁵University College Groningen, University of Groningen, Groningen, The Netherlands

The stability of polycyclic aromatic hydrocarbons (PAHs) upon soft X-ray absorption is of crucial relevance for PAH survival in X-ray dominated regions. PAH stability depends on molecular size but also on the degree of hydrogenation that is related to H₂ formation in the interstellar medium. In this project, we intend to reveal the changes of electronic structure caused by hydrogenation and the impact of hydrogenation on the stability of the carbon backbone for cationic pyrene and its hydrogenated derivatives by analysis of near C K-edge soft X-ray photoions. In our experiments, the PAH cations were trapped in a cryogenic radiofrequency linear ion trap and exposed to monochromatic X-rays with energies from 279 eV to 300 eV. The photo-products were mass-analyzed by means of time-of-flight spectroscopy. Partial ion yields were then studied as a function of photon energy. X-ray absorption spectra computed by time-dependent density functional theory (TD-DFT) aided the interpretation of the experimental results. A very good agreement between experimental data and TD-DFT with short-range corrected functionals for all PAH ions was reached. The near-edge X-ray absorption mass spectra exhibit clear peaks due to C 1s transitions to singly occupied molecular orbitals and to low-lying unoccupied molecular orbitals. In contrast to coronene cations, where hydrogen attachment drastically increases photostability of coronene, the influence of hydrogenation on photostability is substantially weaker for pyrene cations. Here, hydrogen attachment even destabilizes the molecular structure. An astrophysical model describes the half-life of PAH ions in interstellar environments.

E-mail: t.a.schlatholter@rug.nl

Mon. Not. R. Astron. Soc. **523**(1), 865–875 (2023)

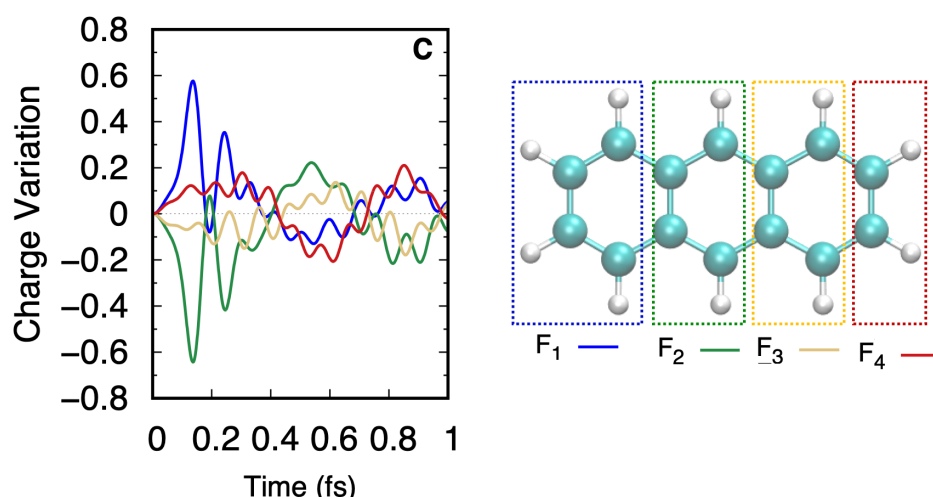
<https://doi.org/10.1093/mnras/stad1341>

Addressing electronic and dynamical evolution of molecules and molecular clusters : DFTB simulations of energy relaxation in Polycyclic Aromatic Hydrocarbons

Mathias Rapacioli¹, Maysa Yusef Buey¹, and Fernand Spiegelman¹

¹Laboratoire de Chimie et Physique Quantique (LCPQ/FERMI), UMR5626, Université de Toulouse (UPS) and CNRS, 118 Route de Narbonne, F-31062 Toulouse, France

We present a review of the capacities of the Density Functional based Tight Binding (DFTB) scheme to address the electronic relaxation and dynamical evolution of molecules and molecular clusters following energy deposition via either collision or laser excitation. The basics and extensions of DFTB for addressing those systems and in particular their electronic states and their dynamical evolution are reviewed. Applications to PAH molecules and clusters, carbonaceous systems of major interest in astrochemical/astrophysical context, are reported. A variety of processes are examined and discussed such as collisional hydrogenation, fast collisional processes and induced electronic and charge dynamics, collision-induced fragmentation, photo-induced fragmentation, relaxation in high electronic states, electronic- to-vibrational energy conversion and statistical versus non-statistical fragmentation. The review illustrates how simulations may help to unravel different relaxation mechanisms depending on various factors such as system size, specific electronic structure or excitation conditions, in close connection with experiments



Ultrafast charge evolution for an anthracene after collision with a 100 keV proton

E-mail: mathias.rapacioli@irsamc.ups-tlse.fr

Phys. Chem. Chem. Phys., **26**:1499 (2024)

<https://doi.org/10.1039/D3CP02852F>

Mixed Cluster Ions of Magnesium and C₆₀

Anna Maria Reider¹, Jan Mayerhofer¹, Paul Martini^{1,2}, Paul Scheier¹, Olga V. Lushchikova¹

¹Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Innsbruck, Austria

²Department of Physics, Stockholm University, Stockholm, Sweden

Magnesium clusters exhibit a pronounced nonmetal-to-metal transition, and the neutral dimer is exceptionally weakly bound. In the present study, we formed pristine Mg_n^{z+} (n = 1–100, z = 1–3) clusters and mixed (C₆₀)_mMg_n^{z+} clusters (m = 1–7, z = 1, 2) upon electron irradiation of neutral helium nanodroplets doped with magnesium or a combination of C₆₀ and magnesium. The mass spectra obtained for pristine magnesium cluster ions exhibit anomalies, consistent with previous reports in the literature. The anomalies observed for C₆₀Mg_n⁺ strongly suggest that Mg atoms tend to wet the surface of the single fullerene positioning itself above the center of a pentagonal or hexagonal face, while, for (C₆₀)_mMg_n^{z+}, the preference for Mg to position itself within the dimples formed by fullerene cages becomes apparent. Besides doubly charged cluster ions, with the smallest member Mg₂²⁺, we also observed the formation of triply charged ions Mg_n³⁺ with n > 24. The ion efficiency curves of singly and multiply charged ions exhibit pronounced differences compared to singly charged ions at higher electron energies. These findings indicate that sequential Penning ionization is essential in the formation of doubly and triply charged ions inside doped helium nanodroplets.

E-mail: Olga.Lushchikova@uibk.ac.at

J. Phys. Chem. A, **128**, 848–857 (2024)

<https://doi.org/10.1021/acs.jpca.3c06902>

Optical constants of exoplanet haze analogs from 0.3 to 30 microns : comparative sensitivity of spectrophotometry and ellipsometry

T. Drant^{1,2}, E. Garcia-Caurel³, Z. Perrin¹, E. Sciamma-O'Brien⁴, N. Carrasco¹, L. Vettier¹, T. Gatier¹, J.-B. Brubach⁶, P. Roy⁶, D. Kitzmann⁷, K. Heng^{2,8,9}

¹University of Paris Saclay, OVSQ, LATMOS, Guyancourt, France

²Ludwig Maximilian University, Faculty of Physics, Observatory of Munich, Munich, Germany

³Ecole Polytechnique, LPICM, Palaiseau, France

⁴NASA Ames Research Center, Moffet Field, CA, USA

⁵LESIA, Observatoire de Paris, Université PSL, CNRS, Sorbonne Université, Meudon, France

⁶Synchrotron SOLEIL, Saint-Aubin, France

⁷University of Bern, Center for Space and Habitability, Bern, Switzerland

⁸University of Bern, ARTORG Center for Biomedical Engineering Research, Bern, Switzerland

⁹University of Warwick, Department of Physics, Coventry, United Kingdom

Samples are produced in a simulated N₂-dominated atmosphere with two different abundance ratios of CO₂ and CH₄ using the PAMPRE plasma reactor at LATMOS. We find that both haze analogs present a significantly lower extinction coefficient in the optical and near-Infrared range compared to the first analogs of Khare et al. (1984). Our haze analog produced in a relatively reduced gas mixture (CO₂/CH₄ = 0.25) exhibits infrared properties surprisingly similar to the Titan analogs of Khare et al. (1984). An increased absorbing power is however observed for our oxidized analog (CO₂/CH₄ = 1.5) confirming previous findings by Gavilan et al. (2018). In addition to the work of He et al. (2023), these data suggest a strong impact of the atmospheric composition on the absolute values of *k*. Existing data obtained in a broad spectral range (Khare et al. (1984), He et al. (2023), present study) must be used to constrain retrieval models and correctly interpret future observations with the JWST and ARIEL space telescopes. The data presented in this paper can be found in the Optical Constants Database (<https://ocdb.smce.nasa.gov/>). The reliability of the optical technique (spectrophotometry and ellipsometry) and calculations is meticulously assessed to better understand the impact on the retrieved refractive indices. *k* values are subjected to large errors in the optical and near-Infrared range that likely contributes to the strong discrepancies in the existing data. In the UV and mid-Infrared, the different calculations lead to rather small errors on *k*, the discrepancies observed in existing data therefore reflect the difference in composition between the haze analogs. For the refractive index *n*, errors of 1-3% are observed with both optical techniques and the different models. The refractive index is very sensitive to the optical method and to the model used, the discrepancy between both techniques overcome the uncertainty given by each. Based on our analysis, we find that UV-Visible reflection ellipsometry provides very accurate *n* and *k* with every model used. The Swanepoel method is proven to be very accurate although larger errors on *n* are expected in the UV as spectroscopic transmission is mainly sensitive to absorption. In the MIR, we suggest the use of direct spectroscopic calculations to avoid the strong degeneracy of an indirect ellipsometric model.

E-mail: thomas.drant@latmos.ipsl.fr

Astronomy & Astrophysics, **682**, A6, 14 pages (2024)

<https://doi.org/10.1051/0004-6361/202346820>

The Influence of Hydrogenation on Photofragmentation and Electronic Structure of PAH Cations and Its Astrophysical Implications

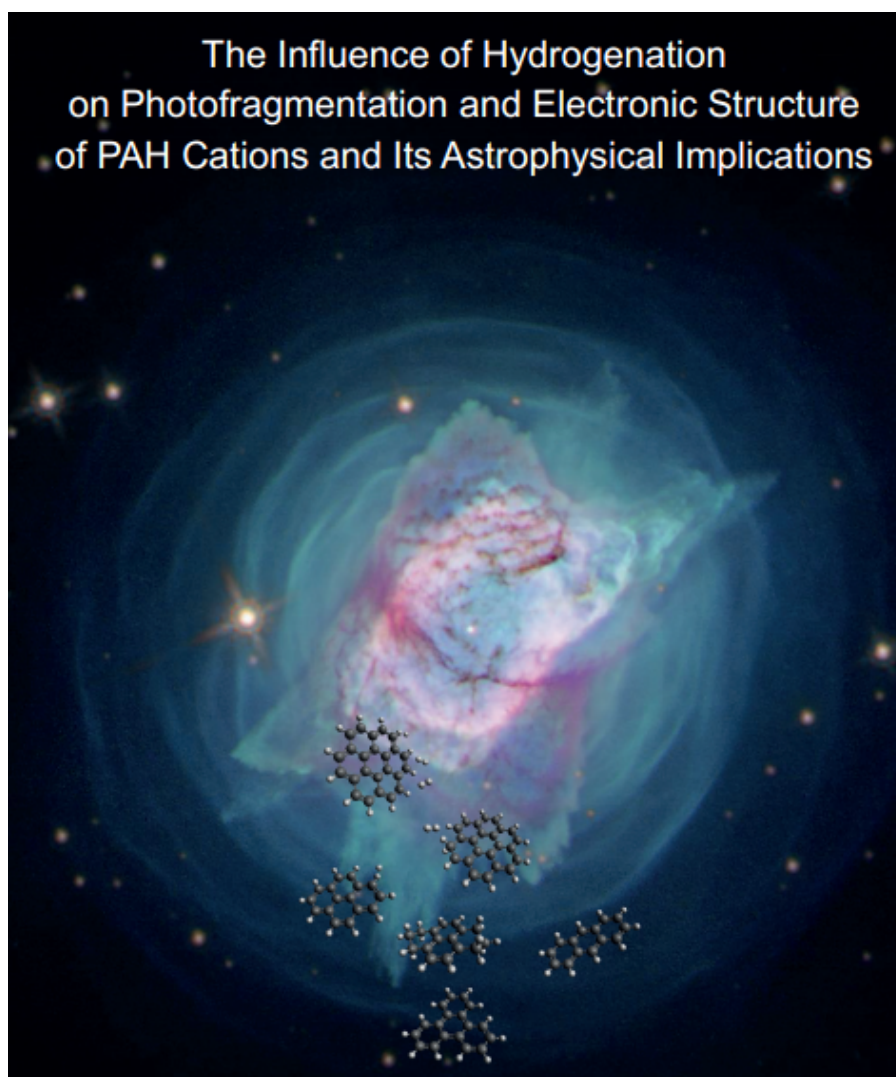
Yining Huo

Institution: Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands

Advisor: Dr. T. A. Schlathöler (Zernike Institute for Advanced Materials, University College Groningen)

Advisor: Prof. dr. R. A. Hoekstra (Co-advisor, Zernike Institute for Advanced Materials, Advanced Research Center for Nanolithography (ARCNL))

Polycyclic aromatic hydrocarbon (PAH) molecules are distributed in the interstellar medium (ISM) and contribute to thermal equilibrium and chemical abundance. One of the most important contributions is the catalytic formation of H_2 from atomic hydrogen on the surface of PAHs. The influence of hydrogenation on stability of the PAH carbon backbone has become a topic of astronomical interest.



The front cover of the thesis.

In this thesis, five prototypical PAH cations and their hydrogenated counterparts were exposed to the X-ray photons around the C K-edge. The near edge X-ray absorption mass spectrometry (NEXAMS) technique was adopted where photoproducts were recorded as a function of photon energies by means of time-of-flight mass spectrometry. The NEXAMS scans of all molecular ions were compared to time-dependent density functional theory (TD-DFT) calculations to interpret the resonant transitions. The photostability was quantitatively analyzed to show that it depends on PAH size, geometry and the state of hydrogenation. As for large and compact PAHs such as coronene, H loss is an efficient way to protect the carbon backbone. By combination of NEXAMS analysis and TD-DFT calculations, an astrophysical model was developed to predict the lifetime of PAH cations in nebula NGC 7027. In order to figure out the influence of heteroatomic nitrogen, the NEXAMS scan of protonated acridine was also investigated and compared to its hydrocarbon counterpart hydrogenated anthracene.

E-mail: huoyining1209@gmail.com

Website: <https://doi.org/10.33612/diss.806984479>



Meetings

2nd COST NanoSpace Joint Scientific Meeting 1st Announcement

**Istanbul, Turkey
16–19 April, 2024**

<https://nanospacejm2.erbaharlab.com/>

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 2nd Action Meeting Scope:

This is the second NanoSpace Joint Scientific Meeting (in person), which will increase the interaction and collaboration among the diversity of disciplines and researchers of the Action. Special WG1 and WG3 sessions as well as NanoSpace Database session will be part of the scientific program. The program will include a Management Committee (MC) meeting.

The specific 2nd Action Joint Meeting Scope is to increase the interactions and collaborations between the diverse disciplines (laboratory astrophysics, theoretical chemistry and physics, astronomy, among others) and researchers (especially from ITC and young researchers) present in NanoSpace towards a common language and understanding of the action's challenge.

Deadline for registration (free) and abstract submission: 15th March 2024

Organizing committee:

- Prof. Dogan Erbahar, Dogus University, Turkey
- Prof. Lufti Arda, Bahcesehir University, Turkey
- Mr. Eftal Gezer, Gebze Technical University, Turkey
- Ms. Dilara Ickecan, Marmara University, Turkey
- 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 Materiaux Jean Rouxell, France
- Dr. Polona Umek, Jozef Stefan Institute, Slovenia
- Dr. Alicja Domracka, CNRS - CIMAP, France
- Dr. Cornelia Jäger, MPIA, Germany

The Action NanoSpace in the internet: <https://research.iac.es/proyecto/nanospace/>

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

Apply to join the COST Action NanoSpace: <https://www.cost.eu/actions/CA21126/#tabs+Name:Working%20Groups%20and%20Membership>

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.

E-mail for contact: derbahar@dogus.edu.tr, agarcia@iac.es

EAS2024-S6

Symposium S6

“European Laboratory Astrophysics in the JWST era”

**Padova, Italy
1–5 July, 2024**

<https://eas.unige.ch/EAS2024/session.jsp?id=S6>

We are pleased to announce the Symposium S6 “European Laboratory Astrophysics in the JWST era” <https://eas.unige.ch/EAS2024/session.jsp?id=S6> at the European Astronomical Society (EAS) annual meeting 2024 <https://eas.unige.ch/EAS2024/>, which will be held in Padova, Italy, from 1–5 July 2024.

This symposium aims to foster new collaborations between experts in laboratory astrophysics and observational astrophysics. With the ground-breaking data from JWST, ALMA and the up-coming ELT, there is a strong need to establish productive links between the relevant communities.

The symposium will cover a variety of topics: Ices, Tracers of Astrochemistry, Molecular Spectroscopy and Reactivity, Protoplanetary Discs and Planets, Plasmas and Dust in Extreme Environments, as well as PAHs and Fullerenes.

All interested researchers are invited to submit an abstract through the EAS website by March 4th: https://eas.unige.ch/EAS_meeting/abstract_submission.jsp

Please note that meeting is planned to be a fully hybrid and on-line presentations will be possible except for invited speakers. More information can be found on the session’s webpage: <https://eas.unige.ch/EAS2024/session.jsp?id=S6>. Registration fee waivers and/or grants provided by EAS are also available on request: https://eas.unige.ch/EAS_meeting/grants.jsp For any inquiries on the Symposium S6 please feel free to contact us.

Important dates:

- Very early bird registration deadline: **26 February 2024**
- Abstract submission deadline: **4 March 2024**
- Early bird registration deadline: **29 April 2024**
- Regular registration deadline: **30 June 2024**
- Symposium S6 “European Laboratory Astrophysics in the JWST era”: **1–2 July 2024**

Please distribute this information so that it reaches all the communities concerned and makes this symposium a success.

E-mail for contact: christine.joblin@irap.omp.eu

AstroPAH Newsletter

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

astropah@strw.leidenuniv.nl

Next issue: 21 March 2024

Submission deadline: 8 March 2024