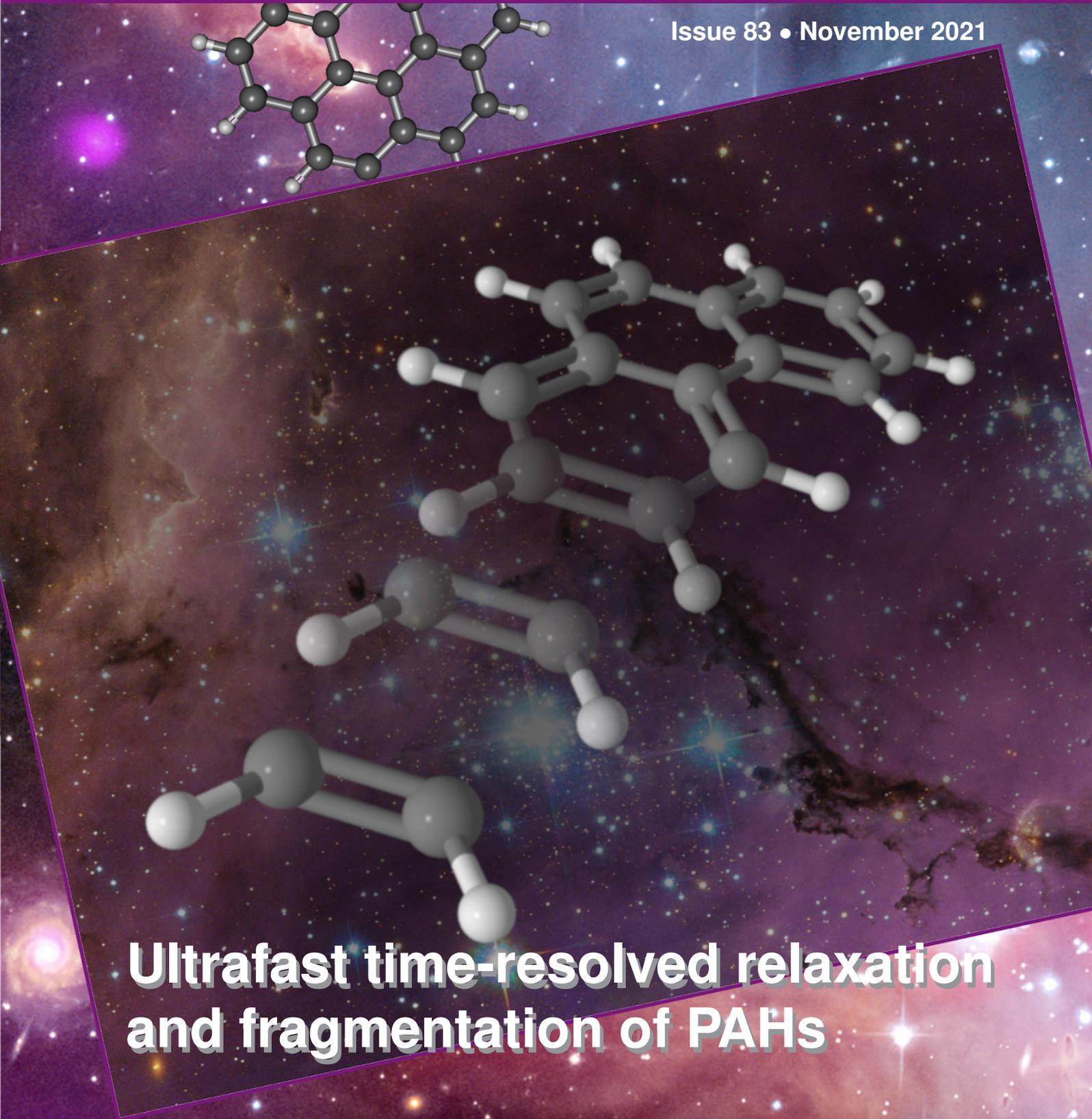


AstroPAH

A Newsletter on Astronomical PAHs

Issue 83 • November 2021



**Ultrafast time-resolved relaxation
and fragmentation of PAHs**



Editorial

Dear Colleagues,

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

Our Picture of the Month represents recent experimental work investigating relaxation and fragmentation patterns of PAHs under extreme UV conditions. Noticeable on this picture are the fragments indicative of dissociation pathways involving acetylene loss. For more information regarding this experimental work, see our Abstracts section (J. Lee et al. 2021).

This month, our In Focus is an interview with Dr. Elisabetta Micelotta who was one of the founding editor of AstroPAH and a member of our editorial board until last September. Elisabetta is an expert in the field of nanoscience in space and has moved from academia to industry. We are very happy to have her share her experiences with us this month.

This month we have received an extravaganza of abstract contributions! They add up to a grand total of 20 abstracts in this issue! Thank you to all as always for sharing your most exciting and recent research with all of us!

We are also happy to share the recent publication of Dr. Ameek Kaur Sidhu's thesis on PAH emission in photodissociation regions. Congratulations!

In the announcement section, you can find the details for two job openings, one for a Principal Scientist position in Crystallization at Nanoform in Helsinki, and the other for an Assistant Professor position in the Origins of Life project at the University of Amsterdam!

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! Next month will already be our last issue of 2021, so please continue sending us your contributions! 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: 16 December 2021.
Submission deadline: 3 December 2021.**

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PAH Picture of the Month

The Picture of the Month illustrates recent work highlighted in the Abstracts section (J. Lee et al., Nature Communications, 12:6107 (2021)) on recent experiments investigating the relaxation and fragmentation of PAHs under extreme ultraviolet light conditions. The PAHs showed ultrafast relaxation in all charge states and preferred dissociation pathways consistent with acetylene loss.

Credits: Picture by Diksha Garg and Denis S. Tikhonov. Background image by ESA/NASA/Hubble

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An Interview with Elisabetta Micelotta

Dr. Elisabetta Micelotta has a PhD in Astrophysics from Leiden University. She has extensive experience in the field of nanoscience in space, with focus on the formation and processing of PAHs and organic nanoparticles under extreme conditions. In the past, she has been a researcher at NASA Goddard Space Flight Center (USA), the University of Western Ontario (Canada) and the University of Helsinki, and a Marie Curie Fellow at Institut d'Astrophysique Spatiale (France). She now works in a drug particle engineering and nanotechnology company called Nanoform in Helsinki, Finland, where she leads the Science & Technology Team.



Can you tell us how you got into PAH-related research, and your current research project?

My original PhD project was about large interstellar dust grains, however, I soon started to notice that some small molecular brothers were also part of the family, and they seemed to be very important. At some point, I also noticed that, while the infrared signature of PAHs seemed to be present in shocked regions like supernova remnants, there were no physical models explaining what would happen to a PAH molecule in such environments. That was step number one. Discovering that Xander Tielens noticed the same fact was step number two. He became my PhD supervisor and I started working on PAHs. Now I lead the Science & Technology Team in a company called Nanoform, where I investigate the formation of nanoparticles of small molecules used as active pharmaceutical ingredients (APIs). If you wonder what is the connection with PAHs, check out the molecular structure of the most common medicines in your cabinet :).

What did it mean for you to be part of the AstroPAH editorial team? What aspect did you like best?

I am one of the co-founders of the newsletter and during these years I saw what great people can achieve when they work together. In the editorial team I have met friends I can count on, even if we live across the globe. And I'm amazed and delighted by the harmony that characterized our collaboration. This has been a fantastic journey, thank you all.

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

I did my Master at the University of Milan in the field of astroparticle physics, working on a CERN+NASA experiment. I continued working on the same project as a research fellow for almost two years, before moving to Leiden for my PhD. After graduation, I have had research positions in different countries: US, Canada, France, and Finland. I lived in different places already as a kid, with my family, so for me moving to a new country to start a new job was natural, and I enjoyed it. In each place, I met incredible people and learned a lot. I believe that doing a few postdocs far from home is important for prospective scientists. However, this should be a career's stage with a well-defined beginning and an even better-defined end. At one point, I had to decide about my next step. I learned that a professor at the University of Helsinki co-founded a company to produce nanoparticles for the health-care sector. We agreed to have a chat. Three weeks later, after three job interviews, I signed my contract to work as a scientist. So, leaving academia it's what allowed me to stay in the field.

Astrochemistry is a very multidisciplinary field. Can you comment on how you collaborate and communicate with experimentalists, observers, modelers and theoreticians... and what you like about such interactions?

Multidisciplinarity is my credo and my reality, even more now than before. I am an astrophysicist and I work with scientist from fields ranging from computer science to pharmaceutical technology, not to mention the collaboration with people from other departments. I think that the key to communicate is to be curious, humble and eager to learn. What I like about such interactions is learning about fields very different from mine from skilled professionals, with the goal of finding together new solutions to our common challenges.

What was the most important advice somebody gave you?

I will take the liberty to mention two, that I believe are particularly relevant for the readers of AstroPAH.

1. There are no sealed compartments in Science.
2. Learn how to fit your key message in one sentence. No matter the topic, no matter the situation.

How do you balance your professional and personal life?

I think that, in my case, flexibility is the key. Of course, this is possible because I have a very supporting family. In this respect, I can mention another important advice that I received in the past. During a career event organized for Marie Curie Fellows, a young male speaker told us the following: "If you want to have a career in science, choose the right life partner". He was addressing this especially to women, but I think that it can be applied to anyone.

What do you do outside of work?

Trying things that I never did before! For instance, last winter I tried cross-country skiing and I have to say that it has been quite an impactful experience. Since I managed to survive and all in one piece, I am waiting for the snow to try again. Apart from such extreme sports, I enjoy books, music, dance, and movies. And listening to people talking about something they know, and they are passionate about, no matter what the topic is. This is one of the greatest pleasures in life.

Anything else you would like to share with AstroPAH readers?

If you are a talented and passionate scientist who wants to continue to do pioneering research, remember that there are also many possibilities outside academia. Start to look at the job listings on LinkedIn and you will be surprised by the number of vacancies for "Scientists". If you don't believe me, go to the "Announcements" section of this issue of the newsletter (p. 28), and then we can talk ;).



Abstracts

Characterizing the PAH Emission in the Orion Bar

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We present 5–14 μm spectra at two different positions across the Orion Bar photodissociation region (PDR) obtained with the Infrared Spectrograph onboard the Spitzer Space Telescope and 3.3 μm PAH observations obtained with the Stratospheric Observatory for Infrared Astronomy (SOFIA). We aim to characterize emission from Polycyclic Aromatic Hydrocarbon (PAH), dust, atomic and molecular hydrogen, argon, sulfur, and neon as a function of distance from the primary illuminating source. We find that all the major PAH bands peak between the ionization front and the PDR front, as traced by H_2 , while variations between these bands become more pronounced moving away from this peak into the face-on PDRs behind the PDR front and at the backside of the H II region. While the relative PAH intensities are consistent with established PAH characteristics, we report unusual behaviours and attribute these to the PDR viewing angle and the strength of the FUV radiation field impinging on the PDRs. We determine the average PAH size which varies across the Orion Bar. We discuss subtle differences seen between the cationic PAH bands and highlight the photo-chemical evolution of carbonaceous species in this PDR environment. We find that PAHs are a good tracer of environmental properties such as the strength of the FUV radiation field and the PAH ionization parameter.

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<http://arxiv.org/abs/2110.12073>

Time-resolved relaxation and fragmentation of polycyclic aromatic hydrocarbons investigated in the ultrafast XUV-IR regime

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Polycyclic aromatic hydrocarbons (PAHs) play an important role in interstellar chemistry and are subject to high energy photons that can induce excitation, ionization, and fragmentation. Previous studies have demonstrated electronic relaxation of parent PAH monocations over 10–100 femtoseconds as a result of beyond-Born-Oppenheimer coupling between the electronic and nuclear dynamics. Here, we investigate three PAH molecules: fluorene, phenanthrene, and pyrene, using ultrafast XUV and IR laser pulses. Simultaneous measurements of the ion yields, ion momenta, and electron momenta as a function of laser pulse delay allow a detailed insight into the various molecular processes. We report relaxation times for the electronically excited PAH*, PAH⁺ and PAH²⁺ states, and show the time-dependent conversion between fragmentation pathways. Additionally, using recoil-frame covariance analysis between ion images, we demonstrate that the dissociation of the PAH²⁺ ions favors reaction pathways involving two-body breakup and/or loss of neutral fragments totaling an even number of carbon atoms.

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<https://www.nature.com/articles/s41467-021-26193-z/>

IRMPD spectroscopy of a PAH cation using FELICE: The infrared spectrum and photodissociation of dibenzo[a,l]pyrene

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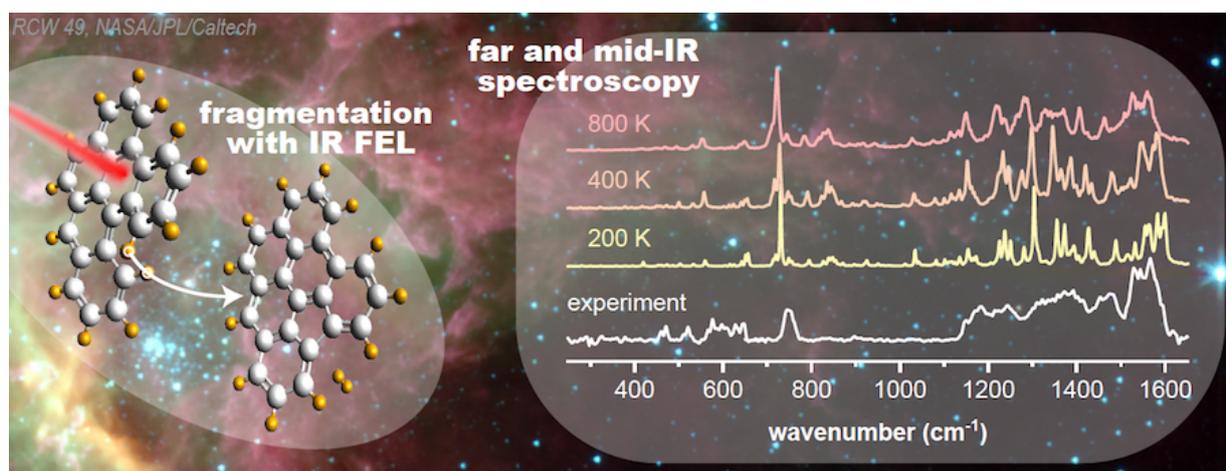
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We present the experimental InfraRed Multiple Photon Dissociation (IRMPD) spectrum and fragmentation mass spectrum of the irregular, cationic PAH dibenzo[a,l]pyrene ($C_{24}H_{14}^+$) in the 6–40 μm / 250–1650 cm^{-1} range. The use of the the Free-Electron Laser for IntraCavity Experiments (FELICE) enabled us to record its Far-InfraRed (FIR) spectrum for the first time. We aim to understand how irregularity affects the infrared spectrum and fragmentation chemistry of PAHs. Dibenzo[a,l]pyrene is an asymmetric, non-planar molecule, for which all vibrational modes are in principle IR-active. Calculated harmonic Density Function Theory (DFT) and anharmonic Density Functional based Tight Binding Molecular Dynamics (DFTB-MD) spectra show a large wealth of bands, which match the experiment well, but with a few differences. The periphery of the molecule contains several edge geometries, but out of all possible modes in the 11–14 μm out-of-plane C–H bending region, only one band at 13.5 μm is prominent. This fact and the richness of the C–C stretching range make irregular PAHs a possible contributor to D-class interstellar spectra. The fragmentation mass spectra reveal facile 2H-loss and no [2C,2H]-loss, which is attributed to the sterically hindered, non-planar cove region, which could protect irregular PAHs from radiation damage.



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<https://doi.org/10.1016/j.jms.2021.111545>

<https://arxiv.org/abs/2110.09249>

Polycyclic aromatic hydrocarbons and the ionized gas in galaxies with active nuclei

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We present a study for a sample of galaxies with active nuclei to characterize the main type of PAH molecules present in these objects and the local physical conditions of their irradiating sources, as well as the characteristics of the residing ionized gas, by combining optical and infrared data. Photoionization models were built with the CLOUDY code to reproduce optical emission line ratios in combination with PAH intensity ratios. We find that the species containing 10–82 carbon atoms are the most abundant in the sample. We suggest that family of species with only two or three fused rings of and a nitrogen hanging, such as small aromatic amides are important targets worthy of consideration in future experimental/theoretical as well as observational studies. We find that the AGN photoionization models reproduce most of the observational data in the $\log(6.2/11.3)$ versus $\log([N II]\lambda 6584/H\alpha)$ diagram with the optical to X-ray spectral index of $\alpha_{\text{ox}} = -1.4$. The flux of small PAH, as well as the flux of ionized PAHs and PANH, decrease as the logarithm of the ionization parameter ($\log U$) increases. The 6.2/11.3 PAH intensity ratio presents anti correlation between the oxygen abundance and $\log U$, in the sense that the 6.2/11.3 ratio decreases as the oxygen abundance and $\log U$ increases. Finally, we found that the ionization degree of PAH species increases with the decreasing of the 11.3/7.7 ratio and the $\log U$, in agreement with the models proposed by Draine & Li.

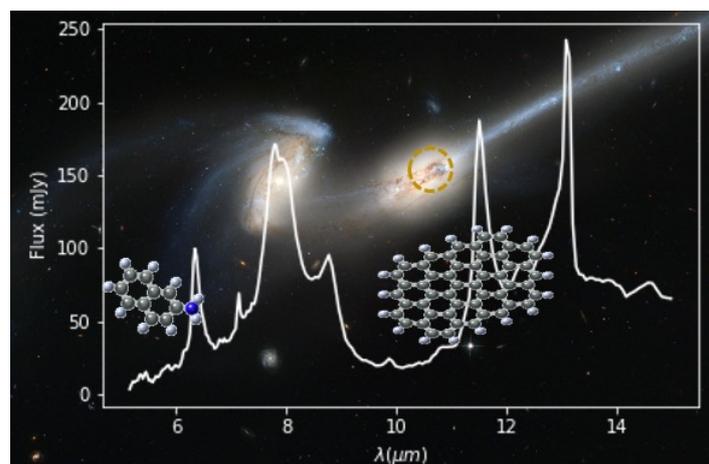


Figure 1 – More relevant species in NGC 4676 galaxy

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Gas phase laboratory formation of astronomically relevant large PAH/organic molecule clusters

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Polycyclic aromatic hydrocarbon (PAH) molecules may play an essential role in the prebiotic compound evolution network in interstellar clouds. In this work, an experimental study of large, astronomically relevant PAH-organic molecule clusters is presented. With the initial molecular precursors dicoronylene (DC, C₄₈H₂₀), Pyroglutamic acid (Pga, C₅H₇NO₃), DC-Proline (Pro, C₅H₉NO₂), and DC-Pyroglutaminol (Pgn, C₅H₉NO₂), our experiments indicate that PAH-organic molecule cluster cations (e.g., (Pga)₁₋₂C₄₈H_n⁺, (Pro)₁₋₂C₄₈H_n⁺, and (Pgn)₁₋₆C₄₈H_n⁺), and carbon cluster-organic molecule cluster cations (e.g., (Pga)C₄₈⁺, (Pro)₁₋₂C₄₈⁺, and (Pgn)₁₋₆C₄₈⁺) are gradually formed through an ion-molecule collision reaction pathway in the presence of a strong galactic interstellar radiation field. These laboratory studies provide a gas-phase growth route toward the formation of complex prebiotic compounds in a bottom-up growth process, as well as insight into their chemical-evolution behavior in the interstellar medium.

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Gas-phase Formation of Cationic Fullerene/Amino Acid Clusters: Evidence for the “Magic Number” Chemical Reactivity of Fullerene Cations

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An experimental and theoretical investigation on the chemical reactivity of fullerene cations (C_n^+ , $n = [36, 60]$) with amino acid molecules (e.g., isoleucine, $C_{14}H_{11}NO_2$) is performed. The results show that, in the gas phase, fullerene cations can react with amino acid molecules to form fullerene/amino acid cluster cations with high efficiency. The formation rate constants for the ion–molecule collision reactions between fullerene cations and isoleucine are estimated under the pseudo-first-order reaction condition. We find the formation rate constants increase gradually with a declining C-atom number of fullerene cations (C_n^+ , $n = [46, 60]$), and depict a plateau in the reactivity for smaller fullerene cations (C_n^+ , $n = [36, 44]$). More importantly, by comparing to its neighbor fullerenes, the magic number of C-atom counts (54, 58) that process with enhanced chemical reactivity are determined. We also obtained the molecular structures and binding energies for the fullerene-monoisoleucine adducts by quantum chemical calculations, which give a good explanation for the magic number chemical reactivity and the enhanced chemical reactivity of smaller fullerene cations. We infer that our results demonstrate the importance of ion–molecule reactions to the formation of large and complex fullerene-amino acid derivatives in the ISM. The high reactivity of fullerene species may indicate that amino acid molecules or other related prebiotic compounds can accrete on small interstellar carbon dust grains.

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Gas-phase formation of cationic fullerene/9-aminoanthracene clusters: an indicator for interstellar dust growth

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Growth of clusters by adduction of monomers — as the first step in dust particle growth — is an area of much interest in astronomy. We focus on the fullerene/9-aminoanthracene cluster species, to illustrate the competition between the van der Waals bonding growth and the covalent bonding growth model versus the charge transfer model in the large cluster formation process. The experimental results show that fullerene-fragment(C_{56} and C_{58}) /9-aminoanthracene cluster cations, e.g. $[(C_{14}H_{11}N)_n C_{56}]^+$ and $[(C_{14}H_{11}N)_n C_{58}]^+$, $n=[1,7]$, are efficiently formed, while C_{60}^+ is insensitive to the cluster's formation. With laser irradiation, all the fullerene/9-aminoanthracene clusters dissociate into 9-aminoanthracene and fullerene cations. The mechanisms for the reactions of fullerene cations and 9-aminoanthracene were investigated by theoretical calculations, under the assumption that the molecular geometries found for the formed complexes correspond to the global energy minima: the absence of C_{60}^+ clusters is mainly due to the charge transfer channel's competition; $[(C_{14}H_{11}N)C_{58}]^+$ has three types of isomers, with van der Waals or covalent bonds, mainly depending on the reaction sites of fullerene cations. Importantly, in the size grown process, for the fullerene/9-aminoanthracene cluster there exists a geometry configuration conversion between the van der Waals and covalent bonding modes. The largest fullerene/9-aminoanthracene clusters, e.g. $[(C_{14}H_{11}N)_7 C_{58}]^+$ (240 atoms, ~ 4 nm in size), are likely in a multishelled geometry, i.e. seven 9-aminoanthracene molecules surrounding fullerene cations in two layers, which can directly build the relationship between molecular clusters and carbonaceous grains. Nitrogen matters! The specific side chains (e.g. $-NH_2$) play an important role in the growth of interstellar dust.

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Gas phase laboratory study on the PAHs/amino acid cluster cations

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As an important class of carbon reservoirs in the interstellar medium (ISM), polycyclic aromatic hydrocarbon (PAH) molecules play an important role in the evolutionary network of prebiotic molecules. Here, the experimental evidence of astronomically relevant amino-acid derivatives — PAH/amino-acid clusters — is provided, and we study their ion–molecular collision reactions in the gas phase. With the initial molecular precursors dicoronylene (DC, C₄₈H₂₀)/alanine (Ala, C₃H₇NO₂) and DC/isoleucine (Ile, C₆H₁₃NO₂), the experiments indicate that PAH–amino-acid cluster cations (e.g. (Ala)C₄₈H_{0–19}⁺ and (Ile)C₄₈H_{0–19}⁺) and graphene–amino-acid cluster cations (e.g. (Ala)_nC₄₈⁺ and (Ile)_nC₄₈⁺, n=1, 2, 3, 4) are efficiently formed in a strong interstellar radiation field. In addition, the structure of clusters and the binding energy of their formation pathways are studied by a quantum chemistry calculation method: gas-phase reactions (ion–molecule reactions) between PAH cations with amino acids readily occur (exothermic energy around 2.0–4.7 eV), and these newly formed clusters have a complex molecular configuration (C–O and C–N bond type). These laboratory studies provide a cluster growth pathway (through an ion–molecule reaction) towards the formation of amino-acid derivatives in a bottom-up process and insight into their chemical evolution behaviour, opening up aromatic-based chemistry that is available to the species (dehydrogenated PAHs or graphene molecules) that formed from the photofragmentation process of PAHs in interstellar environments. When conditions are suitable (e.g. have similar molecular abundance spatial distributions in the ISM), amino acid derivatives can form efficiently, and newly built large PAH/amino acid clusters may be widespread in space.

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Gas phase formation of carbon cluster (fullerenes and graphenes)/prebiotic sugar complexes

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Among the constituent molecular classes of proteins and nucleic acids, the presence of Ribose and deoxy-Ribose in space remains unclear. Here, we provide experimental evidence of astronomically related sugar derivatives — carbon cluster (fullerenes and graphenes)/prebiotic sugar complexes — and study their formation processes in the gas phase. The results show that, with PAH cations (dicoronylene, DC, C₄₈H₂₀⁺)/(2-deoxy-D-Ribose, dR, C₅H₁₀O₄, and dehydrated 2-deoxy-D-Ribose, DedR, C₅H₈O₃) and fullerene cations (C₆₀⁺)/(dR and DedR) as the initial molecular precursors, two series of graphene–prebiotic sugar cluster cations (graphene/dR and graphene/DedR, e.g., (dR)C_n⁺ and (DedR)C_n⁺) and two series of fullerene–prebiotic sugar cluster cations (fullerene/dR and fullerene/DedR, e.g., (dR)(DedR)₂C_n⁺, (DedR)₃C_n⁺, and (dR)₂(DedR)C_n⁺) are formed through an ion–molecule reaction pathway under the influence of a strong radiation field. The structures of the newly formed complexes and the binding energies of these formation reactions are initially theoretically calculated. These laboratory studies attest to the importance of ion–molecule reaction synthesis routes for the chemical complexity in space, demonstrating that the gas phase interstellar materials could directly lead to the formation of large and complex sugar derivatives in a bottom-up growth process. The chemical evolution in space in which single molecules are transformed into complex molecules produces a wide variety of organic compounds (e.g., carbon cluster (fullerenes and graphenes)/prebiotic sugar complexes). For their astrobiological implications, this opens up aromatic based biogenic chemistry that is available to the parent of PAHs or fullerenes in the interstellar environments.

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Exploring the Dust Content of Galactic Halos with Herschel. IV. NGC 3079

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We present the results from an analysis of deep *Herschel* far-infrared observations of the edge-on disk galaxy NGC 3079. The PSF-cleaned PACS images at 100 and 160 μm display a $25 \times 25 \text{ kpc}^2$ X-shape structure centered on the nucleus that is similar in extent and orientation to that seen in $\text{H}\alpha$, X-rays, and the far-ultraviolet. One of the dusty filaments making up this structure is detected in the SPIRE 250 μm map out to $\sim 25 \text{ kpc}$ from the nucleus. The match between the far-infrared filaments and those detected at other wavelengths suggests that the dusty material has been lifted out of the disk by the same large-scale galactic wind that has produced the other structures in this object. A closer look at the central $10 \times 10 \text{ kpc}^2$ region provides additional support for this scenario. The dust temperatures traced by the 100-to-160 μm flux ratios in this region are enhanced within a biconical region centered on the active galactic nucleus, aligned along the minor axis of the galaxy, and coincident with the well-known double-lobed cm-wave radio structure and $\text{H}\alpha$ -X-ray nuclear superbubbles. PACS imaging spectroscopy of the inner 6-kpc region reveals broad [C II] 158 μm emission line profiles and OH 79 μm absorption features along the minor axis of the galaxy with widths well in excess of those expected from beam smearing of the disk rotational motion. This provides compelling evidence that the cool material traced by the [C II] and OH features directly interacts with the nuclear ionized and relativistic outflows traced by the $\text{H}\alpha$, X-ray, and radio emission.

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Orion Bar as a window to the evolution of PAHs

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We investigate the mid-infrared (IR) emission in the Orion Bar photodissociation region, using archival photometric and spectroscopic observations from UKIRT, *Spitzer*, ISO, and SOFIA telescopes. Specifically, we consider flux densities of the emission bands at 3.3, 3.4, 3.6, 6.6, 7.7, 11.2 μm in several locations and a spectrum from 3 to 45 μm in one location. We study the behaviour of band flux ratios, which are sensitive to external conditions, as revealed by their variations with the distance from an ionizing source. Assuming that the mid-IR emission arises mostly from polycyclic aromatic hydrocarbons (PAHs), and that a weak emission feature at 3.4 μm is related to PAHs with extra hydrogen atoms (H-PAHs), we trace variations of the ratios using a model for PAH evolution. Namely, we estimate how populations of PAHs of different sizes, hydrogenation and ionization states change across the Orion Bar over a time interval approximately equal to its lifetime. The obtained ensembles of PAHs are further used to calculate the corresponding synthetic spectra and band flux densities. The model satisfactorily describes the main features of the ratios $I_{3.6}/I_{11.2}$, $I_{7.7}/I_{11.2}$, $I_{7.7}/I_{3.6}$ and $I_{3.3}/I_{3.4}$. We conclude that the best coincidence between modelling and observations is achieved if C loss of PAHs is limited by the number of carbon atoms $N_C = 60$, and the band at 3.4 μm may indeed be attributed to H-PAHs. We confirm that large cations dominate at the surface of the PDR but small neutral PAHs and anions are abundant deeper in the molecular cloud.

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Ultrafast Vibrational Relaxation Dynamics in XUV-Excited Polycyclic Aromatic Hydrocarbon Molecules

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Unraveling ultrafast molecular processes initiated by energetic radiation provides direct information on the chemical evolution under extreme conditions. A prominent example is interstellar media where complex molecules such as polycyclic aromatic hydrocarbons (PAHs) are excited by energetic photons. Until recently, ultrafast dynamics following such excitations remained largely unexplored due to the lack of relevant technologies. Here, we use time-resolved mass spectrometry combining ultrashort femtosecond XUV and IR pulses, to investigate the dynamics induced by high-energy photon excitation in PAHs. We demonstrate that excited cations relax through a progressive loss of vibrational selectivity, created at the early-stage dynamics, and which represents the first steps of a complete intramolecular vibrational energy redistribution. This process is in competition with the recently revealed correlation-band dynamics. These results might have direct consequences for the development of XUV molecular physics and other fields such as astrochemistry.

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IR-photon quenching of delayed electron detachment from hot pentacene anions

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Spontaneous and photo-induced delayed electron detachment from pentacene anions was measured in the electrostatic ion storage ring TMU E-ring. We have investigated pentacene molecular anions ($C_{22}H_{14}^-$), a member of the polycyclic aromatic hydrocarbon (PAH) family with mass 278 u. The spectroscopy and photophysics of PAHs in the gas-phase are active research fields in astrophysics and astrochemistry. Recurrent fluorescence has been found to be an important cooling mechanism for several PAH cations, similar to the previous identification of radiative cooling as an important stabilizing factor suppressing fullerene decay. In contrast, little experimental information on these delayed processes for PAH anions has been obtained so far. On the other hand, it has been proposed that the majority of the negative charge carriers in interstellar molecular clouds are in the form of PAH anions. The pentacene anion is of special interest in this context because it has an electronic excited state, which exhibits exceptionally strong absorption, slightly below the electron detachment threshold E_{th} .

The dissipation mechanisms of the internal energy of the stored hot pentacene anions were inferred both from the temporal profile of the spontaneous detachment and from the laser-firing time dependence of the photo-induced temporal profile. Simulations based on statistical emission processes reproduced the observed behaviors, providing the value for the radiative cooling rates in the time range of a few tens of milliseconds. Using the obtained information on the competition between electron detachment and radiative cooling, we discuss the anion survival probabilities as a function of the initial internal energies and the nature of the observed quasi-exponential decrease in the temporal profile of the spontaneous detachment at long times. We concluded that the observed quasi-exponential decrease originates in single-photon quenching of electron detachment in the internal energy region close to the detachment threshold E_{th} .

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Interstellar Extinction and Elemental Abundances: Individual Sight Lines

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While it is well recognized that both the Galactic interstellar extinction curves and the gas-phase abundances of dust-forming elements exhibit considerable variations from one sightline to another, as yet most of the dust extinction modeling efforts have been directed to the Galactic average extinction curve, which is obtained by averaging over many clouds of different gas and dust properties. Therefore, any details concerning the relationship between the dust properties and the interstellar environments are lost. Here we utilize the wealth of extinction and elemental abundance data obtained by space telescopes and explore the dust properties of a large number of individual sightlines. We model the observed extinction curve of each sightline and derive the abundances of the major dust-forming elements (i.e., C, O, Si, Mg and Fe) required to be tied up in dust (i.e., dust depletion). We then confront the derived dust depletions with the observed gas-phase abundances of these elements and investigate the environmental effects on the dust properties and elemental depletions. It is found that for the majority of the sightlines the interstellar oxygen atoms are fully accommodated by gas and dust and therefore there does not appear to be a “missing oxygen” problem. For those sightlines with an extinction-to-hydrogen column density $A_V/N_H \gtrsim 4.8 \times 10^{-22} \text{ mag cm}^2 \text{ H}^{-1}$ there are shortages of C, Si, Mg and Fe elements for making dust to account for the observed extinction, even if the interstellar C/H, Si/H, Mg/H and Fe/H abundances are assumed to be protosolar abundances augmented by Galactic chemical evolution.

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C₆₀ Cation as the Carrier of the $\lambda 9577$ Å and $\lambda 9632$ Å Diffuse Interstellar Bands: Further Support from the VLT/X-Shooter Spectra

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Ever since their first detection over 100 years ago, the mysterious diffuse interstellar bands (DIBs), a set of several hundred broad absorption features seen against distant stars in the optical and near infrared wavelength range, largely remain unidentified. The close match both in wavelengths and in relative strengths recently found between the experimental absorption spectra of gas-phase buckminsterfullerene ions (C₆₀⁺) and four DIBs at $\lambda 9632$ Å, $\lambda 9577$ Å, $\lambda 9428$ Å and $\lambda 9365$ Å (and, to a lesser degree, a weaker DIB at $\lambda 9348$ Å) suggests C₆₀⁺ as a promising carrier for these DIBs. However, arguments against the C₆₀⁺ identification remain and are mostly concerned with the large variation in the intensity ratios of the $\lambda 9632$ Å and $\lambda 9577$ Å DIBs. In this work, we search for these DIBs in the ESO VLT/X-shooter archival data and identify the $\lambda 9632$ Å, $\lambda 9577$ Å, $\lambda 9428$ Å, and $\lambda 9365$ Å DIBs in a sample of 25 stars. While the $\lambda 9428$ Å and $\lambda 9365$ Å DIBs are too noisy to allow any reliable analysis, the $\lambda 9632$ Å and $\lambda 9577$ Å DIBs are unambiguously detected and, after correcting for telluric water vapor absorption, their correlation can be used to probe their origin. To this end, we select a subsample of nine hot, O- or B0-type stars of which the stellar Mg II contamination to the $\lambda 9632$ Å DIB is negligibly small. We find that their equivalent widths, after normalized by reddening to eliminate their common correlation with the density of interstellar clouds, exhibit a tight, positive correlation, supporting C₆₀⁺ as the carrier of the $\lambda 9632$ Å and $\lambda 9577$ Å DIBs.

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Where Have All the Interstellar Silicon Carbides Gone?

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The detection of the 11.3 μm emission feature characteristic of the Si–C stretch in carbon-rich evolved stars reveals that silicon carbide (SiC) dust grains are condensed in the outflows of carbon stars. SiC dust could be a significant constituent of interstellar dust since it is generally believed that carbon stars inject a considerable amount of dust into the interstellar medium (ISM). The presence of SiC dust in the ISM is also supported by the identification of presolar SiC grains of stellar origin in primitive meteorites. However, the 11.3 μm absorption feature of SiC has never been seen in the ISM and oxidative destruction of SiC is often invoked. In this work we quantitatively explore the destruction of interstellar SiC dust through oxidation based on molecular dynamics simulations and density functional theory calculations. We find that the reaction of an oxygen atom with SiC molecules and clusters is exothermic and could cause CO-loss. Nevertheless, even if this is extrapolable to bulk SiC dust, the destruction rate of SiC dust through oxidation could still be considerably smaller than the (currently believed) injection rate from carbon stars. Therefore, the lack of the 11.3 μm absorption feature of SiC dust in the ISM remains a mystery. A possible solution may lie in the currently believed stellar injection rate of SiC (which may have been overestimated) and/or the size of SiC dust (which may actually be considerably smaller than submicron in size).

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Dust destruction and survival in the Cassiopeia A reverse shock

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Core-collapse supernovae (CCSNe) produce large ($\gtrsim 0.1 M_{\odot}$) masses of dust, and are potentially the primary source of dust in the Universe, but much of this dust may be destroyed before reaching the interstellar medium. Cassiopeia A (Cas A) is the only supernova remnant where an observational measurement of the dust destruction efficiency in the reverse shock is possible at present. We determine the pre- and post-shock dust masses in Cas A using a substantially improved dust emission model. In our preferred models, the unshocked ejecta contains 0.6–0.8 M_{\odot} of 0.1 μm silicate grains, while the post-shock ejecta has 0.02–0.09 M_{\odot} of 5–10 nm grains in dense clumps, and $2 \times 10^{-3} M_{\odot}$ of 0.1 μm grains in the diffuse X-ray emitting shocked ejecta. The implied dust destruction efficiency is 74–94 % in the clumps and 92–98 % overall, giving Cas A a final dust yield of 0.05–0.30 M_{\odot} . If the unshocked ejecta grains are larger than 0.1 μm , the dust masses are higher, the destruction efficiencies are lower, and the final yield may exceed 0.5 M_{\odot} . As Cas A has a dense circumstellar environment and thus a much stronger reverse shock than is typical, the average dust destruction efficiency across all CCSNe is likely to be lower, and the average dust yield higher. This supports a mostly-stellar origin for the cosmic dust budget.

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The impact of metallicity-dependent dust destruction on the dust-to-metals ratio in galaxies

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The ratio of the mass of interstellar dust to the total mass of metals (the dust-to-metals/DTM ratio) tends to increase with metallicity. This can be explained by the increasing efficiency of grain growth in the interstellar medium (ISM) at higher metallicities, with a corollary being that the low DTM ratios seen at low metallicities are due to inefficient stellar dust production. This interpretation assumes that the efficiency of dust destruction in the ISM is constant, whereas it might be expected to increase at low metallicity; the decreased cooling efficiency of low-metallicity gas should result in more post-shock dust destruction via thermal sputtering. We show that incorporating a sufficiently strong metallicity dependence into models of galaxy evolution removes the need for low stellar dust yields. The contribution of stellar sources to the overall dust budget may be significantly underestimated, and that of grain growth overestimated, by models assuming a constant destruction efficiency.

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Survival of polycyclic aromatic hydrocarbon knockout fragments in the interstellar medium

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Laboratory studies play a crucial role in understanding the chemical nature of the interstellar medium (ISM), but the disconnect between experimental timescales and the timescales of reactions in space can make a direct comparisons between observations, laboratory, and model results difficult. Here we study the survival of reactive fragments of the polycyclic aromatic hydrocarbon (PAH) coronene, where individual C atoms have been knocked out of the molecules in hard collisions with He atoms at stellar wind and supernova shockwave velocities. Ionic fragments are stored in the DESIREE cryogenic ion-beam storage ring where we investigate their decay for up to one second. After 10 ms the initially hot stored ions have cooled enough so that spontaneous dissociation no longer takes place at a measurable rate; a majority of the fragments remain intact and will continue to do so indefinitely in isolation. Our findings show that defective PAHs formed in energetic collisions with heavy particles may survive at thermal equilibrium in the interstellar medium indefinitely, and could play an important role in the chemistry in there, due to their increased reactivity compared to intact or photo-fragmented PAHs.

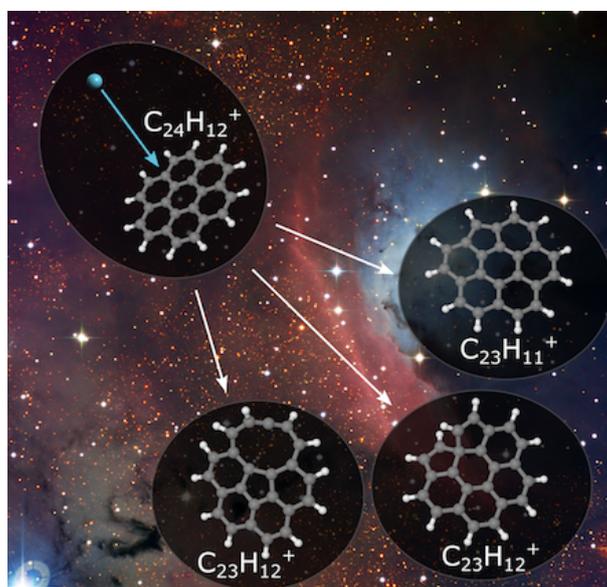


Figure 2 – Examples of fragments produced when a single C atom is knocked out of a coronene cation in a collision with an energetic particle.

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Characterizing Spatial Variations of PAH Emission in the Reflection Nebula NGC 1333

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Infrared emission features at 3.3, 6.2, 7.7, 8.6, and 11.2 μm , attributed to polycyclic aromatic hydrocarbons, show variations in relative intensity, shape, and peak position. These variations depend on the physical conditions of the photodissociation region (PDR) in which strong PAH emission arises, but their relationship has yet to be fully quantified. We aim to better calibrate the response of PAH species to their environment using observations with matching apertures and spatial resolution. We present observations from the Field-Imaging Far-Infrared Line Spectrometer (FIFI-LS) on board the Stratospheric Observatory for Infrared Astronomy (SOFIA) of the gas cooling lines [OI] 63, 146 μm and [CII] 158 μm in the reflection nebula NGC 1333 and use archival dust continuum observations from the Photodetector Array Camera and Spectrometer (PACS) on board Herschel. We employ PDR modelling to derive the physical conditions and compare these with the characteristics of the PAH emission as observed with the Infrared Spectrometer (IRS) on board Spitzer. We find distinct spatial characteristics for the various PAH spectral components. We conclude that the ionic bands (6.2, 7.7, 8.6, and 11.0) and the 7–9 μm emission are due to multiple PAH sub-populations and that the plateaus are distinct from the features perched on top. The 6–9 μm PAH emission exhibit a significant change in behaviour between the irradiated PDR and diffuse outskirts, confirming these bands arise from multiple PAH sub-populations with different underlying molecular properties. We find multiple promising relationships between PAH ratios and the FUV radiation field strength but no clear correlations with the PAH ionization parameter.

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THESIS

Revisiting polycyclic aromatic hydrocarbon emission in Photodissociation regions

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Advisor: Profs. Els Peeters and Jan Cami (University of Western Ontario)

The mid-infrared (IR) spectrum of almost all objects in the Universe is dominated by a set of strong emission features characteristic of a class of large organic molecules made of carbon and hydrogen known as polycyclic aromatic hydrocarbons (PAHs). These molecules account for $\sim 15\%$ of the cosmic carbon and $\sim 20\%$ of the total IR power of the Milky Way and star-forming galaxies. They are strong absorbers of ultraviolet (UV) photons and release the absorbed energy through vibrational transitions that result in strong IR emission features. PAHs play a critical role in the evolution of the interstellar medium (ISM) as they drive much of the ISM's heating and ionization balance. As a result, detailed knowledge of the molecular astrophysics of PAHs, including a thorough understanding of their molecular properties and their interactions with the environment in which they reside, is crucial to understand the evolution of the ISM. Although decades of experimental, theoretical, and observational work have helped gain important insights into the behaviour of PAHs in the ISM, our understanding is far from complete. In this thesis, we investigate the astrophysical behaviour of PAHs from both an observational and theoretical standpoint.

Our observational study focuses on identifying the key parameters that drive the PAH behaviour in two well-known Galactic reflection nebulae, NGC 2023 and NGC 7023, using a Principal Component Analysis. We find that the amount of PAH emission, which represents the PAH abundance and excitation, and the PAH charge state are the only two parameters that drive their behaviour in both environments. In our theoretical study, we develop a model that determines the charge distribution of PAHs and uses it to compute the PAH emission spectrum in astrophysical environments. The relative strengths of the PAH emission features predicted by our model in the Orion Bar, NGC 2023, NGC 7023, the Horsehead nebula, and the diffuse ISM compare well to those obtained from observations. Furthermore, the results of our model highlight the necessity of experimentally determined electron-recombination rates of PAHs and the molecular characteristics of PAH anions, both of which are crucial in understanding PAH behaviour but for which the data is scarce to date.

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Announcements

Principal Scientist Crystallization Nanoform, Helsinki, Finland

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- PhD in Physics, Materials Science, Chemistry or Chemical Engineering preferred, or a related field, with a strong background in Crystallization Science.
- Solid experience with Crystallization Science, ideally from both a theoretical and experimental perspective. Familiarity with process design and development would be advantageous.
- Candidates with theoretical and experimental background from both academia and industry are welcome to apply.
- Familiarity with condensed-matter modelling and/or (multi-scale) molecular modelling of self-assembly of (pharmaceutical) materials in equilibrium and out-of-equilibrium conditions.
- Familiarity with supercritical fluids theoretical/experimental fundamentals and/or technologies is advantageous, but it is not a pre-requisite. Continuous learning is a must.
- Fluent English (written and spoken).
- Effective oral and written communication skills.

Personal Attributes:

- Scientific open mind, curiosity & enthusiasm. Willingness and capability of learning in a fast and efficient way from different domains to find solutions to complex and challenging problems.
- Ability to act as a strong team player while providing scientific and technical leadership on multiple projects.

What we offer you

- An opportunity to do unique and pioneering research and have a real impact.

You'll have:

- Scientific Independence
- Access to state-of-the-art experimental facilities and solid technical support.
- Adequate resources to do the science.
- Excellent IT and administrative support.
- Attractive compensation package with broad employee benefits selection.
- A great international team to join with highly skilled and motivated colleagues.
- Encouraging and forward-looking team spirit.
- You'll be part of a team that invents world-class solutions for the pharma industry, and ultimately for the patient.
- We provide extensive learning opportunities. You'll be able to utilize your skills and competencies widely as we continuously create something new.
- We like challenges and want everyone to enjoy solving them together.

You will get to be part of a unique growth company in the pharma industry.

If you have any questions, please contact Dr. Elisabetta Micelotta or Prof. Niklas Sandler:
elisabetta.michelotta@nanoform.com; niklas.sandler@nanoform.com

Please submit your application (cover letter and CV) by 15th December 2021.

Deadline: 15 December 2021

E-mail for contact: elisabetta.michelotta@nanoform.com

E-mail for contact: niklas.sandler@nanoform.com

Webpage: <https://tinyurl.com/scientist-crystallization>

Webpage: <https://nanoform.com/en/>

Assistant Professor of Interdisciplinary Teaching Related to Origins of Life

Anton Pannekoek Institute, University of Amsterdam, The Netherlands

Advertised by Annemieke Petrignani

JOB DESCRIPTION

We seek to fulfil a tenure-track teaching position (UD) in interdisciplinary origins of life, in strong connection with the Anton Pannekoek Institute for Astronomy (API). We are looking for a candidate who would like to teach across science programs and conduct research programs in the areas of origins of life.

The candidate will coordinate and contribute to the development of a faculty-wide initiative called InterSpecials that is to be implemented across the research and teaching areas of the Faculty of Science (FNWI) at University of Amsterdam (UvA). The InterSpecial initiative is an educational innovation, aimed to teach students both interdisciplinary skills and specialized expertise. The Origins InterSpecial acts as pilot and focuses on the interdisciplinary origins-of-life theme. The applicant will be requested to develop a pedagogical framework for this origin(s)-of-life initiative, as well as to develop new teaching methods and trajectories, and to mentor students through the interdisciplinary learning line. The applicant is also expected to develop their own research within the origins initiative and coordinate it with other researchers in an interdisciplinary framework. The educational duties will cover about 50% of the work. The remaining 50% are dedicated to active research of the UD, in any of the areas associated with the Origin-of-life theme.

We particularly encourage applications from prospective members who can enhance the diversity of backgrounds and ideas in our group. The FNWI is committed to diversity in all its forms and is committed to be inclusive.

WHAT ARE YOU GOING TO DO

You are expected:

- to coordinate the development and implementation of a faculty-wide Origins InterSpecial initiative and participate to teaching and coaching students;
- to be active in the fundamental and/or applied research related to our origins of life initiative, publishing in high level international journals;
- to teach origins of life related courses at the BSc and MSc levels across the faculty of science;
- to foster the connections between science and research;
- to present your work at leading conferences;

- to be willing to build up a research group of internationally outstanding level;
- to be willing to support potential rollout of the Origin InterSpecial initiative to other interdisciplinary areas;
- to be active in the attraction of external funding;
- to supervise students, including BSc, MSc and PhD as well as postdocs;
- to actively contribute to departmental duties.

REQUIREMENTS

What do we require:

- A PhD in Astronomy, Astrophysics, Physics, Planetary Science, Chemistry, Biology or Informatics, or related fields.
- An affinity to work on origin of life initiatives and to teach on the related topics.
- An affinity for interdisciplinary work and functioning in a team.
- The ability and willingness to teach and conduct research.
- Demonstrable willingness to perform administrative, organizational tasks, and to build up curriculum activities.
- Excellent communication skills.
- Willingness to work on public outreach.
- Teaching experience will be a strong plus.
- Experience in interdisciplinary teaching, course development and/or teaching material to diverse students will be an advantage.
- The applicant is expected to obtain teaching qualification BKO level within two years and a SKO level within five years.

CONDITIONS OF EMPLOYEMENT

Fixed-term contract: 18 months

Our offer:

The initial appointment will be for a period of 18 months, to evaluate the suitability of the candidate. During this period three evaluations will take place. On the basis of a positive evaluation, the position will become permanent after 18 months.

The starting salary will be in accordance with university regulations for academic personnel, and depending on experience and qualifications. It will range from a minimum €3,807 to €5,211 (scale 11) gross per month (salary scale) based on full-time employment.

This is exclusive 8% holiday allowance and 8.3% end-of-year bonus. A favourable tax agreement, the '30% ruling', may apply to non-Dutch applicants. The Collective Labour Agreement of Dutch Universities is applicable.

EMPLOYER

University of Amsterdam

With over 6,000 employees, 30,000 students and a budget of more than 600 million euros, the University of Amsterdam (UvA) is an intellectual hub within the Netherlands. Teaching and research at the UvA are conducted within seven faculties: Humanities, Social and Behavioural Sciences, Economics and Business, Law, Science, Medicine and Dentistry. Housed on four city campuses in or near the heart of Amsterdam, where disciplines come together and interact, the faculties have close links with thousands of researchers and hundreds of institutions at home and abroad.

The UvA's students and employees are independent thinkers, competent rebels who dare to question dogmas and aren't satisfied with easy answers and standard solutions. To work at the UvA is to work in an independent, creative, innovative and international climate characterised by an open atmosphere and a genuine engagement with the city of Amsterdam and society.

DEPARTMENT

Faculty of Science – Anton Pannekoek Institute for Astronomy

The Faculty of Science has a student body of around 7,000, as well as 1,600 members of staff working in education, research or support services. Researchers and students at the Faculty of Science are fascinated by every aspect of how the world works, be it elementary particles, the birth of the universe or the functioning of the brain.

The FNWI offers a complete undergraduate (BSc) and graduate (MSc, PhD) teaching program in various disciplines that focuses on integrating students in research early in their education. The applicant should be committed to contribute in innovative ways to the excellence of our teaching programs, and to foster the connections between science and research.

Scientists at FNWI have access to a wide variety of national funding lines at the Dutch research organization NWO, and to European funding lines like ERC grants and FP7 programs and networks. Scientists at UvA have set an interdisciplinary collaborative research and training program on the origins and fundamental aspects of life, as part of the national Origin Center. UvA is also part of the National Astronomy Education Committee NOVA, the Dutch Top Research School. In this context, the department of Astronomy (the Anton Pannekoek Institute, API) has a long tradition of excellence in astronomical research, including a program on star and planet formation, and exoplanets; it is currently in the process of strengthening its group in origins research.

The Anton Pannekoek Institute for Astronomy furthers research, teaching and public understanding of astronomy. It conducts astronomical research and trains astronomers from bachelor to postdoctoral level, aiming at world-leading levels and activities.

ADDITIONAL INFORMATION

Do you have questions about this vacancy? Or do you want to know more about our organisation? Please contact: Jean-Michel Désert, Annemieke Petrignani and/or Carsten Dominik (email addresses given below).

Deadline: 31 December 2021

E-mail for contact: desert@uva.nl

E-mail for contact: A.Petrignani@uva.nl

E-mail for contact: dominik@uva.nl

Webpage: <https://tinyurl.com/job-originsoflife>

AstroPAH Newsletter

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

astropah@strw.leidenuniv.nl

Next issue: 16 December 2021

Submission deadline: 3 December 2021