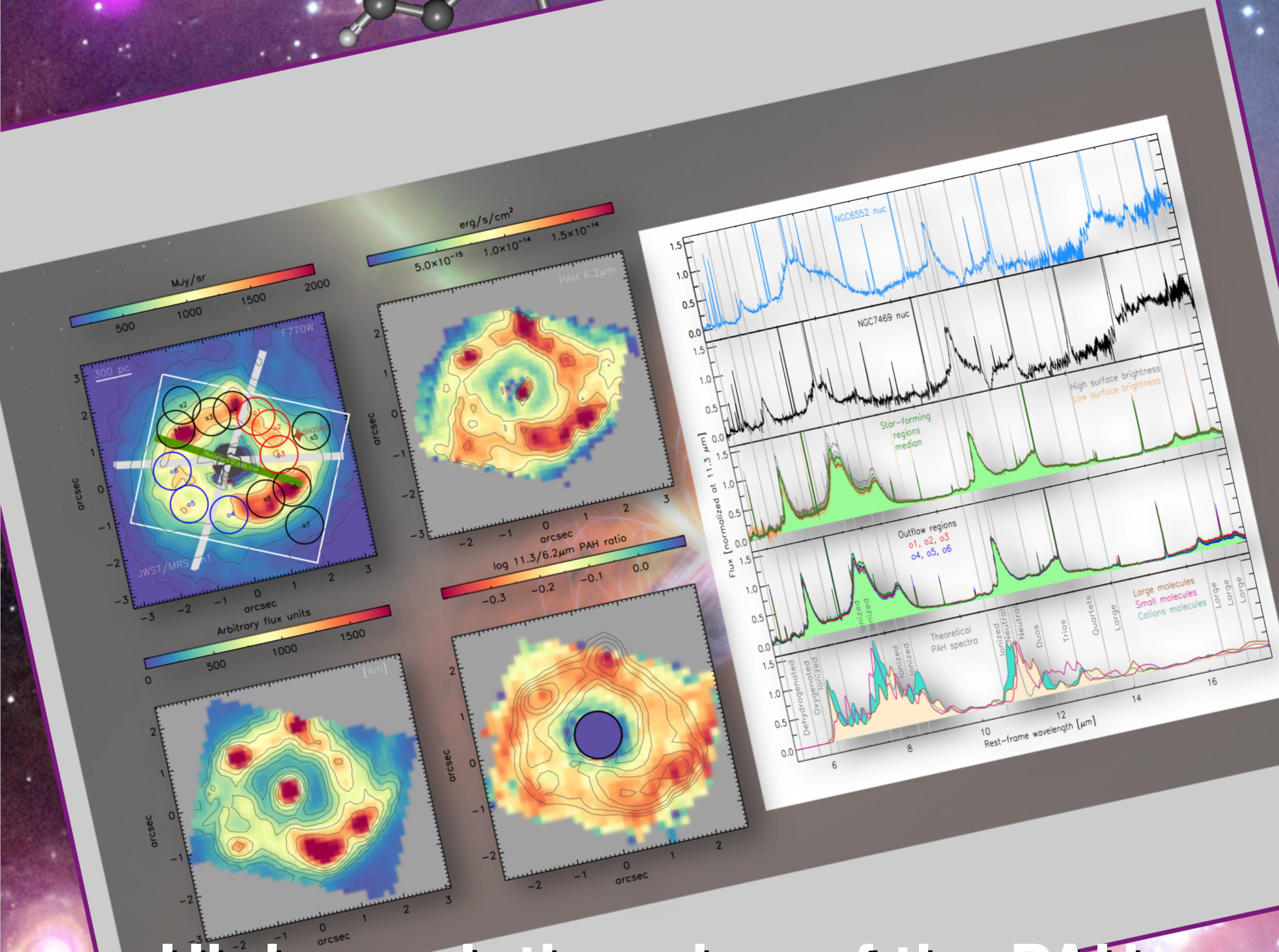
AstroPAH

A Newsletter on Astronomical PAHs

Issue 94 • December 2022



High resolution view of the PAH emission using JWST/MRS data

Editorial

Dear Colleagues,

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

To commemorate JWST's launch anniversary this December, we dedicate the Picture of the Month and the In Focus section of this issue to highlighting the science results from four Early Release Science (ERS) programs. We thank Lee Armus and Aaron Evans (ERS Programme 1328), Olivier Berné, Emilie Habart and Els Peeters (ERS Programme 1288, PDRs4All), Ryan Lau (ERS Programme 1349, WR DustERS), and Melissa McClure, Adwin Boogert and Harold Linnartz (ERS Programme 1309, IceAge) for contributing to this special In Focus. Also a reminder that all are welcome to share their results and research with us and to be featured in our In Focus.

The James Webb Space Telescope Cycle 2 Call for Proposals has now been released. This Call includes Observations and funding for Archival Research and Theoretical Research Programs. Up to 5,000 hours will be available in this cycle. Proposal deadline is January 27, 2023.

As always, we have a trove of exciting abstracts. We also want to draw your attention to two conference announcements. The registration is now open for the 2023 Kavli-IAU Astrochemistry Symposium: "From the First Galaxies to the Formation of Habitable Worlds", which will be held in Traverse City, MI, USA, July 10–14, 2023. The AOGS 2023, which will be held in Singapore from 30 July to 4 August, 2023, will have an astrochemistry-relevant planetary science session titled "Astrochemical Processes Leading to the Formation of Planetary Bodies in the Solar System". Registration and abstract submission are now open.

If you are on Instagram, be sure to check out our next PAH of the Month, an interesting dehydrogenated PAH.

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.

We wish you pleasant and relaxing holidays! AstroPAH will be back in February after we return from our annual January break.

The Editorial Team

Next issue: 23 February 2023.
Submission deadline: 10 February 2023.

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PAH Picture of the Month

High angular resolution view of the PAH emission in Seyfert galaxies using JWST/MRS data by García-Bernete et al. 2022. On the left are the maps of the central 6 region of NGC 7469, which include the AGN and the circum-nuclear ring of star formation. The maps indicate that the PAH emission mainly traces the star-forming regions. On the right are continuum-subtracted spectra showing the PAH emission together with the fine-structure lines.

Credits: Plots: García-Bernete et al. 2022. Background image credit: Artist's impression of an active supermassive black hole by ESO/L. Calçada.

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Celebrating JWST

A highlight of the PAH-related science results

Introduction

Dr. Ameek Sidhu

The launch of the James Webb Space Telescope (JWST) on December 25, 2021, marked the beginning of a golden era in infrared (IR) astronomy. With four scientific instruments onboard, the Near Infrared Camera (NIRCam), the Near-Infrared Spectrograph (NIRSpec), the Mid-Infrared Instrument (MIRI), and the Fine Guidance Sensor/Near Infrared Imager and Slitless Spectrograph (FGS-NIRISS), JWST provides imaging and spectroscopy from 0.6 to 28.8 µm. The first five public JWST images, released in July 2022, revealed an unprecedented view of the Universe, spanning from different stages of star evolution to the most profound views of the early Universe. The field of PAH astrophysics is also on the verge of a revolution in this golden era of IR spectroscopy, as PAHs emit strongly in the IR wavelength region. For the first time, we will obtain the full spectral coverage of PAH emission over small spatial scales. This will enable detailed studies of PAH emission characteristics, shedding light on the molecular properties of the interstellar PAH family. Moreover, the detailed observations of PAHs in the near and far Universe combined with the observations of gas and dust in a wide variety of astrophysical environments will be critical in obtaining the complete picture of PAH evolution in the interstellar medium.

To commemorate JWST's launch anniversary this December, we dedicate this issue to highlighting the science results from four Early Release Science (ERS) programs. The ERS programs were designed to educate the community about the potential and capabilities of the telescope. Here, we invite the Principal Investigators from four of the thirteen ERS programs to highlight their first astrochemistry-related science results.

ERS Programme 1328

A JWST Study of the Starburst-AGN Connection in Merging LIRGs

PIs: Lee Armus and Aaron Evans

Galactic mergers, which can trigger massive starbursts and powerful AGN via the fueling of super-massive black holes, are a key component of galaxy evolution. These periods of rapid evolution are often enshrouded by dust, making observations at short wavelengths extremely difficult. The James Webb Space Telescope is set to transform our understanding of infrared and merging galaxies, providing a detailed look at the physics of star formation and black hole growth in nearby and distant systems.

In Director's Discretionary Time, Early Release Science program 1328 (Co-PI's: L. Armus, A. Evans), "A JWST Study of the Starburst-AGN Connection in Merging Luminous Infrared Galaxies", we are observing four nearby, Luminous Infrared Galaxies (LIRGs) selected from the Great Observatories All-sky LIRG Survey (GOALS). The targets, **NGC 7469** (IRAS 23007+0836, UGC 12332), **NGC 3256** (IRAS 10257-4338), **VV114** (IRAS 01053-1746, Arp 236) and **II Zw 096** are representative of the range of galaxy properties in GOALS, such as relative starburst and AGN power, merger stage, luminosity, and spectral feature strengths. With NIRSpec, NIRCam and MIRI, we are measuring the dynamics and physical conditions in the atomic and warm molecular gas and the dust on scales of 50-100 pc in the nuclei of local LIRGs at unprecedented sensitivity.

Three of the four ERS targets have been observed and the initial results have been published in a series of papers available on astro-ph. Among these papers are four that describe the properties of the high-speed outflowing wind and the star-forming regions and ISM in the circum-nuclear region of the Seyfert 1.5 type galaxy, NGC 7469. In particular, with the IFU data, we find direct evidence for excess warm and turbulent molecular gas and AGN feedback on the PAH populations within 300 pc of the nucleus (Lai et al. 2022, U et al. 2022). The size and ionization of PAHs in the star-forming ring vary moderately at a level of 30% probed by the PAH inter-band ratios. The largest change in the PAH band ratios occurs in the radial direction when moving from the ring towards the central AGN where the grains appear to increase in size and become more ionized.

JWST is allowing us to study multiple PAH features and map changing grain properties in external galaxies on sub-kpc scales in the mid-infrared for the first time. More detailed analysis of the full spectroscopic and imaging datasets are ongoing.

The GOALS JWST ERS team consists of more than 30 scientists in 8 countries representing 18 institutions. A full description of GOALS, as well as highlights of and links to our recent publications, can be found on the GOALS team website.

Team Website: https://goals.ipac.caltech.edu/

ERS Programme 1288: PDRs4All

Radiative Feedback from Massive Stars as Traced by Multiband Imaging and Spectroscopic Mosaics

PIs: Olivier Berné, Emilie Habart, and Els Peeters

Mechanical and radiative feedback from massive stars drive the evolution of interstellar matter in our Galaxy and throughout the Universe, from the era of vigorous star formation at redshifts of 1–3 to the present day. Photo-Dissociation Regions (PDRs), where far-ultraviolet photons (E $<$ 13.6 eV) from these stars create a largely neutral but warm region of gas and dust, are ideal laboratories to study these main feedback processes.

“PDRs4All” obtained breathtaking JWST images and spectra of the Orion Nebula and the proto-typical PDR, the Orion Bar. These observations reveal a hyper-structured molecular cloud edge. Indeed, for the first time, we spatially resolve the PDR in the IR, exposing the individual spectral signatures from the key zones and sub-regions within the ionized gas, the atomic PDR, the molecular PDR, and the molecular cloud with unprecedented detail. We identify and characterize an incredibly rich inventory of spectral features, showcasing emission of H I recombination lines with upper levels as high as 50, He I and He II lines, ionic lines tracing the ionized and neutral gas, C I recombination lines, fluorescence lines of O I and NI, a wealth of H_2 rovibrational and rotational lines, as well as CO, CH^+ and HD emission lines, and the aromatic infrared bands.

Due to the proximity of the Orion Nebula and the unprecedented spatial resolution of JWST, this incredibly rich dataset reveals the physical and chemical anatomy of PDRs showcasing its steep edges and inhomogeneous structure at scales inaccessible before (see Fig.1). As such, this dataset revises the commonly used, 2D stratified structure (or cartoon) of the PDR anatomy and will benchmark and transform PDR models for the JWST era.

In addition, the PDRs4All dataset includes several proplyds, i.e. planet-forming disks around low-mass stars. The evolution of such disks in stellar clusters is believed to be significantly affected by far-UV photons that heat the gas and lead to mass-loss through photo-evaporation. Direct detection and characterization of these photo-evaporating flows however require a combination of high spatial and spectral resolution. The PDRs4All dataset, combined with Atacama Large Millimeter Array (ALMA) observations, reveals the photo-evaporation flow of the 203-506 protoplanetary disk, located near the Trapezium cluster in the Orion Nebula, and allows the first direct characterization of a photo-evaporating flow. A mass-loss rate of the order of 10^{-7} $\mathrm{M}_{\odot}$/yr is derived, which is in agreement with 1D dynamical models where small dust grains in the flow provide a large UV opacity. This is compatible with the detection of large amounts of PAH molecules in the flow which efficiently absorb UV.

Team Website: https://pdrs4all.org/

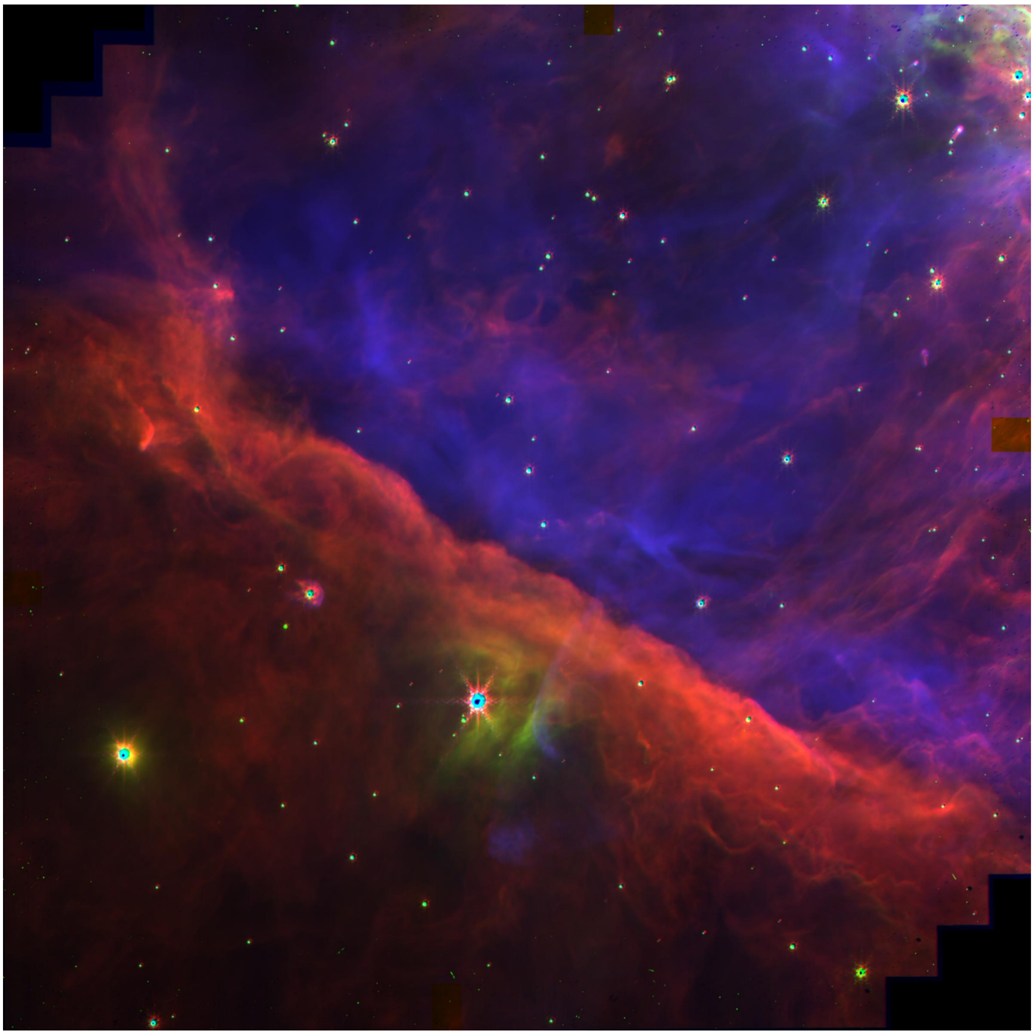

Figure 1 *– Composite image (3 colors) with filters showing key tracers of ionized gas, aromatic hydrocarbons, dust and molecular gas: F187N (blue), F335M (red), F470N (green).*

References

1. *"PDRs4All: A JWST Early Release Science Program on radiative feedback from massive stars", Berné, Habart, Peeters et al. 2022, PASP 134, 1035*
2. *"PDRs4All II: JWST's NIR and MIR imaging view of the Orion Nebula", Habart, Peeters, Berné et al. 2023, in prep.*
3. *"PDRs4All III: JWST's NIR spectroscopic view of the Orion Bar", Peeters, Berné, Habart et al. 2023, in prep.*
4. *"PDRs4All IV: A molecular photoevaporation flow from a young protoplanetary disk as revealed by JWST", Berné, Habart, Peeters et al. 2023, in prep.*

ERS Programme 1309: Ice Age

Chemical Evolution of Ices during Star Formation

PIs: Dr. Melissa McClure, Dr. Adwin Boogert and Prof. Harold Linnartz

Icy grain mantles are the main reservoir for volatile elements in star-forming regions across the Universe, as well as the formation site of prebiotic complex organic molecules (COMs) seen in our Solar System. In the "Ice Age" JWST Early Release Science program (PID 1309, 32 hours), we trace the evolution of pristine and complex ice chemistry in a representative low-mass star-forming region through observations of: the dark molecular cloud itself, a pre-stellar core, a Class 0 protostar, a Class I protostar, and a protoplanetary disk. These observations reveal the chemical evolution of the reservoir of material that will form comets and planetary atmospheres.

We are mapping the spatial distribution of ices down to $\sim$ 20–50 AU in these targets to identify when, and at what visual extinction, the formation of each ice species begins. Comparing high spectral resolution (R $\sim$ 1500–3000) and sensitivity (S/N $\sim$ 100–300) observations from 3 to 15 µm to template laboratory and radiative transfer model spectra will allow us to search for new COMs, as well as distinguish between different ice morphologies, thermal histories, and mixing environments.

The analysis of these data is producing science enabling products beneficial to Cycle 2 proposers. A newly updated public laboratory ice database will provide feature identifications for all of the expected ices. This database, organized by co-PI Prof. Harold Linnartz and Dr. Will Rocha at the Leiden Laboratory for Astrophysics was released this summer (the Leiden Ice Database for Astrochemistry - LIDA), and is described in Rocha et al. (2022), which is a highlighted article in A&A. A chemical model by Ice Age team members Prof. Rob Garrod and Dr. Miwha Jin was used to predict ice abundances for the Class 0 envelope in a paper published this summer (Jin et al. 2022), and other team members are working to produce a further grid of chemical models for the other star formation stages with varying UV fields to simulate other environments. We anticipate that these resources will be particularly useful for astrochemistry and spectroscopy of fainter, extended targets like star forming regions of the SMC/LMC or more distant galaxies.

The team is working to overcome several difficulties with the data calibration, pipeline, and MIRI instrument to reduce the data that was taken in the summer, and we anticipate more data in February. Co-PI Dr. Adwin Boogert and Dr. Helen Fraser are leading a team working to improve the pipeline algorithms for extraction of NIRCam WFSS spectra in crowded fields with strong, spatially variable background emission and contaminating bright or extended sources. The first results paper is in press at Nature Astronomy (McClure et al. 2023, accepted December 1st, 2022), led by PI Dr. Melissa McClure, showcasing high fidelity NIRSpec Fixed Slit, MIRI LRS, and NIRCam WFSS mode observations of the densest lines of sight observed in a molecular cloud. This paper has been an enormous team effort involving three instruments and a team of 42 co-authors. The spectra reveal the many weak ice features, including for the first time in quiescent cloud material the ice species OCN-, OCS, and ^{13}CO along with functional groups for COMs, likely ethanol and acetaldehyde. The presence of these features suggests that ice complexity starts at an early, pre-stellar stage in the molecular cloud. The results will be published within the next month, with an embargoed press release.

Team Website: http://jwst-iceage.org/

ERS Programme 1349: WR DustERS

Establishing Extreme Dynamic Range with JWST: Decoding Smoke Signals in the Glare of a Wolf-Rayet Binary

PI: Dr. Ryan Lau

Dust is a key ingredient in the formation of stars and planets. However, the dominant channels of dust production throughout cosmic time are still unclear. With its unprecedented sensitivity and spatial resolution in the mid-IR, JWST is the ideal platform to address this issue by investigating the dust abundance, composition, and production rates of various dusty sources. In particular, colliding-wind Wolf-Rayet (WR) binaries are efficient dust producers in the local Universe, and likely existed in the earliest galaxies. To study these interesting objects, we have conducted JWST observations of the colliding-wind binaries WR140 (Fig. 2) and WR137 to study WR dust composition, abundance, and formation mechanisms.

Figure 2 *– The two stars in Wolf-Rayet 140 produce shells of dust every eight years that look like rings, as seen in this image from NASA's James Webb Space Telescope. Each ring was created when the stars came close together and their stellar winds collided. Credit: NASA/ESA/CSA/STScI/JPL-Caltech*

In our ERS program (ERS 1349 - WR DustERS), we utilized three key JWST observing modes:

1. The Medium-Resolution Spectrometer (MRS) on the Mid-Infrared Instrument (MIRI)
2. The Imager on the Mid-Infrared Instrument (MIRI)
3. Aperture Masking Interferometry (AMI) mode with the Near Infrared Imager and Slitless Spectrograph (NIRISS)

We have published initial results from our MIRI Imager and MRS observations of WR140 in Nature Astronomy. The MIRI observations reveal the presence of more than 17 circumstellar dust shells around WR140 formed by the binary system over the past 140 years, and the spectroscopic signatures of the circumstellar dust is consistent with "Unidentified Infrared Band" features. Our results indicate that dust-forming carbon-rich WR binaries like WR140 are enriching the interstellar medium with carbon-rich aromatic compounds and carbonaceous dust.

Team Website: https://www.ir.isas.jaxa.jp/ ryanlau/WRDustERS/index.html

Abstracts

Study of vibrational spectra of polycyclic aromatic hydrocarbons with phenyl side group

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Computational study of polycyclic aromatic hydrocarbons (PAHs) with phenyl side group substituted at different positions is reported. The infrared spectral variations due to the position of phenyl substitution, ionization state and the size of the molecules are discussed and possible contribution of phenyl-PAHs to the mid-infrared emission features from astrophysical objects is analyzed. Structurally phenyl group substitution at 2^{nd} position gives more stable species compared to substitution at other positions. Phenyl-PAHs exhibit new aromatic bands near 695 and 741 cm^{-1} (14.4 and 13.5 µm), due to contribution from quintet C–H wag, that compare well with minor features at 14.2 and 13.5 µm observed in several astrophysical objects. Just as in plain PAHs, the C–C stretch vibrational modes ($\sim$1600 cm^{-1}) have negligible intensity in neutrals, but the cations of all phenyl-PAHs exhibit significantly strong phenyl group C–C stretch peak close to class B type 6.2 µm astrophysical band. In 2-phenylpyrene, it is the neutral molecule that exhibits this strong feature in the 6.2 µm range along with other features that match with sub-features at 6.66 and 6.9 µm, observed in astronomical spectra of some late type objects. The substitution of phenyl side group at solo position shifts the C–C stretch mode of parent PAH close to the region of 6.2 µm astrophysical band. The results indicate possibility of phenyl-PAHs in space and the bottom-up formation of medium sized compact PAHs with phenyl side group in carbon rich cool circumstellar shells. Phenyl-PAHs need to be considered in modelling mid-infrared emission spectra of various astrophysical objects.

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The mid-infrared molecular inventory towards Orion IRc2

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We present the first high spectral resolution mid-infrared survey in the Orion BN/KL region, covering 7.2 to 28.3 µm. With SOFIA/EXES we target the enigmatic source Orion IRc2. While this is in the most prolifically studied massive star-forming region, longer wavelengths and molecular emission lines dominated previous spectral surveys. The mid-infrared observations in this work access different components and molecular species in unprecedented detail. We unambiguously identify two new kinematic components, both chemically rich with multiple molecular absorption lines. The “blue clump” has $v_{\mathrm{LSR}}=-7.1\pm0.7$ km s^{-1} and the “red clump” 1.4 ± 0.5 km s^{-1}. While the blue and red clumps have similar temperatures and line widths, molecular species in the blue clump have higher column densities. They are both likely linked to pure rotational H_2 emission also covered by this survey. This work provides evidence for the scenario that the blue and red clumps are distinct components unrelated to the classic components in the Orion BN/KL region. **Comparison to spectroscopic surveys towards other infrared targets in the region show that the blue clump is clearly extended.** We analyze, compare, and present in depth findings on the physical conditions of C_2H_2, $^{13}CCH_2$, CH_4, CS, H_2O, HCN, $H^{13}CCN$, HNC, NH_3, and SO_2 absorption lines and an H_2 emission line associated with the blue and red clumps. We also provide limited analysis of H_2O and SiO molecular emission lines towards Orion IRc2 and the atomic forbidden transitions [FeII], [SI], [SIII], and [NeII].

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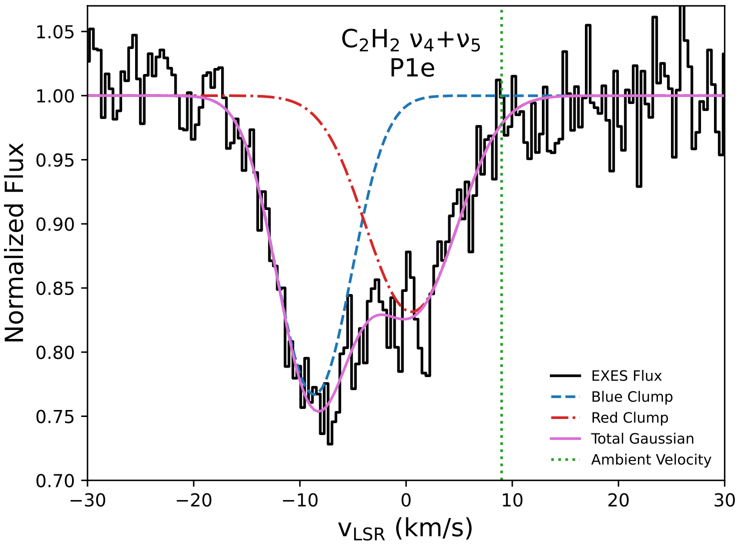

Gaussian fit for the P1e transition of the $\nu_5 + \nu_4$ band of C_2H_2. Black is the normalized EXES flux. Magenta is the total Gaussian fit, while the blue and red belong respectively to the blue clump and the red clump. The vertical, green dotted line indicates the systematic, ambient cloud velocity 9 km s^{-1}(Zapata et al. 2012)

GOALS-JWST: Tracing AGN Feedback on the Star-Forming ISM in NGC 7469

Thomas S.-Y. Lai, Lee Armus, and the GOALS Team

IPAC, California Institute of Technology, Pasadena, CA, USA

We present *James Webb Space Telescope (JWST)* Mid-InfraRed Instrument (MIRI) integral-field spectroscopy of the nearby merging, luminous infrared galaxy, NGC 7469. This galaxy hosts a Seyfert type-1.5 nucleus, a highly ionized outflow, and a bright, circumnuclear star-forming ring, making it an ideal target to study AGN feedback in the local Universe. We take advantage of the high spatial/spectral resolution of *JWST*/MIRI to isolate the star-forming regions surrounding the central active nucleus and study the properties of the dust and warm molecular gas on $\sim$100 pc scales. The starburst ring exhibits prominent Polycyclic Aromatic Hydrocarbon (PAH) emission, with grain sizes and ionization states varying by only $\sim$30%, and a total star formation rate of 10–30 $M_\odot$/yr derived from fine structure and recombination emission lines. Using pure rotational lines of H_2, we detect 1.2×10^7 $M_\odot$ of warm molecular gas at a temperature higher than 200 K in the ring. All PAH bands get significantly weaker towards the central source, where larger and possibly more ionized grains dominate the emission, likely the result of the ionizing radiation and/or the fast wind emerging from the AGN. The small grains and warm molecular gas in the bright regions of the ring however display properties consistent with normal star-forming regions. These observations highlight the power of *JWST* to probe the inner regions of dusty, rapidly evolving galaxies for signatures of feedback and inform models that seek to explain the co-evolution of supermassive black holes and their hosts.

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The Astrophysical Journal Letters (in publication)

https://arxiv.org/pdf/2209.06741.pdf

Theoretical study of infrared and ultraviolet spectra of fourteen isomers of C_{24} and comparison with astronomical observations

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The present paper discusses the infrared features of C_{24} based on the Density Functional Theory (DFT) calculation and suggests some of the features observed in celestial objects may be attributed to C_{24}. We also calculate the electronic absorption spectra of the C_{24} isomers to compare with the bump feature at 217 nm in the interstellar extinction curve. The C_{24} isomers are of four groups viz. cage, planar, bowl, and ring forms, and the present study considers their neutral and charged states. The structural parameters are reported for the first time. The planar structure is the most stable and the ring structure has a significant dipole moment observed. We extract theoretical infrared spectra of fourteen isomers in their neutral and charged states at the B3LYP /6-311++G** level of theory. The time-dependent density functional theory (TDDFT) approach is used to calculate the electronic transitions, the absorbance, and the HOMO to LUMO gaps of the 14 C24 isomers in their neutral and charged states. Upon ionization, significant changes are observed in the infrared and electronic absorption spectra, and the structural parameters. Average theoretical spectra of the cage, planar, bowl, and ring of the C_{24} isomer show the features at 6.2 µm, 7.65 µm, 8.65 µm, 11.3 µm, 12.8 µm, and 35.6 µm, which match with the features in the observed spectra of the reflection nebulae, NGC 2023 and NGC 7023. A sign of a bump in the ultraviolet at around 218 nm is observed in the electronic absorption spectra.

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Reparameterized semi-empirical methods for computing anharmonic vibrational frequencies of multiply-bonded hydrocarbons

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Reparameterized semi-empirical methods can reproduce gas-phase experimental vibrational frequencies to within 24 cm^{-1} or better for a 100-fold decrease in computational cost in the anharmonic fundamental vibrational frequencies. To achieve such accuracy and efficiency, the default parameters in the PM6 semi-empirical model are herein optimized to reproduce the experimental and high-level theoretical vibrational spectra of three small hydrocarbon molecules, C_2H_2, *c*-C_2H_2, and C_2H_4, with the hope that these same parameters will be applicable to large polycyclic aromatic hydrocarbons (PAHs). This massive cost reduction allows for the computation of explicit anharmonic frequencies and the inclusion of resonance corrections that have been shown to be essential for accurate predictions of anharmonic frequencies. Such accurate predictions are necessary to help to disentangle the heretofore unidentified infrared spectral features observed around diverse astronomical bodies and hypothesized to be caused by PAHs, especially with the upcoming influx of observational data from the *James Webb Space Telescope*. The optimized PM6 parameters presented herein represent a substantial step in this direction with those obtained for ethylene (C_2H_4) yielding a 37% reduction in the mean absolute error of the fundamental frequencies compared to the default PM6 parameters.

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The Spectral Features and Detectability of Small, Cyclic Silicon Carbide Clusters

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Rovibrational spectral data for several tetra-atomic silicon carbide clusters (TASCCs) are computed in this work using a CCSD(T)-F12b/cc-pCVTZ-F12 quartic force field. Accurate theoretical spectroscopic data may facilitate the observation of TASCCs in the interstellar medium which may lead to a more complete understanding of how the smallest silicon carbide (SiC) solids are formed. Such processes are essential for understanding SiC dust grain formation. Due to SiC dust prevalence in the interstellar medium, this may also shed light on subsequent planetary formation. Rhomboidal Si_2C_2 is shown here to have a notably intense (247 km mol^{-1}) anharmonic vibrational frequency at 988.1 cm^{-1} (10.1 µm) for ν_2, falling into one of the spectral emission features typically associated with unknown infrared bands of various astronomical regions. Notable intensities are also present for several of the computed anharmonic vibrational frequencies including the cyclic forms of C_4, SiC_3, Si_3C, and Si_4. These features in the 6 to 10 µm range are natural targets for infrared observation with the *James Webb Space Telescope*'s MIRI instrument. Additionally, *t*-Si_2C_2, *d*-Si_3C, and *r*-SiC_3 each possess dipole moments of greater than 2.0 D making them interesting targets for radioastronomical searches especially since *d*-SiC_3 is already known in astrophysical media.

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Fragmentation of the PAH cations of Isoviolanthrene and Dicoronylene: A case made for interstellar cyclo[n]carbons as products of universal fragmentation processes

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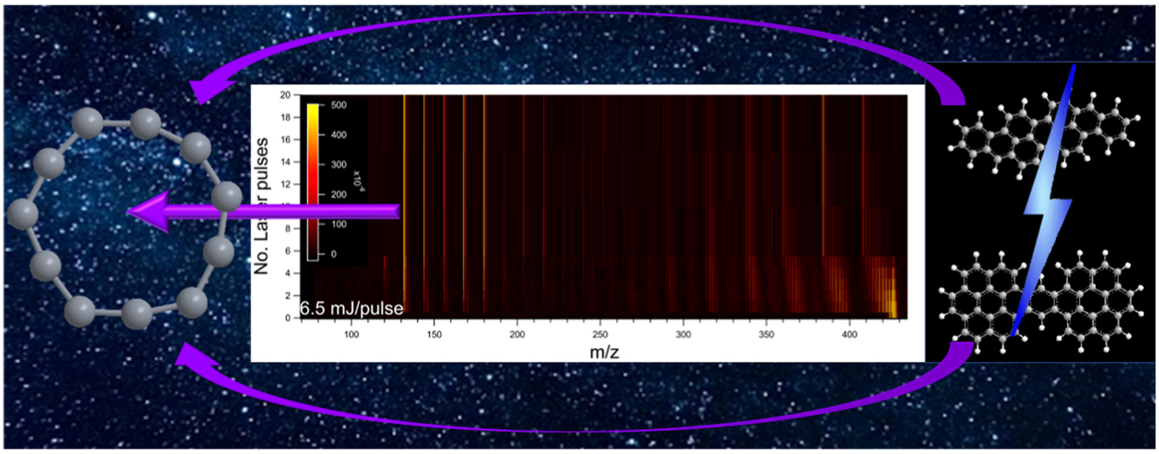
The photo-induced fragmentation pathways of the cationic forms of isoviolanthrene ($C_{34}H_{18}$) and dicoronylene ($C_{48}H_{20}$) are systematically studied with mass spectrometry employing an ion trap coupled with a laser system. The mass spectra of these structurally different species display similar fragmentation products, akin to previous work on three dibenzopyrene isomers, but also display some differences. The products formed in the largest yields are pure carbon clusters, which are likely in the form of ionized cyclo[n]carbons (n = 11–15). These findings are relevant to get a full picture of the molecular makeup of interstellar space, particularly in heavily irradiated regions where polycyclic aromatic hydrocarbon (PAH) molecules are omnipresent and subject to harsh irradiation and are broken down into smaller components. These interstellar species are expected to include the carbon clusters observed here, but which are not identified in space yet.



Graphical abstract depicting the two-dimensional TOF-MS representation of the laser-induced photofragmentation of large PAH cations, leading to the formation of ionized carbon clusters.

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Gas-phase hydrogen/deuterium exchange on large, astronomically relevant cationic PAHs

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[4]CAS Center for Excellence in Quantum Information and Quantum Physics, Hefei National Laboratory for Physical Sciences at the Microscale, and Department of Chemical Physics, University of Science and Technology of China, Hefei, China

To examine the gas-phase hydrogen/deuterium exchange on large, astronomically relevant cationic polycyclic aromatic hydrocarbons (PAHs), the ion-molecule collision reaction between $C_{42}H_{18}{}^{+}$ (hexa-peri-hexabenzocoronene cations, HBC^{+}) and D atoms is studied. The experimental results show that the deuterated HBC cations ($[C_{42}H_{m}D_{n}]^{+}$, m+2×n up to $\sim$ 54) are efficiently formed, and an effective hydrogen/deuterium exchange is determined. The structure of newly formed deuterated HBC cations and the bonding energy for these reaction pathways are investigated with quantum theoretical calculations. The exothermic energy for each reaction pathway is relatively high, and the existence of competition between deuteration and dedeuteration and of hydrogen/deuterium exchange is confirmed. A kinetic model is constructed to simulate the deuteration and hydrogenation processes and the hydrogen/deuterium exchange on HBC^{+} as a function of the reaction time over the experimental and typical astrophysical conditions. We infer that if we do not consider other chemical evolution processes (e.g., photoevolution), then cationic PAHs will reach the final equilibrium state (reaction with H/D atoms) very quickly regardless of the initial state of PAHs, and deuterated cationic PAHs are scarce in the interstellar medium (ISM).

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https://iopscience.iop.org/article/10.3847/1538-4357/ac96ee/pdf

Destructive Processing of Silicon Carbide Grains: Experimental Insights into the Formation of Interstellar Fullerenes and Carbon Nanotubes

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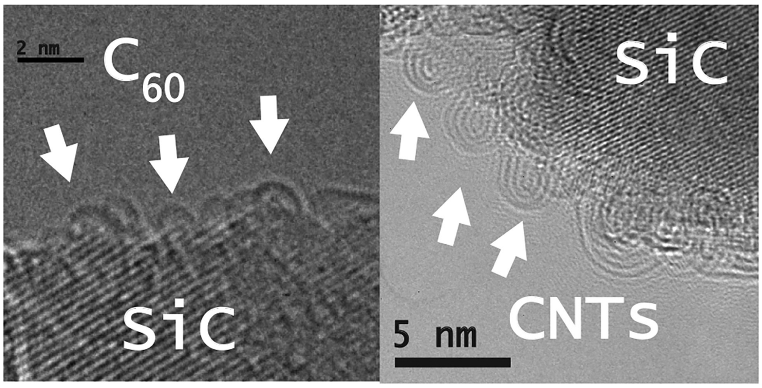
The detection of the fullerenes C_{60} and C_{70} in the interstellar medium (ISM) has transformed our understanding of chemical complexity in space. These discoveries also raise the possibility for the presence of even larger molecules in astrophysical environments. Here we report in situ heating of analog silicon carbide (SiC) presolar grains using transmission electron microscopy (TEM). These heating experiments are designed to simulate the temperature conditions occurring in post-AGB stellar envelopes. Our experimental findings reveal that heating the analog SiC grains to the point of decomposition initially yields hemispherical C_{60}-sized nanostructures, with five- and six-membered rings, which transform into multiwalled carbon nanotubes (MWCNTs) if held isothermally $>$2 min. These MWCNTs are certainly larger than any of the currently observed interstellar fullerene species, both in overall size and number of C atoms. These experimental simulations suggest that such MWCNTs are likely to form in post-AGB circumstellar material, where the structures, along with the smaller fullerenes, are subsequently injected into the ISM.



C_{60}-sized nanobuds and multiwalled carbon nanotubes (CNTs), formed from thermal decomposition of silicon carbide (SiC). Credits: ACS (J. Phys. Chem. A 2022, 126, 34, 5761-5767)

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Journal of Physical Chemistry A, **126**, 5761–5767 (2022)

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On the presence of metallofullerenes in fullerene-rich circumstellar envelopes

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The presence of neutral C_{60} fullerenes in circumstellar environments has been firmly established by astronomical observations as well as laboratory experiments and quantum-chemistry calculations. However, the large variations observed in the C_{60} 17.4μm/18.9μm band ratios indicate that either additional emitters should contribute to the astronomical IR spectra or there exist unknown physical processes besides thermal and UV excitation. Fullerene-based molecules such as metallofullerenes and fullerene-adducts are natural candidate species as potential additional emitters, but no specific species has been identified to date. Here we report a model based on quantum-chemistry calculations and IR spectra simulation of neutral and charged endo(exo)hedral metallofullerenes, showing that they have a significant contribution to the four strongest IR bands commonly attributed to neutral C_{60}. These simulations may explain the large range of 17.4μm/18.9μm band ratios observed in very different fullerene-rich circumstellar environments like those around planetary nebulae and chemically peculiar R Coronae Borealis stars. Our proposed model also reveals that the 17.4μm/18.9μm band ratio in the metallofullerenes simulated IR spectra mainly depends on the metal abundances, ionization level, and endo/exo concentration in the circumstellar envelopes. We conclude that metallofullerenes are potential emitters contributing to the observed IR spectra in fullerene-rich circumstellar envelopes. Our simulated IR spectra indicate also that the James Webb Space Telescope has the potential to confirm or refute the presence of metallofullerenes (or even other fullerene-based species) in circumstellar enviroments.

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The Astrophysical Journal (accepted on 23/11/22, in press)

https://arxiv.org/abs/2212.05981
http://research.iac.es/preprints/?c=view&pre_id=22079

Meetings

2023 Kavli-IAU Astrochemistry Symposium

Astrochemistry VIII - From the First Galaxies to the Formation of Habitable Worlds

Park Place Hotel, Traverse City, MI, USA
10 - 14 July, 2023

https://events.mpe.mpg.de/event/14/

Astrochemistry is at the heart of many astrophysical fields, from the early Universe to star- and planet-formation and evolution in our Milky Way and local galaxies, to exoplanet atmospheres, and to our Solar System. Decades-long concerted efforts of astronomers and theoretical/experimental chemists have provided a solid foundation for using molecules as powerful diagnostic tools of the physical and chemical structure, dynamics, and history of a multitude of astrophysical objects, allowing connections and glimpses into the life cycle of the interstellar medium, as well as into the growth of chemical complexity in space. The great sensitivity, high angular resolution and frequency coverage of telescopes such as ALMA have allowed unprecedented views of stellar and planet nurseries. JWST with its sensitive near- to mid-infrared spectrometers will soon open a new sensitive and sharp observing window into major molecular ingredients such as water, carbon dioxide, as well as other key organic species. JWST will allow us to probe composition of ices on interstellar and planet-forming scales, enabling studies of the linked-chemistry of exoplanetary atmospheres and protoplanetary disks. It is therefore timely for the eighth IAU Symposium on Astrochemistry that will allow the ever-growing astrochemical community to meet and discuss recent achievements and future challenges, including the possibilities of new synergies with other related fields.

If you are interested in joining us, please fill out the form:

Registration Form

Looking forward to seeing you all in Traverse City!

On behalf on the organising committee,

- Paola Caselli, Ted Bergin & Jes Jorgensen

E-mail for contact: caselli@mpe.mpg.de

Asia Oceania Geosciences Society 2023

Astrochemical Processes Leading to the Formation of Planetary Bodies in the Solar System

Singapore
30 July - 4 August, 2023

https://www.asiaoceania.org/aogs2023/public.asp?page=home.asp

We are excited to share with you the opening of our session titled "Astrochemical Processes Leading to the Formation of Planetary Bodies in the Solar System", now open for abstract submissions, at the upcoming Asia Oceania Geosciences Society 2023 Annual Meeting. The AOGS will mark its 20th Annual Meeting and will be held in Singapore on July 30th – August 4th 2023. This session intends to bring together researchers in the fields of planetary science, astrophysics, astrochemistry, and atmospheric science whose work focuses on the study of molecular interactions towards the formation of organic compounds in planetary environments, including comets, asteroids, planetary object (planets, dwarf planets, and moons) surfaces, and planetary object atmospheres. This also includes studies covering the formation of simple chemical precursors up to larger and more complex macromolecular organic compounds.

Research areas that are encouraged include, but are not limited to, all spectral ranges of laboratory investigations, particle (electrons, protons, cosmic rays) and radiation (ultraviolet, extreme ultraviolet, X-ray photons), interaction with all phases of matter including ices and tholins, and theoretical and laboratory cross sections and reaction rates, with emphasis on applications to planetary, cometary, and astronomical observations. Experimentalists, observers, theorists, and modelers are all encouraged to present their work to disseminate and advance scientific knowledge in this very interdisciplinary field, further discuss emerging ideas and insights on planetary science, astrophysics, and astrochemistry. It is important to promote the dialogues among interdisciplinary researchers, in Asia, Oceania, and the rest of the world, and to increase collaborations and the cross fertilization of ideas to ensure the continual growth of scientific understanding in our community.

Deadline for abstract submission: February 14th 2023.

Notification announcements: March 21st - 28th 2023.

Registration and abstract submission are now open:

Registration and Abstract Submission

Looking forward to seeing you all in Singapore!

The session conveners,

- David Dubois (NASA Ames Research Center), Asper Chen (National Center University) & Michel Nuevo (NASA Ames Research Center)

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Announcements

PhD Studentship Available in Astrocatalysis

Advertised by Martin R. S. McCoustra

This PhD opportunity will be in the Laboratory Astrochemistry research group at Heriot-Watt University, Edinburgh. This project, aligned with the recently funded EPSRC project Astrocatalysis: In Operando Studies of Catalysis and Photocatalysis of Space-abundant Transition Metals (AstroCat, EP/W023024/1), will provide students with the opportunity to explore the cutting edge of laboratory astrochemistry and modern catalytic science. The project also aligns with goals of the COST Action 21126 - Carbon molecular nanostructures in space (NanoSpace).

Details of the project and any deadlines can be found here at Catalysis in the Laboratory Astrochemistry of Nanocarbon Formation in Space (CAstroCat) at Heriot-Watt University on FindAPhD.com.

This scholarship is only open to students eligible for UK ‘home’ fee status. This would be UK students but also include students who are settled in the UK, free from immigration controls and who have been in the UK for at least 3 years.

Deadline: 31 March 2023

E-mail for contact: m.r.s.mccoustra@hw.ac.uk

Webpage: https://www.findaphd.com/phds/project/catalysis-in-the-laboratory-astrochemistry-of-nanocarbon-formation-in-space-castrocat/?p153691

AstroPAH Newsletter

http://astropah-news.strw.leidenuniv.nl — Next issue: 23 February 2023

astropah@strw.leidenuniv.nl — Submission deadline: 10 February 2023