A Newsletter on Astronomical PAHs

Issue 96 • March 2023

c)

Synthesis of N-graphene in astronomical ice

a)

Editorial

Dear Colleagues,

Welcome to our new AstroPAH volume no. 96! We hope all of you are healthy and doing well!

Our PAH Picture of the Month features N-graphene synthesized in astronomical ices as seen in transmission electron microscopy (TEM). From left to right are shown the TEM snapshot of a large N-graphene sheet, the zoomed-in hexagonal patter, and the corresponding diffraction pattern. More information can be found in the Sivaraman et al. publication listed in our Abstracts.

Many thanks to all of you again for all your contributions covering PAH synthesis pathways, radical-radical reactions, and galactic PAH content.

We would like to draw your attention to three future meeting announcements: the Laboratory Astrophysics Workshop (ICE 2024) in Hawaii next year, the JWST COST NanoSpace Training School this coming summer, and a "Surface Astrochemistry"mini-symposium later this year organized by the European Conference on Surface Science.

If you are on Instagram, be sure to check out our next PAH of the Month!

We hope you enjoy reading our newsletter, and we thank you for your dedication and interest in AstroPAH! Please continue sending us your contributions, and if you wish to contact us for a future In Focus or other ideas, feel free to use our email.

The Editorial Team

Next issue: 20 April 2023. Submission deadline: 7 April 2023.

AstroPAH Newsletter Editorial Board:

Editor-in-Chief

Prof. Alexander Tielens Leiden Observatory (The Netherlands)

Executive Editors

Dr. Isabel Aleman Institute of Mathematics and Statistics, University of São Paulo (Brazil)

Dr. Ella Sciamma-O'Brien NASA Ames Research Center (USA)

Editors

Dr. David Dubois

NASA Ames Research Center BAER Institute (USA)

Dr. Helgi Rafn Hróðmarsson

Laboratoire Inter-Universitaire des Systèmes Atmosphériques (France)

Dr. Rijutha Jaganathan

Aarhus University (Denmark)

Dr. Donatella Loru

Deutsches Elektronen-Synchrotron (Germany)

Dr. Julianna Palotás University of Maryland (USA)

Dr. Ameek Sidhu University of Western Ontario (Canada)

Dr. Sandra Wiersma Institute de Recherche en Astrophysique et Planétologie (France)

Contact us:

astropah@strw.leidenuniv.nl http://astropah-news.strw.leidenuniv.nl Click here to Subscribe to AstroPAH Click here to Contribute to AstroPAH

Follow us on:

Contents

PAH Picture of the Month	1
Editorial	2
Recent Papers	4
Meetings	21

PAH Picture of the Month

N-graphene synthesized in astronomical ice revealed by high-resolution transmission electron microscopy (HR-TEM). a) HR-TEM image of a large sheet of N-graphene. b) zoom-in of the exagonal pattern of Ngraphene. c) corresponding diffraction pattern. More information can be found in Sivaraman et al. 2013

Credits: Sivaraman et al. 2023.

This newsletter is edited in LTEX. Newsletter Design by: Isabel Aleman. Image Credits: Background image in this page: NASA, ESA, and the Hubble Heritage Team (STScI/AURA). Headers background: X-ray and optical image composition. X-ray by Chandra: NASA/CXC/Univ.Potsdam/L.Oskinova et al; Optical by Hubble: NASA/STScI; Infrared by Spitzer: NASA/JPL-Caltech.

Abstracts

Evolution of grain size distribution with enhanced abundance of small carbonaceous grains in galactic environments

Hiroyuki Hirashita^{1,2}

¹Institute of Astronomy and Astrophysics, Academia Sinica, Taipei, Taiwan ²Theoretical Astrophysics, Department of Earth and Space Science, Osaka University, Osaka, Japan

We propose an updated dust evolution model that focuses on the grain size distribution in a galaxy. We treat the galaxy as a one-zone object and include five main processes (stellar dust production, dust destruction in supernova shocks, grain growth by accretion and coagulation, and grain disruption by shattering). In this paper, we improve the predictions related to small carbonaceous grains, which are responsible for the 2175 Å bump in the extinction curve and the polycyclic aromatic hydrocarbon (PAH) emission features in the dust emission spectral energy distribution (SED), both of which were underpredicted in our previous model. In the new model, we hypothesize that small carbonaceous grains are not involved in interstellar processing. This avoids small carbonaceous grains being lost by coagulation. We find that this hypothetical model shows a much better match to the Milky Way (MW) extinction curve and dust emission SED than the previous one. The following two additional modifications further make the fit to the MW dust emission SED better: (i) The chemical enrichment model is adjusted to give a nearly solar metallicity in the present epoch, and the fraction of metals available for dust growth is limited to half. (ii) Aromatization for small carbonaceous grains is efficient, so that the aromatic fraction is unity at grain radii \lesssim 20 Å. As a consequence of our modelling, we succeed in obtaining a dust evolution model that explains the MW extinction curve and dust emission SED at the same time.

E-mail: hirashita@asiaa.sinica.edu.tw

Mon. Notices Royal Astron. Soc., 518:3827 (2022)

https://ui.adsabs.harvard.edu/abs/2023MNRAS.518.3827H/abstract

Unconventional Pathway in the Gas-Phase Synthesis of 9H-Fluorene ($C_{13}H_{10}$) via the Radical–Radical Reaction of Benzyl (C_7H_7) with Phenyl (C_6H_5)

Chao He¹, Ralf I. Kaiser¹, Wenchao Lu², Musahid Ahmed², Pavel S. Pivovarov³, Oleg V. Kuznetsov³, Marsel V. Zagidullin³, and Alexander M. Mebel⁴

¹Department of Chemistry, University of Hawaii at Manoa, Honolulu, Hawaii 96822, USA

²Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

³Samara National Research University, Samara 443086, Russian Federation

⁴Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199, USA

The simplest polycyclic aromatic hydrocarbon (PAH) carrying a five-membered ring—9Hfluorene ($C_{13}H_{10}$)—is produced isomer-specifically in the gas phase by reacting benzyl (C_7H_7) with phenyl (C_6H_5) radicals in a pyrolytic reactor coupled with single photon ionization mass spectrometry. The unconventional mechanism of reaction is supported by theoretical calculations, which first produces diphenylmethane and unexpected 1-(6methylenecyclohexa-2,4-dienyl)benzene intermediates ($C_{13}H_{12}$) accessed via addition of the phenyl radical to the ortho position of the benzyl radical. These findings offer convincing evidence for molecular mass growth processes defying conventional wisdom that radicalradical reactions are initiated through recombination at their radical centers. The structure of 9H-fluorene acts as a molecular building block for complex curved nanostructures like fullerenes and nanobowls providing fundamental insights into the hydrocarbon evolution in high temperature settings.

E-mail: ralfk@hawaii.edu

Angew. Chem. Int. Ed., 62:e202216972 (2023)

https://onlinelibrary.wiley.com/doi/10.1002/anie.202216972

Exotic Reaction Dynamics in the Gas-Phase Preparation of Anthracene ($C_{14}H_{10}$) via Spiroaromatic Radical Transients in the Indenyl–Cyclopentadienyl Radical–Radical Reaction

Chao He¹, Ralf I. Kaiser¹, Wenchao Lu², Musahid Ahmed², Yahaira Reyes³, Stanislaw F. Wnuk³, and Alexander M. Mebel³

¹Department of Chemistry, University of Hawaii at Manoa, Honolulu, Hawaii 96822, USA

²Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

³Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199, USA

The gas-phase reaction between the 1-indenyl ($C_9H_7^{\bullet}$) radical and the cyclopentadienyl ($C_5H_5^{\bullet}$) radical has been investigated for the first time using synchrotron-based mass spectrometry coupled with a pyrolytic reactor. Soft photoionization with tunable vacuum ultraviolet photons afforded for the isomerselective identification of the production of phenanthrene, anthracene, and benzofulvalene ($C_{14}H_{10}$). The classical theory prevalent in the literature proposing that radicals combine only at their specific radical centers is challenged by our discovery of an unusual reaction pathway that involves a barrierless combination of a resonantly stabilized hydrocarbon radical with an aromatic radical at the carbon atom adjacent to the traditional C1 radical center; this unconventional addition is followed by substantial isomerization into phenanthrene and anthracene via a category of exotic spiroaromatic intermediates. This result leads to a deeper understanding of the evolution of the cosmic carbon budget and provides new methodologies for the bottom-up synthesis of unique spiroaromatics that may be relevant for the synthesis of more complex aromatic carbon skeletons in deep space.

E-mail: ralfk@hawaii.edu

J. Am. Chem. Soc., 145:3084-3091 (2023)

https://pubs.acs.org/doi/10.1021/jacs.2c12045

A unified reaction network on the formation of fivemembered ringed polycyclic aromatic hydrocarbons (PAHs) and their role in ring expansion processes through radical-radical reactions

Wang Li¹, Long Zhao^{1,2}, and Ralf I. Kaiser³

¹National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, China

²School of Nuclear Science and Technology, University of Science and Technology of China, Hefei, Anhui 230027, China

³Department of Chemistry, University of Hawaii at Manoa, Honolulu, Hawaii 96822, USA

Exploiting a chemical microreactor in combination with an isomer-selective product identification through fragment-free photoionization utilizing tunable vacuum ultraviolet (VUV) light in tandem with the detection of the ionized molecules by a high resolution reflection time-of-flight mass spectrometer (Re-TOF-MS), the present investigation reveals molecular mass growth processes to four distinct polycyclic aromatic hydrocarbons carrying two six- and one five-membered ring (C₁₃H₁₀): 3H-cyclopenta[a]naphthalene, 1Hcyclopenta[b]naphthalene, 1H-cyclopenta[a]naphthalene, and fluorene in the gas phase. Temperatures of 973 and 1023 K simulating conditions in combustion settings along with circumstellar envelopes of carbon-rich stars and planetary nebulae. These reactions highlight the importance of methyl-substituted aromatic reactants (biphenyl, naphthalene) which can be converted to the methylene $(-CH_2^{\bullet})$ motive by hydrogen abstraction or photolysis. Upon reaction with acetylene, methylene-substituted aromatics carrying a hydrogen atom at the ortho position of the ring can be then converted to cyclopentadieneannulated aromatics thus providing a versatile pathway to five-membered ring aromatics at elevated temperatures.

E-mail: ralfk@hawaii.edu

Phys. Chem. Chem. Phys., 25:4141 (2023)

https://pubs.rsc.org/en/content/articlelanding/2023/cp/d2cp05305e/unauth

Absence of nuclear PAH emission from a compact starburst: The case of the type-2 quasar Mrk 477

C. Ramos Almeida^{1,2}, D. Esparza-Arredondo^{1,2}, O. González-Martín³, I. García-Bernete⁴, M. Pereira-Santaella^{5,6}, A. Alonso-Herrero⁷, J. A. Acosta-Pulido^{1,2}, P. S. Bessiere^{1,2}, N. A. Levenson⁸, C. N. Tadhunter⁹, D. Rigopoulou⁴, M. Martínez-Paredes¹⁰, S. Cazzoli¹¹, and B. García-Lorenzo^{1,2}

¹Instituto de Astrofísica de Canarias, La Laguna, Tenerife, Spain

²Departamento de Astrofísica, Universidad de La Laguna, Tenerife, Spain

³Instituto de Radioastronomía and Astrofísica (IRyA-UNAM), Morelia, Mexico

⁴Department of Physics, University of Oxford, Oxford, UK

⁵Centro de Astrobiología (CSIC-INTA), Torrejón de Ardoz, Madrid, Spain

⁶Observatorio Astronómico Nacional (OAN-IGN)-Observatorio de Madrid, Madrid, Spain

⁷Centro de Astrobiología (CAB), CSIC-INTA, Madrid, Spain

⁸Space Telescope Science Institute, Baltimore, USA

⁹Department of Physics & Astronomy, University of Sheffield, Sheffield, UK

¹⁰Korea Astronomy and Space Science Institute 776, Daejeon, Republic of Korea

¹¹Instituto de Astrofísica de Andalucía – CSIC, Granada, Spain

Mrk 477 is the closest type-2 quasar, at a distance of 163 Mpc. This makes it an ideal laboratory for studying the interplay between nuclear activity and star formation with a great level of detail and signal-to-noise. Here we present new mid-infrared (mid-IR) imaging and spectroscopic data with an angular resolution of 0.4 arcsec (~300 pc) obtained with the Gran Telescopio Canarias instrument CanariCam. The N-band (8-13 μ m) spectrum of the central ~400 pc of the galaxy reveals [S IV] λ 10.51 μ m emission, but no 8.6 or 11.3 μ m polycyclic aromatic hydrocarbon (PAH) features, which are commonly used as tracers of recent star formation. This is in stark contrast with the presence of a nuclear starburst of ~300 pc in size, an age of 6 Myr, and a mass of 1.1 × 10⁸ M_☉, as constrained from ultraviolet Hubble Space Telescope observations. Considering this, we argue that even the more resilient, neutral molecules that mainly produce the 11.3 μ m PAH band are most likely being destroyed in the vicinity of the active nucleus despite the relatively large X-ray column density, log N_H=23.5 cm⁻², and modest X-ray luminosity, 1.5×10⁴³ erg s⁻¹. This highlights the importance of being cautious when using PAH features as star formation tracers in the central region of galaxies to evaluate the impact of feedback from active galactic nuclei.

E-mail: cra@iac.es

Astronomy & Astrophysics, 669:L5 (2023)

https://www.aanda.org/articles/aa/full_html/2023/01/aa45409-22/aa45409-22.html https://arxiv.org/abs/2212.01258

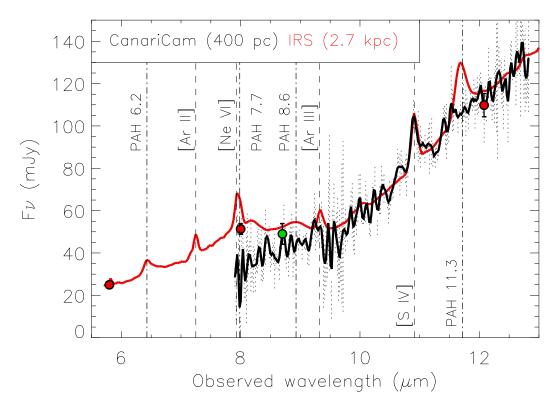


Figure 1 – GTC/CanariCam nuclear spectrum of Mrk 477 (0.5 arcsec~400 pc; solid black line, with errors indicated as dotted lines). Weak silicate absorption and [S IV]λ10.51 µm emission are the only spectral features detected. The solid red line corresponds to the IRS spectrum (3.6 arcsec~2.7 kpc), which, in addition to the ionized and warm molecular hydrogen emission lines, shows clear PAH emission bands at 6.2, 7.7, 8.6, and 11.3 µm. Filled dots are the fluxes obtained from images in the CanariCam Si-2 filter (in green), IRAC 5.8 and 8 µm, and WISE 12 µm bands (in red).

Probing Computational Methodologies in Predicting Mid-Infrared Spectra for Large Polycyclic Aromatic Hydrocarbons (PAHs)

B. Kerkeni 1,2,3 , I. García-Bernete¹, D. Rigopoulou¹, D. P. Tew⁴, P. F. Roche¹, and D. C. Clary⁴

¹Department of Physics, University of Oxford, Oxford, OX1 3RH, United Kingdom

²ISAMM, Université de la Manouba, La Manouba 2010 Tunisia

³Département de Physique, LPMC, Faculté des Sciences de Tunis, Université de Tunis el Manar, Tunis 2092, Tunisia

⁴Department of Chemistry, University of Oxford, Oxford, OX1 3QZ, United Kingdom

We extend the prediction of vibrational spectra to large sized Polycyclic Aromatic Hydrocarbon (PAH) molecules comprising up to \sim 1500 carbon atoms by evaluating the efficiency of several computational chemistry methodologies. We employ classical mechanics methods (Amber and Gaff) with improved atomic point charges, semi-empirical (PM3, and DFTB) and density functional theory (B3LYP) and conduct global optimizations and frequency calculations in order to investigate the impact of PAH size on the vibrational band positions. We primarily focus on the following mid-infrared (MIR) emission bands 3.3, 6.2, 7.7, 8.6, 11.3, 12.7 and 17.0 μm. We developed a general Frequency Scaling Function (\mathcal{FSF}) to shift the bands and to provide a systematic comparison versus the three methods for each PAH. We first validate this procedure on IR scaled spectra from the NASA Ames PAH Database, and extend it to new large PAHs. We show that when the FSF is applied to the Amber and Gaff IR spectra, an agreement between the normal mode peak positions with those inferred from the B3LYP/4-31G model chemistry is achieved. As calculations become time intensive for large sized molecules $N_{\rm C} > 450$, this proposed methodology has advantages. The FSF has enabled extending the investigations to large PAHs where we clearly see the emergence of the 17.0 µm feature, and the weakening of the 3.3 µm one. We finally investigate the trends in the 3.3 μ m/17.0 μ m PAH band ratio as a function of PAH size and its response following the exposure to fields of varying radiation intensities.

10

E-mail: boutheina.kerkeni@physics.ox.ac.uk

Mon. Notices Royal Astron. Soc., 513:3663-3681 (2022)

https://doi.org/10.1093/mnras/stac976

A high-resolution study of near-IR diffuse interstellar bands, search for small-scale structure, time variability, and stellar features

J. V. Smoker^{1,2}, A. Müller³, A. Monreal Ibero^{4,5,6}, M. Elyajouri⁷, C. J. Evans^{2,8}, F. Najarro⁹, A. Farhang¹⁰, N. L. J. Cox¹¹, J. Minniti¹², K. T. Smith¹³, J. Pritchard¹⁴, R. Lallement⁷, A. Smette¹, H. M. J. Boffin¹⁴, M. Cordiner, and J. Cami^{16,17,18}

¹European Southern Observatory, Alonso de Cordova 3107, Vitacura, Santiago, Chile

²UK Astronomy Technology Centre, Royal Observatory, Blackford Hill, Edinburgh EH9 3HJ, UK

³Max-Planck-Institut fur Astronomie, Königstuhl 17. 69117 Heidelberg, Germany

⁴Leiden Observatory, Leiden University, PO Box 9513, 2300 RA Leiden, The Netherlands

⁵Instituto de Astrofísica de Canarias, C/ Vía Láctea s/n, E-38205 La Laguna, Tenerife, Spain

⁶Departamento de Astrofísica, Universidad de La Laguna, E-38200 La Laguna, Tenerife, Spain

⁷GEPI, Observatoire de Paris, PSL Research University, CNRS, Place Jules Janssen, 92190 Meudon, France ⁸European Space Agency, ESA Office, Space Telescope Science Institute, 3700 San Martin Drive, Baltimore, MD 21218, USA

⁹Departamento de Astrofísica, Centro de Astrobiología, CSIC-INTA, Ctra. Torregjon a Ajalvir km. 4, 28850-Madrid,Spain

¹⁰School of Astronomy, Institute for Research in Fundamental Sciences, 19395-5531 Tehran, Iran

¹¹ACRI-ST, Centre d'Etudes et de Recherche de Grasse (CERGA), 10 Av. Nicolas Copernic, 06130 Grasse, France

¹²Nicolaus Copernicus Astronomical Center, Polish Academy of Sciences, Bartycka 18, 00-716 Warsaw, Poland

¹³AAAS Science International, Clarendon House, Clarendon Road, Cambridge CB2 8FH, UK

¹⁴European Southern Observatory, Karl-Schwarzschild-Str. 2 85748 Garching bei München, Germany

¹⁵NASA Goddard Space Flight Center, 8800 Greenbelt Road, Greenbelt, MD 20771, USA

¹⁶Department of Physics and Astronomy, The University of Western Ontario, London, ON N6A 3K7, Canada

¹⁷Institute for Earth and Space Exploration, The University of Western Ontario, London, ON N6A 3K7, Canada ¹⁸SETI Institute, 189 Bernardo Ave, Suite 100, Mountain View, CA 94043, USA

The diffuse interstellar bands (DIBs) are a set of hundreds of unidentified absorption features that appear almost ubiquitously throughout the interstellar medium. Most DIBs appear at optical wavelengths, but some are in the near-infrared. We aim to characterise near-infrared DIBs at high spectral resolving power towards multiple targets. We observed 76 early-type stars at a resolving power of 50,000 (velocity resolution $\sim 6 \text{ kms}^{-1}$) and signal-to-noise ratios of several hundreds using the CRyogenic high-resolution InfraRed Echelle Spectrograph (CRIRES). These data allow us to investigate the DIBs around 1318.1, 1527.4, 1561.1, 1565.1, 1567.0, 1574.4, and 1624.2 nm. Example spectra are shown in Fig. 2. We detected a total of six DIB features and 17 likely stellar features through comparisons with a model spectrum computed with CMFGEN.

Additionally, we measured equivalent widths of the DIBs at 1318.1 and 1527.4 nm using observations with X-shooter towards ten very highly reddened (3.2 < E(B - V) < 6.5) Cepheid variable stars and towards four stars observed at low values of precipitable water vapour as well as by using other archive data. We measured correlations (correlation coefficient $r \sim 0.73-0.96$, depending on the subsample used) between DIB equivalent width and reddening for the DIBs at 1318.1, 1561.1, 1565.1, and 1567.0 nm. Comparing the near-infrared DIBs with 50 of the strongest optical DIBs, we find correlations r > 0.8 between the 1318, 1527, 1561, 1565, and 1567 nm and the optical DIBs 5705, 5780, 6203, 6283, and 6269 Å. The 5797 Å DIB is less well correlated with the near-infrared DIBs. The DIB at 9632.1 Å, which is likely C_{60}^+ , is not well correlated with the 1318.1 nm DIB. Partial

correlation coefficients using E(B - V) as the covariate were also determined. For stars earlier than B2, the 1318.1 nm DIB is affected by an emission line on its blue wing that is likely stellar in nature, although we cannot rule out an interstellar or circumstellar origin for this line caused by, for example, a DIB in emission. The 1318.1 nm DIB also has an extended red wing. The line is reasonably well fitted by two Gaussian components, although neither the component equivalent width (EW) ratios nor the separation between components are obviously correlated with such indicators as $\lambda\lambda$ 5780/5797 and reddening. The EW at 1318 nm correlates with H I with EW(1318 nm)/E(B - V) decreasing with f(H₂).

Five pairs of stars within one arcmin of each other show very similar 1318.1 nm DIB profiles. Possible variation in the 1318.1 nm feature is seen between HD 145501 and HD 145502 (separated by 41 arcsec, equivalent to 7200 au) and HD 168607 and HD 168625 (separated by 67 arcsec, equivalent to 0.52 pc on the plane of the sky). Seventeen sightlines have repeat CRIRES observations separated by 9.9 years. No time variability was detected in the 1318.1 nm DIB in the CRIRES data nor in the 5780.5 Å, 5797.1 Å, 1318.1 nm, and 1527.4 nm DIBs. Tentative time variation is observed in the C_{60}^+ DIBs at 9577 and 9632 Å towards HD 183143, although it is very close to the noise level and requires confirmation. The Near Infrared (NIR) DIBs observed occur more in more UV-irradiated regions than the 5797 Å DIB allowing the study of heavily reddened sightlines. Future searches for time variability in DIBs will require either higher quality data, larger intervals between epochs, or both.

E-mail: jsmoker@email.com E-mail: jcami@uwo.ca

Astronomy & Astrophysics, in press, 2023

https://arxiv.org/abs/2212.03563

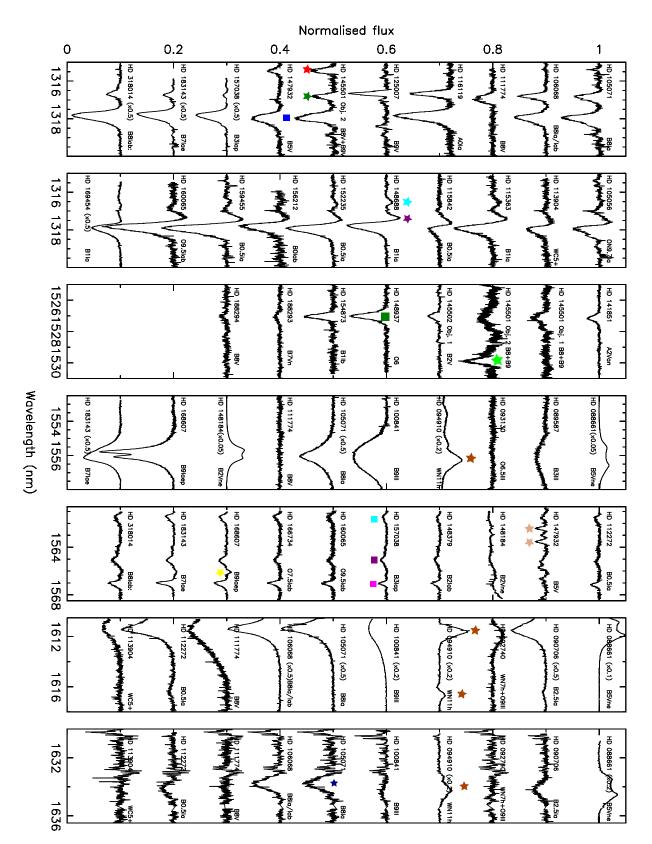


Figure 2 – Normalised CRIRES spectra showing examples of observed stellar and interstellar features. The ordinate is the normalised flux plus an offset with the abscissa as the wavelength in nm. Stellar lines: Red stars: 1315.4 nm; Green: 1316.8 nm; Cyan: 1316.5 nm (EmL); Purple: 1317.3 nm (EmL, uncertain); Light Green: 1529.9 nm; Yellow: 1566.1 nm (EmL); Gold: 1562.4, 1563.0, and 1563.5 nm; Navy: 1633.8; Brown: 1555.7, 1616.7, and 1634.2 nm (EmL). Not shown: 1610.9 nm, 1625.3 nm and 1626.1 nm features. DIBs: Blue squares: 1318.1 nm; Green: 1527.1 nm; Cyan: 1561.1 nm; Purple: 1565.1 nm; Pink: 1567.0 nm. Not shown: broad and weak feature around 1564.4 nm.

13

Evidence that Shocks Destroy Small PAH Molecules in Low-luminosity Active Galactic Nuclei

Lulu Zhang^{1,2}, Luis C. Ho^{1,2}, and Aigen Li^3

¹Kavli Institute for Astronomy and Astrophysics, Peking University, Beijing 100871, China ²Department of Astronomy, School of Physics, Peking University, Beijing 100871, China ³Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211, USA

We combined mapping-mode mid-infrared Spitzer spectra with complementary infrared imaging to perform a spatially resolved study of polycyclic aromatic hydrocarbons (PAHs) emission from the central regions of 66 nearby galaxies, roughly evenly divided into starforming systems and low-luminosity active galactic nuclei (AGNs). In conjunction with similar measurements available for quasars, we aim to understand the physical properties of PAHs across a broad range of black hole accretion power, with the goal of identifying observational diagnostics that can be used to probe the effect of AGNs on the host galaxy. Whereas the PAH emission correlates tightly with far-ultraviolet luminosity in star-forming regions, the spatially resolved regions of AGNs tend to be PAH-deficient. Moreover, AGN regions exhibit on average smaller PAH 6.2µm/7.7µm and larger PAH 11.3µm/7.7µm band ratios. Although the current data are highly restrictive, they suggest that these anomalous PAH band ratios cannot be explained by the effects of the AGN radiation field alone. Instead, they hint that small grains may be destroyed by the combined effects of radiative processes and shocks, which are plausibly linked to jets and outflows preferentially associated with highly sub-Eddington, radiatively inefficient AGNs. While guasars also present a PAH deficit and unusual PAH band ratios, their characteristics differ in detail compared to those observed in more weakly accreting AGNs, a possible indicator of fundamental differences in their modes of energy feedback.

E-mail: I.I.zhang@pku.edu.cn

Astrophys. J., 939:22 (2022)

https://doi.org/10.3847/1538-4357/ac930f

Estimating Molecular Gas Content in Galaxies from PAH Emission

Lulu Zhang^{1,2} and Luis C. Ho^{1,2}

¹Kavli Institute for Astronomy and Astrophysics, Peking University, Beijing 100871, China ²Department of Astronomy, School of Physics, Peking University, Beijing 100871, China

Emission from polycyclic aromatic hydrocarbons (PAHs), a commonly used indicator of star formation activity in galaxies, also has the potential to serve as an effective empirical tracer of molecular gas. We use a sample of 19 nearby galaxies with spatially resolved mid-infrared Spitzer spectroscopy, multi-wavelength optical and mid-infrared imaging, and millimeter interferometric CO(1–0) maps to investigate the feasibility of using PAH emission as an empirical proxy to estimate molecular gas mass. PAH emission correlates strongly with CO emission on sub-kpc scales over the diverse environments probed by our sample of starforming galaxies and low-luminosity active galactic nuclei. The tight observed correlation, likely a consequence of photoelectronic heating of the diffuse interstellar gas by the PAHs, permits us to derive an empirical calibration to estimate molecular gas mass from the luminosity of PAH emission that has a total scatter of only \sim 0.2–0.25 dex. Mid-infrared bands sensitive to PAH emission (e.g., the Spitzer/IRAC4 and WISE/W3 filters) can also be used as a highly effective substitute for this purpose.

15

E-mail: I.I.zhang@pku.edu.cn

Astrophys. J., 943:1 (2023)

https://doi.org/10.3847/1538-4357/aca8f1

The Contribution of Evolved Stars to PAH Heating and Implications for Estimating Star Formation Rates

Lulu Zhang 1,2 and Luis C. Ho 1,2

¹Kavli Institute for Astronomy and Astrophysics, Peking University, Beijing 100871, China ²Department of Astronomy, School of Physics, Peking University, Beijing 100871, China

Emission from polycyclic aromatic hydrocarbons (PAHs) is a promising tool for estimating star formation rate (SFR) in galaxies, but the origin of its sources of excitation, which include not only young but possibly also old stars, remains uncertain. We analyze Spitzer mid-infrared mapping-mode spectroscopic observations of the nuclear and extra-nuclear regions of 33 nearby galaxies to study the contribution of evolved stars to PAH emission. In combination with photometric measurements derived from ultraviolet, $H\alpha$, and infrared images, the spatially resolved spectral decomposition enables us to characterize the PAH emission, SFR, and stellar mass of the sample galaxies on sub-kpc scales. We demonstrate that the traditional empirical correlation between PAH luminosity and SFR has a secondary dependence on specific SFR, or, equivalently, stellar mass. Ultraviolet-faint regions with lower specific SFRs and hence greater fraction of evolved stars emit stronger PAH emission at fixed SFR than ultraviolet-bright regions. We reformulate the PAH-based SFR estimator by explicitly introducing stellar mass as a second parameter to account for the contribution of evolved stars to PAH excitation. The influence of evolved stars can explain the sub-linear correlation between PAH emission and SFR, and it can partly account for the PAH deficit in dwarf galaxies and low-metallicity environments.

16

E-mail: I.I.zhang@pku.edu.cn

Astrophys. J., 943:60 (2023)

https://doi.org/10.3847/1538-4357/acab60

Spatially resolved mid-infrared observations of the circumstellar environment of the born-again object FG Sge

Keiichi Ohnaka¹ and Benjamín A. Jara Bravo¹

¹Instituto de Astrofísica, Universidad Andrés Bello, Santiago, Chile

FG Sge has evolved from the hot central star of the young planetary nebula Hen 1-5 to a G–K supergiant in the last 100 years. It is one of the three born-again objects currently identified, which are considered to have undergone a thermal pulse in the post-AGB evolution. We present mid-infrared spectro-interferometric observations of FG Sge and probe its dusty environment. FG Sge was observed with MIDI at the Very Large Telescope Interferometer at baselines of 43 and 46 m between 8 and 13 µm. The circumstellar dust environment of FG Sge was spatially resolved, and the Gaussian fit to the observed visibilities results in a FWHM of \sim 10.5 mas. The observed mid-infrared visibilities and the spectral energy distribution can be fairly reproduced by optically thick ($\tau_V \approx 8$) spherical dust shell models consisting of amorphous carbon with an inner radius $r_{\rm in}$ of ~30 R_{\star} (corresponding to a dust temperature of 1100 ± 100 K). The dust shell is characterized with a steep density profile proportional to $r^{-3.5\pm0.5}$ from the inner radius $r_{\rm in}$ to $(5-10) \times r_{\rm in}$, beyond which it changes to r^{-2} . The dust mass is estimated to be $\sim 7 \times 10^{-7} M_{\odot}$, which translates into an average total mass-loss rate of $\sim 9 \times 10^{-6} M_{\odot}$ yr⁻¹ as of 2008 with a gas-to-dust ratio of 200 adopted. In addition, the 8-13 µm spectrum obtained with MIDI with a field of view of 200 mas does not show a signature of the polycyclic aromatic hydrocarbon (PAH) emission, in marked contrast to the spectra taken with the Spitzer Space Telescope six and 20 months before the MIDI observations with wide slit widths of 3.6–10". This implies that the PAH emission originates from an extended region of the optically thick dust envelope. The dust envelope of FG Sge is much more compact than that of the other born-again stars Sakurai's object and V605 Agl, which might reflect the difference in the evolutionary status. The PAH emission from the extended region of the optically thick dust envelope likely originates from the material ejected before the central star became H-deficient, and it may be excited by the UV radiation from the central star escaping through gaps among dust clumps and/or the bipolar cavity of a disk-like structure.

17

E-mail: k1.ohnaka@gmail.com

Astronomy & Astrophysics, 668:A119 (2022)

https://doi.org/10.1051/0004-6361/202244921

Enhanced star formation through the high-temperature formation of H_2 on carbonaceous dust grains

Francesco Grieco $^{1,2},\;$ Patrice Theulé $^3,\;$ Ilse De Looze $^2,\;$ and $\;$ François Dulieu 1

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

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

³Aix Marseille Université, CNRS, CNES, LAM, Marseille, France

The microphysics of molecular hydrogen formation has implications on galactic-scale star formation rates over cosmic times. It is the cooling agent needed to initiate the cloud collapse regulating the star formation efficiency. H_2 formation is inefficient in the gas phase under typical interstellar conditions, needing dust grains as catalysts. Small carbonaceous grains with sizes from 4 to 100–200 Angstrom, including Polycyclic Aromatic Hydrocarbons (PAHs), have been shown to increase the H₂ formation rates due to their large surface-tovolume ratios. H₂ formation on PAHs was previously thought to reduce above temperatures of 50 K and H atom recombination was believed to be highly efficient only below 20 K. Until now, both laboratory experiments and theoretical modeling have suggested that H₂ cannot form on grains with temperatures above 100K. Here we report evidence, through direct laboratory measurements, of the high efficiency formation of H₂ at temperatures up to 250K on a carbonaceous surface mimicking interstellar dust. By pushing their formation towards warmer temperatures, the H₂ molecules could start contributing significantly to the cooling of warmer gas (50 K-250 K). This will have a huge impact on our understanding of H₂ formation in nearby galaxies and its efficiency in high-redshift galaxies where the CMB (Cosmic Microwave Background) already pushes dust temperatures above 20 K.

E-mail: francesco.grieco@ugent.be

Nat. Astron. (2023)

https://www.nature.com/articles/s41550-023-01902-4

N-graphene synthesized in astrocheimcal ices

B Sivaraman¹, K K Rahul¹, M Ambresh², D Sahu^{1,3}, J K Meka¹, S -L Chou⁴, Y -J Wu⁴, D Gupta^{5,12}, A Das⁶, J -I Lo⁴, B -M Cheng^{7,8}, B N Rajasekhar⁹, Anil Bhardwaj¹, H Hill¹⁰, P Janardhan¹, and N J Mason¹¹

¹Physical Research Laboratory, 380009, Navrangpura, Ahmedabad, India

²Center for Nanoscience, Indian Institute of Science, Bangalore, India

³Academia Sinica, Institute of Astronomy and Astrophysics, Taipei, Taiwan

⁴National Synchrotron Radiation Research Center, Hsinchu, Taiwan

⁵CNRS, IPR (Institute de Physique de Rennes), University of Rennes-1, Rennes, France

⁶Institute of Astronomy Space and Earth Science, Kolkata, India

⁷Tzu-Chi University of Science and Technology, No. 880, Sec.2, Chien-Kuo Rd, 970, Hualien City , Taiwan

⁸Department of Medical Research, Hualien Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Hualien, Taiwan

⁹Atomic and Molecular Physics Division, Bhabha Atomic Research Centre, Mumbai, India

¹⁰International Space University, Strasbourg, France

¹¹School of Physical Sciences, University of Kent, CT2 7NH, Canterbury, UK

¹²Division-I. Physikalisches Institut, Universitat Zu Koln, Koln, Germany

In our quest for the presence of large complex molecules containing a majority of carbon in the interstellar medium (ISM), the search for graphene plays a central role due to its nature in making other carbon structures. Although the ingredients for graphene synthesis are present in the ISM, conclusive laboratory evidence of such formation is lacking. Therefore, in our laboratory experiments simulating the cold ISM conditions, we subjected icy mantles of benzonitrile, an aromatic with a cyanide side chain that has recently been detected in the interstellar medium, to vacuum ultraviolet photon irradiation. The irradiated ice was observed to leave a residue upon warming to room temperature. The residue was removed from the substrate and placed on a Quantifoil grid for electron microscopy analysis. Transmission electron microscopy showed quantum dots (QD) and nitrogen-doped graphene (N-Graphene) sheets. Diffraction and energy-dispersive X-ray spectroscopy revealed the crystalline nature and carbon–nitrogen composition, of the observed graphene sheet. This is the first evidence of QD and N-graphene synthesis in ice irradiation at interstellar temperatures.

E-mail: bhala@prl.res.in

Eur. Phys. J. D, 77: 24 (2023)

https://link.springer.com/content/pdf/10.1140/epjd/s10053-023-00590-z.pdf?pdf=button

Cavity Ring-Down Spectroscopy of Anthracene, 9-Methylanthrac and 2-Methylanthracene in Supersonic Expansion

S Bejaoui^{1,2}, P Bera^{1,2}, F Salama¹, T Lee¹,

¹Space Science and Astrobiology Division, NASA Ames Research Center, Mountain View, CA, USA ²Bay Area Environmental Research Institute, Moffett Field, CA, USA

The S_0S_1 absorption spectra of anthracene ($C_{14}H_{10}$), 9-methylanthracene ($C_{15}H_{12}$), and 2methylanthracene ($C_{15}H_{12}$) are measured in the ultraviolet region between 330 and 375 nm (26,666 to 30,303 cm1) with cavity ring-down spectroscopy in supersonic free-jet expansions of argon. The associated vibronic band systems and their spectroscopic assignments are discussed and compared to previous studies performed using fluorescence excitation and dispersed fluorescence techniques. Density functional theory (DFT) calculations were carried out to study the structures and evaluate the vibrational transitions of the ground and excited states. Time-dependent DFT calculations of the first electronic excited states and Franck-Condon factor calculations were carried out to assist in the assignment of the experimentally measured vibronic bands. The vibronic spectra obtained in absorption agree well with fluorescence excitation spectra in terms of peak positions but exhibit different relative band intensities. We find a very good match between experimentally obtained vibronic line positions and the peak positions of the quantum chemically calculated Franck-Condon excitation lines.

E-mail: salma.bejaoui@nasa.gov

J. Phys. Chem. A (2023)

https://pubs.acs.org/doi/full/10.1021/acs.jpca.2c08994

Meetings

Laboratory Astrophysics Workshop (ICE 2024)

Kauai, Hawaii, USA 18–22 February, 2024

http://uhmreactiondynamics.org/ICE2024.html

Significant new experimental techniques have been developed to investigate the interaction of ionizing radiation (UV, VUV, gamma rays, charged particles) and of neutrals (atoms, radicals, molecules, grains) with surfaces of solids (ices, minerals, carbonaceous compounds) in the Solar System and in the Interstellar Medium (ISM). These processes provide new fundamental insights — sometimes on the molecular level — into the processes that are critical to the chemistry in the ISM, of star and planet forming regions, and on/in icy objects in the Solar System from the formation of the simplest molecule (molecular hydrogen) to astrobiologically important species such as amino acids and sugars. There is an increasing convergence of interests of these fields, so a 'united' workshop is highly desired.

Based on the successful workshops in 2013 and 2015, the third workshop brings together researchers from leading laboratories through invited (senior and junior researchers) as well as contributed talks covering the interaction of (non)ionizing radiation (UV, VUV, gamma rays, charged particles) and neutrals (atoms, radicals, molecules, grains) with low temperature solids (ices, minerals, organics). The talks can be extended to observations, modeling, and electronic structure calculations, if these topics can be linked — as evident from the abstract — to laboratory experiments. The session chairs will adhere strictly to the allocated time limits of the presentations.

Accommodation: The workshop will take place in the Sheraton Coconut Beach Resort in Kapaa, Kauai, Hawaii, USA, starting with a reception and registration on February 18, 2024, at 6 pm (Sunday). Additional hotels are within walking distance.

Transportation: Sheraton Coconut Beach Resort is a short drive (20 minutes) from the airport (LIH). LIH can be reached on non-stop flights from HNL, LAX, SFO, SEA, PHX, and OAK.

Schedule: The conference will run from February 19 - 22, 2024, with a reception scheduled for Sunday evening starting at 6 pm on February 18.

Registration: Registration and abstract submission will begin July 1, 2023, with late registration beginning on November 1, 2023. No refunds will be given after November 1, 2023. This is an in-person conference only.

E-mail for contact: aturner7@hawaii.edu

COST NanoSpace JWST Training School

La Laguna, Tenerife, Spain 19–22 June, 2023

https://research.iac.es/congreso/jwstworkshop2023/

This JWST Training School is organized by the COST Action NanoSpace (CA21126) in collaboration with the Instituto de Astrofísica de Canarias (IAC) and James Webb Space Telescope (JWST) experts from ESA, NASA and the Centro de Astrobiología (CAB). The COST Action NanoSpace (CA21126) brings together researchers and innvotators from 47 countries and several industrial partners. NanoSpace proposes a highly interdisciplinary approach in order to understand the physics and chemistry of carbon molecular nanostructures in space, taking advantage of the recent successful operation of the James Webb Space Telescope (JWST), the new facilities that can better mimic the interstellar medium (ISM) on the ground as well as the recent developments in the computational facilities and in laboratory techniques.

The main goal of the COST NanoSpace JWST Training School is to provide COST Action NanoSpace participants and young researchers the tools on data analysis and proposals preparation for the exploitation of the unprecedent astronomical data from the James Webb Space Telescope (JWST). The COST NanoSpace JWST Training School will provide specific training to reduce JWST imaging and spectroscopic data, with focus on the mid-infrared spectral range. Attendees will get acquainted with the pipeline architecture and data models and will run a set of hands-on exercises, especially using JWST/MIRI data. These are designed to cover specific science cases, demonstrate calibration challenges and how to solve them. The programme will mostly focus on spectroscopy, but will also demonstrate imaging data reduction as well as the tools for proposals preparation.

The school will be in hybrid format (both on-site and on-line) with on-site attendance limited to 80 trainees and with priority given to PhD students and Young Researchers (i.e. researchers under the age of 40), which are strongly encouraged to participate. There is no registration fee and the NanoSpace COST Action will provide financial support (i.e. reimbursement after the event) for a limited number of participants (\sim 30-40), with high priority to those with a primary affiliation in an institution located in an Inclusiveness Target Country (ITC) / Near Neighbour Country (NNC) participating in the Action. The information requested in the on-line registration form will be used to select the final list of registered participants as well as those eligible for financial support, which will be notified in advance of the Training School. The attendees are expected to arrange their own travel and accommodation.

See the website of the COST NanoSpace JWST Training School for more detailed information, registration, programme, organising committees, etc.

Deadline for on-site registration (no registration fee): 10th May 2023 (or when 80 participants have registered, whichever is sooner).

Deadline for on-line registration (no registration fee): 31st May 2023 (no participants limit but with limited support, mainly via the Slack plattform).

22

E-mail for contact: jwst2023@iac.es

Mini-Symposium "Surface Astrochemistry" at the 36th European Conference on Surface Science

Lodz, Poland 28 August—1 September, 2023

https://www.ecoss36.uni.lodz.pl/

I am writing to invite you and your group to submit an abstract for a talk in a mini-symposium "Surface Astrochemistry" at the 36th European Conference on Surface Science (ECOSS36) to be held in Lodz, Poland, August 28 – September 1, 2023. The aim of this mini-symposium (MS) is to provide important knowledge of the recent work (theoretical, experimental, and observational) that has been done in the field of surface science in astrochemistry. This is important in order to update the community on the recent discoveries, which will lead to understanding the big picture of complex and/or prebiotic molecular formation catalyzed by carbonaceous, silicate and/or ice surfaces in space. This MS will be a 2 hour session that opens the floor for discussion of new future research directions. The abstract submission opens on March 13, 2023, and closes on May 14, 2023. More information about the MS will be soon available on the ECOSS36 website. Please, feel free to contact me for any questions. I am looking forward to seeing you in Lodz.

Dario Campisi - MS organizer

E-mail for contact: campisi@theochem.uni-stuttgart.de

AstroPAH Newsletter

http://astropah-news.strw.leidenuniv.nl astropah@strw.leidenuniv.nl Next issue: 20 April 2023 Submission deadline: 7 April 2023

AstroPAH - March 2023 • Issue 96

23