AstroPAH

A Newsletter on Astronomical PAHs

Issue 81 • September 2021

Formation of organic dust in novae

Editorial

Dear Colleagues,

Welcome to our 81st AstroPAH volume! We hope all of you are healthy and doing well!

The Editorial Board would like to express our deepest gratitude to Elisabetta Micelotta who is sadly leaving the AstroPAH board. Thank you Elisabetta for being part of this team since the AstroPAH conception and for the incredible journey over numerous newsletter publications!

As you may have seen, JWST has a new launch date.

Our Picture of the Month illustrates recent work highlighted in our Abstracts on laboratory simulations of carbonaceous dust particles with inclusions of nitrogen in the form of Quenched Nitrogen-included Carbonaceous Composite (CQNCC). This latest study suggests that the spectra of QNCC have a close resemblance to the infrared spectra of dusty classical novae.

In this Newsletter we present an In Focus by Dimitra Rigopoulou and Ismael Garcia-Bernete on “PAHs to probe the AGN - host galaxy connection”, where the authors review PAH properties and emission in the context of Active Galactic Nuclei (AGN) and the relationship between AGN and the dust and gas in the host galaxy.

Our contributed abstracts cover the topic of our Picture of the Month (the nature of organic dust in novae) as well as galactic C_2H distributions, *ab initio* heats of formation for PAHs, and the detection of interstellar cyanoacetyleneallene in TMC-1. You can also find Dr. Dario Campisi’s PhD Thesis in our abstract section.

A senior postdoctoral position in laser molecular spectroscopy at the Berlin Institute of Technology (TU Berlin) are listed in our Announcements section.

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

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

The Editorial Team

Next issue: 21 October 2021.
Submission deadline: 8 October 2021.

Contents

PAH Picture of the Month

A laboratory simulation of carbonaceous dust with inclusion of nitrogen in the form of Quenched Nitrogen-included Carbonaceous Composite (QNCC) showed that the spectra of QNCC have a close resemblance to the observed infrared spectra of novae. See more about this work in the first abstract by Endo et al. (2021).

Credits: The University of Tokyo.

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PAHs to probe the AGN - host galaxy connection

by Dimitra Rigopoulou & Ismael Garcia-Bernete

Supermassive black holes (SMBH) are believed to play an instrumental role in the evolution of their host galaxies, as evidenced by the existence of tight correlations between the SMBH masses and large-scale host properties (e.g. Kormendy & Ho et al. 2013, Heckman & Best 2014). Star-formation (SF) and SMBH growth follow similar evolutionary tracks (e.g. Madau & Dickinson 2014). In addition, theoretical models suggest that feedback from growing SMBH/Active Galactic Nuclei (AGN), in the form of ouflows (as shown in Figure 1) is a key ingredient in models that link the central SMBH to its host galaxy, by shutting off its star-formation and maintaining its quiescence after it has been quenched (e.g., Hopkins et al. 2006, Weinberger et al. 2018). However, because SF is difficult to measure around AGN, there is a lot of uncertainty about the exact nature of the interrelations between the two processes and the important role that AGN feedback plays in regulating galaxy evolution.

Diagnostics at optical wavelengths (e.g. Kauffman et al. 2003) provide tools to probe SF and accretion processes. However, these diagnostics may not be very useful for objects where dust obscuration is significant. Therefore, studying these processes at mid-infrared (mid-IR) wavelengths, where dust extinction is significantly lower compared to optical wavelengths, offers significant advantages. Among the various mid-infrared diagnostics, emission from Polycyclic Aromatic Hydrocarbons (PAHs) has been successfully used to quantify SF in the vicinity of the AGN (e.g. Esquej et al. 2014).

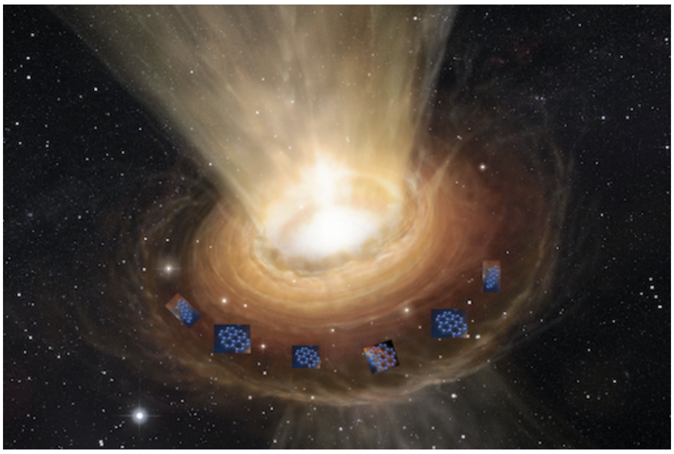

Figure 1 *– Artist impression showing the surroundings of an SMBH at the heart of NGC 3783, an AGN in the southern constellation of Centaurus. A wind of cool material in the polar regions of the dusty torus is visible. PAH emission originates in the dusty region surrounding the SMBH. (Credit: ESO/M. Kornmesser)*

Observations with ISO, Spitzer and ground-based telescopes have provided mid-IR spectra for large samples of local AGN (e.g., Roche et al. 1991, Laurent et al. 2000, Buchanan et al. 2006, Wu et al. 2009). Often, AGN-dominated systems do not show strong PAH features in their nuclear IR spectra. Even when PAH features are detected they often have low equivalent widths compared to those observed in star-forming galaxies. It has been suggested that PAH molecules could be destroyed in the very hard radiation fields of AGN (e.g. Voit 1992). An alternative explanation is that PAH features maybe diluted by the strong AGN continuum, (as suggested by e.g. Alonso-Herrero et al. 2014, Ramos Almeida et al. 2014). Hence it is important to investigate the link between PAH emission and the hardness of the radiation field to better understand the effect that hard radiation fields (such as those seen in AGN) have on PAH molecules.

The detailed characteristics of PAH features, such as their central wavelength, shape and the intensity ratios between different bands, are known to vary (Peeters, Spoon & Tielens 2004). These variations are the result of changes in the structure of the PAH molecules in response to exposure in diverse astrophysical environments. Because each PAH band is attributed to a specific vibrational mode, the ratio between different bands could be used as a diagnostic of PAH properties. For instance, it is well known that the 3.3 μm PAH feature is due to the radiative relaxation of C-H stretching modes, the 6-9 μm features originate from C-C stretching modes while the 11.3 μm feature originates in the C-H out-of-plane bending modes. As a result, the 6-9 μm features will be much more prominent in ionised PAHs, while the converse is true for the 3.3 and 11.3 μm bands. Consequently, the ratios between the C-C and the C-H feature intensities depend on the charge of the PAHs, which is directly related to the physical conditions in the environment where the emission is originating.

Theoretical PAH Spectra

In Rigopoulou et al. (2021), we used theoretically computed spectra of PAHs of different size, structure and charge to construct diagnostic grids in order to investigate how the ratios of the various PAH emission features can be used to trace the ISM conditions of AGN. The theoretical spectra used to generate the grids were computed using Density Functional Theory (DFT). The PAH molecules were built with the Gaussview 5 software while the DFT calculation were performed using Gaussian 16 (Frisch 2016) together with the B3LYP functional along with the 4-31G basis set. Theoretical spectra from the NASA Ames PAH IR Spectroscopic Database (Bauschlicher et al. 2018) were also used in our study. The DFT spectra were subsequently convolved with a specific band shape, line width, and emission temperature to convert them into an emission spectrum similar to those observed in astrophysical environments following the steps described in Rigopoulou et al. (2021). The PAH spectra were subsequently placed in bins of increasing number of carbons, N_c, and, for each bin a spectrum was calculated by averaging the spectra in that bin (PAHs that were found to deviate by more than 3σ from the average value determined in that bin were excluded from further analysis).

Figure 2 shows the 6.2/7.7 vs. 11.3/7.7 PAH ratios from the DFT PAH spectra exposed to radiation fields with a range of energies from the ISRF (filled circles) to $10^3\times$ISRF (stars). The top grid (black lines) represents neutral PAHs, the middle grid (brown lines) represents 50% neutral and 50% ionised PAHs while the bottom one (magenta lines) corresponds to 100% ionized PAHs. The same grids for the 11.3/7.7 vs. 11.3/3.3 ratio plot from DFT PAH spectra exposed to radiation fields with a range of energies from ISRF to $10^3\times$ISRF. Since, so far, the most commonly detected PAH bands in AGN spectra are the 6.2, 7.7 and 11.3 μm, we currently focus on grids involving these band ratios.

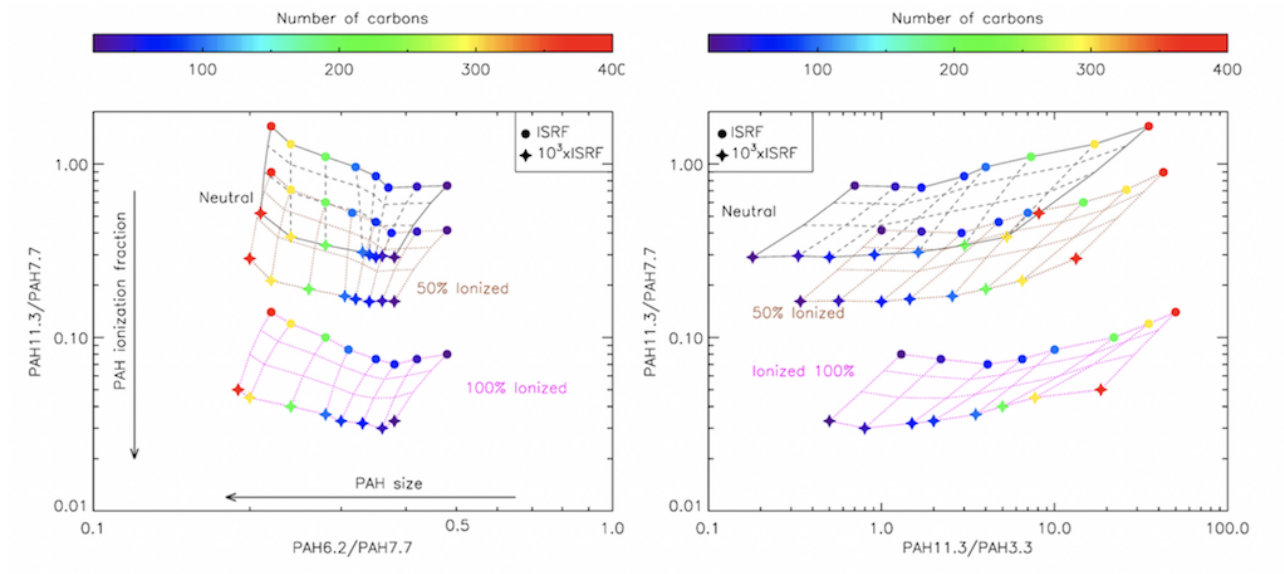

Figure 2 *– Left: The 6.2/7.7 vs. 11.3/7.7 ratio plot from DFT PAH spectra exposed to radiation fields with a range of energies from the ISRF (filled circles) to $10^3\times$ISRF (stars). The top grid (black lines) represents neutral PAHs, the middle grid (brown lines) represents 50% neutral and 50% ionised PAHs while the bottom one (magenta lines) corresponds to 100% ionized PAHs. Right: The same grids for the 11.3/7.7 vs. 11.3/7.7 ratios.*

The Impact of the AGN on the host galaxy

There is increasing evidence that the AGN interacts with the dust and gas in the host galaxy. Using archival staring mode data taken with the Infrared Spectrometer (IRS) on board the Spitzer Space Telescope of AGN and star-forming galaxies, in Garcia-Bernete et al. (2021) we investigated whether PAH band ratios can be used to probe the physical conditions of the ISM in these galaxies. Figure 3 shows the 6.2/7.7 vs. 11.3/7.7 PAH band ratios of AGN-dominated and star-forming galaxies together with the PAH diagnostic grids. It is evident that PAH band ratios can, indeed, be a powerful diagnostic of the physical conditions of the ISM in galaxies. Moreover, the plot indicates that PAH emission from AGN appears to favour larger PAH molecules, on average, than star-forming galaxies. Although the study provided a first insight into the diagnostic power of PAHs to provide information on the PAH size

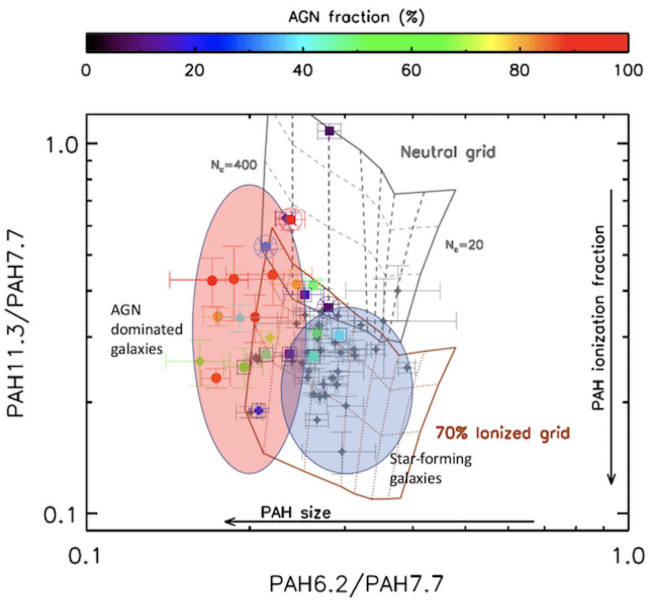

Figure 3 *– PAH diagnostic grids constructed from the band ratios of theoretical PAH spectra. Coloured points represent PAH band ratios measured from AGN and grey points represent data for star-forming galaxies.*

and charge of star-forming galaxies and AGN it was limited by the low spectral/spatial resolution provided by Spitzer/IRS spectra.

To further investigate the impact of the AGN on the host galaxy it is necessary to compare PAH emission from nuclear (central) and circumnuclear (extended) regions of galaxies hosting active nuclei. Differences in the emission from these two regions would give us valuable clues about the influence of the AGN on its host-galaxy. For this purpose we analysed Spitzer/IRS spectral mapping data in order to be able to compare PAH band ratios from the *central* and *circumnuclear* regions. We took as our central region an area covering approximately 5.9″×5.9″. The central AGN spectra were extracted assuming a point-like source, whereas the spectra of the extended regions were computed as the difference between the total galaxy minus the central AGN extracted emission.

Figure 4 shows the PAH band ratios for those AGN where we were able to measure nuclear (central) and extended (circumnuclear) emission. PAH band ratios from the central AGN regions (circles) and extended regions (stars) are compared to our PAH diagnostic grids. Although the study is based on a small sample of AGN (where Spitzer/IRS mapping data were available) some interesting results are already evident: The PAH band ratios measured in the central AGN-dominated spectra are located in the region of large PAH molecules. In contrast, the PAH band ratios derived from the extended AGN regions appear to be closer to the values measured in star-forming galaxies (beige shaded area in Figure 4). We interpret these trends as an indication that the AGN does indeed influence the dust grain distribution (PAH molecules) in the host galaxy. Although our analysis is limited by the low spatial resolution of Spitzer/IRS data we tentatively interpret these trends as *evidence for the destruction of small grains in the central AGN region.*

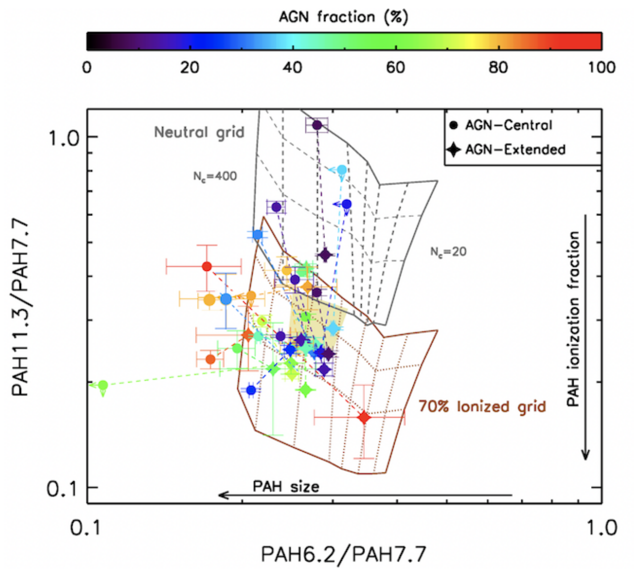

Figure 4 *– PAH 11.3/7.7 vs. 6.2/7.7 grids based on neutral (grey) and ionised (brown) PAH molecules. Small circles denote values corresponding to central AGN PAH ratios. Stars correspond to AGN extended regions.The beige shaded region indicates the range of PAH values seen in star-forming galaxies.*

The imminent launch of the James Webb Space Telescope (JWST, at the time of writing the launch is scheduled for December 18th, 2021) will transform studies of PAHs in AGN by providing an unprecedented level of spectral and spatial detail. With diffraction-limited resolution, JWST will offer superb sensitivity, particularly for low brightness regions. By measuring PAH emission from nuclear and circumnuclear regions in galaxies we will be able to elucidate the impact of the central AGN on its host galaxy and advance our understanding of the survival of PAH molecules in the harshest environments in the Universe.

Prof. Dimitra Rigopoulou is a Professor of Astrophysics in the Galaxy formation and evolution research group at the University of Oxford. Her research focuses on the evolution of galaxies and the growth of structure in the Universe by (i) using multiwavelength datasets to gain new insights into galaxy formation and evolution by contrasting the views provided by radiation emitted in different wavelengths (in particular those in the mid/far-infrared, and submillimetre), and (ii) studying of nearby galaxies where the increased spatial resolution afforded by ground based telescopes and space based observatories enables a better understanding of the physical processes governing galaxy evolution.

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Dr. Ismael Garcia Bernete is a postdoctoral research assistant in the Galaxy formation and evolution research group at the University of Oxford. His primary research interests are in the broad field of galaxy formation and evolution, particularly in understanding the role that active galactic nuclei (AGN) play on the galaxy formation and evolution, the feeding and feedback processes in galaxies, star-formation-AGN connection, and physical conditions of the interstellar medium (ISM).

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References

- *Alonso-Herrero A., et al., 2014, MNRAS, 443,2766*
- *Bauschlicher, C.W. Jr, Ricca, A., Boersma, C., Allamandola, L. J., 2018, ApJ 234, 32*
- *Buchanan, C. L., Kastner, J. H., Forrest, W.J., et al., 2006, ApJ 132, 1890*
- *Esquej, P., et al. 2014, ApJ 780, 66*
- *Frisch, M. J., et al., 2016, Gaussian16 Revision C.01*
- *Garcia-Bernete, I. et al. 2021, MNRAS, submitted*
- *Heckman, T. Best, P.N., 2014, ARA&A 52, 589*
- *Hopkins, P., et al., 2006, ApJ 652, 864*
- *Kauffman, G., et al. 2003, MNRAS, 346, 1055*
- *Kormendy, J., Ho, L.C., 2013, ARA&A 51, 511*
- *Madau, P., Dickinson, M., 2014, ARA&A 52, 415*
- *Peeters, E., Spoon, H.W.W., Tielens, A.G.M, 2004, ApJ 613, 896*
- *Ramos Almeida, C., Alonso-Herrero, A., Esquej, P., et al. 2014, MNRAS 439, 3847*
- *Rigopoulou, D., et al. 2021, MNRAS 504, 5287*
- *Roche, P.F., Aitken, D. K., Smith, C.H., Ward, M.J., 1991, MNRAS 248, 606*
- *Voit, G.M., 1992, MNRAS 258, 161*

- *Weinberger, R., et al., 2018, MNRAS 479, 4056*
- *Wu, Y., et al. 2009, ApJ 701, 658*
- *Laurent, O., Mirabel, I. F., Charmandaris, V., et al. 2000, A&A 359, 887*

On the Nature of Organic Dust in Novae

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Recent astronomical observations and planetary missions have found that complex organics are prevalent throughout the universe, from the solar system to distant galaxies. However, the detailed chemical composition and the synthesis pathway of these organics are still unclear. Circumstellar envelopes represent excellent laboratories to study the abiological synthesis of extraterrestrial organics. Novae, having very short dynamical lifetimes, can put severe constraints on the chemical pathway of organic synthesis. Here, we report a laboratory simulation of carbonaceous dust with inclusion of Nitrogen in the form of Quenched Nitrogen-included Carbonaceous Composite (QNCC). QNCC is produced by the quenched condensation of plasma gas generated from the nitrogen gas, and aromatic and/or aliphatic hydrocarbon solids by applying microwave discharge (2.45 GHz, 300 W). We have shown that the spectra of QNCC have a close resemblance to the observed infrared spectra of novae. The results of the infrared and X-ray analyses suggest that the nitrogen inclusion in the form of amine plays an important role in the origin of the broad 8 μm feature of dusty novae. We conclude that QNCC is at present the best laboratory analog of organic dust formed in the circumstellar medium of dusty classical novae, which carries the unidentified infrared bands in novae via thermal emission process.

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The 3.3 μm Infrared Emission Feature: Observational and Laboratory Constraints on Its Carrier

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We examine the self-consistency of laboratory and observational data for potential carriers of the 3.3 μm infrared emission feature (IEF), a member of the ubiquitous family of strong interstellar IEFs at 3.3, 3.4, 6.2, 7.7, 8.6, 11.2, and 12.7 μm. Previous studies have shown that most Galactic sources (reflection nebulae, HII regions, and planetary nebulae) show 3.3 μm IEFs displaying similar central wavelengths, full widths at half maximum, and profiles. Our study is focused on the band profile designated as Class A, the most prevalent of four classes of observed band profiles. In contrast to the observations, laboratory spectra for gas phase polycyclic aromatic hydrocarbons (PAHs), the widely assumed carriers of the IEFs, display central wavelength shifts, widths, and profiles that vary with temperature and PAH size. We present an extrapolation of the laboratory band shifts and widths for smaller PAHs ($\leq$ 32 carbon atoms) to the larger PAHs ($>$ 50 carbon atoms) that are thought to be the IEF carriers. The extrapolation leads to tight constraints on the sizes of the putative PAH carriers. Reconciling the observations with the implications of the laboratory spectra pose a significant challenge to the PAH and other IEF carrier hypotheses.

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Accurate Heats of Formation for Polycyclic Aromatic Hydrocarbons: A High-Level Ab Initio Perspective

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Polycyclic aromatic hydrocarbons (PAHs) are key reference materials for the validation and parameterization of computationally cost-effective procedures such as density functional theory (DFT), semiempirical molecular orbital theory, and molecular mechanics. We obtain accurate heats of formation (ΔH_f^{298}) for 20 PAHs with up to 18 carbon atoms by means of the explicitly correlated W1-F12 thermochemical procedure. The heats of formation are obtained via atomization reactions and quasiisodesmic reactions involving CH_4, C_2H_4, and C_6H_6 for which accurate experimental ΔH_f^{298} values are available from the ATcT thermochemical network. We show that for large PAHs the differences between W1-F12 heats of formation obtained from atomization and quasiisodesmic reactions increase with the size of the system and range between 1.7 (C_7H_8) and 8.9 (Chrysene, $C_{18}H_{12}$) kJ/mol. This suggests that atomization reactions should be used with caution for obtaining heats of formation for medium-sized systems even when highly accurate thermochemical procedures (such as W1-F12 theory) are used. For eight PAH compounds (toluene, indene, acenaphthylene, biphenyl, diphenylmethane, anthracene, pyrene, and chrysene) our best theoretical values agree with the best experimental values to within $\sim$1 kJ/mol; for six additional systems (indane, naphthalene, biphenylene, acenaphthene, phenanthrene, and m-terphenyl) agreement between theory and experiment is good with deviations ranging between 2–4 kJ/mol. However, for four systems (p-terphenyl, fluorene, pyracene, and pyracyclene) our best W1-F12 values suggest that the experimental ΔH_f^{298} values should be revised by significant amounts ranging from 6.5 and 24.4 kJ/mol.

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Can force fields developed for carbon nanomaterials describe the isomerization energies of fullerenes?

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We evaluate the performance of carbon force fields for 1811 C60 PW6B95-D3/Def2-QZVP isomerization energies. Several force fields (most notably the machine-learning GAP-20 potential) exhibit a high statistical correlation with the DFT isomerization energies. Therefore, linear scaling of the isomerization energies can significantly improve the accuracy. The best scaled force fields attain mean-absolute deviations of 8.5 (GAP-20), 12.3 (LCBOP-I and REBO-II), and 13.3 (ABOP) kcal mol^{-1}, which translate to mean-absolute relative deviations of 4.7% (GAP-20), 6.5% (LCBOP-I), 6.6% (REBO-II) and 7.1% (ABOP). Therefore, these force fields offer a computationally economical way for exploring the relative energies of fullerenes.

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The distribution and origin of C_2H in NGC 253 from ALCHEMI

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Observations of chemical species can provide insights into the physical conditions of the emitting gas however it is important to understand how their abundances and excitation vary within different heating environments. C_2H is a molecule typically found in PDR regions of our own Galaxy but there is evidence to suggest it also traces other regions undergoing energetic processing in extragalactic environments.

Aims: As part of the ALCHEMI ALMA large program, we map the emission of C_2H in the central molecular zone of the nearby starburst galaxy NGC 253 at 1.6” (28 pc) resolution and characterize it to understand its chemical origins.

Methods: We used spectral modeling of the N = 1–0 through N = 4–3 rotational transitions of C_2H to derive the C_2H column densities towards the dense clouds in NGC 253. We then use chemical modeling, including photodissociation region (PDR), dense cloud, and shock models to investigate the chemical processes and physical conditions that are producing the molecular emission.

Results: We find high C_2H column densities of 10^{15} cm^{-3} detected towards the dense regions of NGC 253. We further find that these column densities cannot be reproduced if it is assumed that the emission arises from the PDR regions at the edge of the clouds. Instead, we find that the C_2H abundance remains high even in the high visual extinction interior of these clouds and that this is most likely caused by a high cosmic-ray ionization rate.

Conclusion: C_2H emission in NGC 253 primarily arises from dense gas where the cosmic-ray ionization rate is greater than 10^{14} s^{-1}.

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Astronomy & Astrophysics (2021)

https://doi.org/10.1051/0004-6361/202141233 https://ui.adsabs.harvard.edu/abs/2021arXiv210704580 abstract

PAH Spectroscopy from 1 to 5 μm

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The PAH model predicts many weak emission features in the 1–5 μm region that can resolve significant questions that it has faced since its inception in the mid-80's. These features contain fundamental information about the PAH population that is inaccessible via the much stronger PAH bands in the 5– 20 μm region. Apart from the 3.3 μm band and plateau, PAH spectroscopy across most of the 1–5 μm region has been unexplored due to its low intrinsic intensity. ISO and Akari covered some of this wavelength range, but lacked the combined sensitivity and resolution to measure the predicted bands with sufficient fidelity. The spectroscopic capabilities of the *NIRSpec* instrument on board JWST will make it possible to measure and fully characterize many of the PAH features expected in this region. These include the fundamental, overtone and combination C – D and C ≡ N stretching bands of deuterated PAHs, cyano-PAHs (PAH–C ≡ N), and the overtones and combinations of the strong PAH bands that dominate the 5–20 μm region. These bands will reveal the amount of D tied up in PAHs, the PAH D/H ratio, the D distribution between PAH aliphatic and aromatic subcomponents, and delineate key stages in PAH formation and evolution on an object-by-object basis and within extended objects. If cyano-PAHs are present, these bands will also reveal the amount of cyano groups tied up in PAHs, determine the N/C ratio within that PAH subset, and distinguish between the bands near 4.5 μm that arise from CD versus C ≡ N.

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Detection of interstellar H_2CCCHC_3N: A possible link between chains and rings in cold cores

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Context: The chemical pathways linking the small organic molecules commonly observed in molecular clouds to the large, complex, polycyclic species long suspected of being carriers of the ubiquitous unidentified infrared emission bands remain unclear.
Aims: To investigate whether the formation of mono- and polycyclic molecules observed in cold cores could form via the bottom-up reaction of ubiquitous carbon-chain species with, for example, atomic hydrogen, a search is made for possible intermediates in data taken as part of the GOTHAM (GBT Observations of TMC-1: Hunting for Aromatic Molecules) project.
Methods: Markov chain Monte Carlo (MCMC) source models were run to obtain column densities and excitation temperatures. Astrochemical models were run to examine possible formation routes, including (a) a novel grain-surface pathway involving the hydrogenation of C_6N and HC_6N, (b) purely gas-phase reactions between C_3N and both propyne (CH_3CCH) and allene (CH_2CCH_2), and (c) via the reaction CN + $H_2CCCHCCH$.
Results: We report the first detection of cyanoacetyleneallene (H_2CCCHC_3N) in space toward the TMC-1 cold cloud using the Robert C. Byrd 100 m Green Bank Telescope (GBT). Cyanoacetyleneallene may represent an intermediate between less-saturated carbon chains, such as the cyanopolyynes, that are characteristic of cold cores and the more recently discovered cyclic species, such as cyanocyclopentadiene. Results from our models show that the gas-phase allene-based formation route in particular produces abundances of H_2CCCHC_3N that match the column density of 2×10^{11} cm^{-2} obtained from the MCMC source model, and that the grain-surface route yields large abundances on ices that could potentially be important as precursors for cyclic molecules.

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Behavior of implanted Xe, Kr and Ar in nanodiamond and thin graphene stacks: experiment and modeling

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Implantation and subsequent behaviour of heavy noble gases (Ar, Kr, Xe) in few-layer graphene sheets and in nanodiamonds is studied both using computational methods and experimentally using X-ray absorption spectroscopy. X-ray absorption spectroscopy provides substantial support for the Xe-vacancy (Xe-V) defect as a main site for Xe in nanodiamond. It is shown that noble gases in thin graphene stacks distort the layers, forming bulges. The energy of an ion placed in between flat graphene sheets is notably lower than in domains with high curvature. However, if the ion is trapped in the curved domain, considerable additional energy is required to displace it.

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Profile comparison of the 6–9 μm polycyclic aromatic hydrocarbon bands in starburst-dominated galaxies

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Polycyclic aromatic hydrocarbons (PAHs) are of great astrochemical and astrobiological interest due to their potential to form prebiotic molecules. We analyse the 7.7 and 8.6 μm PAH bands in 126 predominantly starburst-dominated galaxies extracted from the Spitzer/IRS ATLAS project. Based on the peak positions of these bands, we classify them into the different A, B, and C Peeters' classes, which allows us to address the potential characteristics of the PAH emitting population. We compare this analysis with previous work focused on the 6.2 μm PAH band for the same sample. For the first time in the literature, this statistical analysis is performed on a sample of galaxies. In our sample, the 7.7 μm complex is equally distributed in A and B object's class while the 8.6 μm band presents more class B sources. Moreover, 39 per cent of the galaxies were distributed into A class objects for both 6.2 and 7.7 μm bands and only 18 per cent received the same A classification for the three bands. The "A A A" galaxies presented higher temperatures and less dust in their interstellar medium. Considering the redshift range covered by our sample, the distribution of the three bands into the different Peeters' classes reveals a potential cosmological evolution in the molecular nature of the PAHs that dominate the interstellar medium in these galaxies, where B class objects seem to be more frequent at higher redshifts and, therefore, further studies have to be addressed.

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PHD THESIS

Interstellar Catalysts and the PAH Universe

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Organic molecules in interstellar space are important as they influence the structure of galaxies and star formations. Studying catalytic processes in space allows us to understand how molecular species are formed and chemically evolved in the interstellar medium and solar system objects. Quantum chemical methods, such as "Density Functional Theory" (DFT), can be employed to study the chemical pathways for the formation of molecular species, which is challenging with only observations and experiments. This thesis studies, with DFT methods, how polycyclic aromatic hydrocarbons (PAHs), the most abundant organic species in space, catalyze the formation of molecular hydrogen in the interstellar medium. Specifically, how linear PAHs become superhydrogenated and how the presence of Stone Wales defect in PAHs contributes to their catalytic activity for molecular hydrogen formation. In addition, this thesis reports the study of the catalytic activity of forsterite, a silicate mineral abundant in grains, asteroids, and meteorites. Specifically, the presence of Schottky MgO vacancy in forsterite can catalyze the C – H activation of PAHs as the first step to study the breakdown reaction of PAHs in asteroidal settings. The latter is indispensable to understand the formation of the so-called organic inventory of solar system objects.

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Postdoc Position in Molecular Physics / Physical Chemistry / Laboratory Astrophysics

Berlin Institute of Technology (TU Berlin), Germany

Advertised by Otto Dopfer

A (senior) postdoctoral position for up to five years is available in the laser molecular spectroscopy and environmental physics group of Otto Dopfer at the Berlin Institute of Technology (TU Berlin), Germany. The predominantly experimental research of our group involves the laser spectroscopic, mass spectrometric, and quantum chemical investigation of molecules, radicals, ions, clusters, and nanostructures in the gas phase, with strong relevance to a broad range of interdisciplinary topics ranging from materials science to biophysics, catalysis, astrochemistry, environmental chemistry, and plasma physics.

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Experience in several of the following fields is mandatory:

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3. writing of publications, reports, and proposals
4. strong communication and presentation skills

Interested and highly qualified candidates are encouraged to send their application (in a single pdf file) to Prof. Otto Dopfer (dopfer@physik.tu-berlin.de), including a cover letter, a CV (including a list of publications), a statement of qualifications relevant for the position (max. 1 page), a statement of research interests (max. 1 page) as well as names and complete addresses of two referees.

Evaluation of the applications will begin at October 1 (2021) and will continue until the position is filled. The desired starting date is February 1st (2022) but this is negotiable to some extent.

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Deadline for Application: October 31, 2021.

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