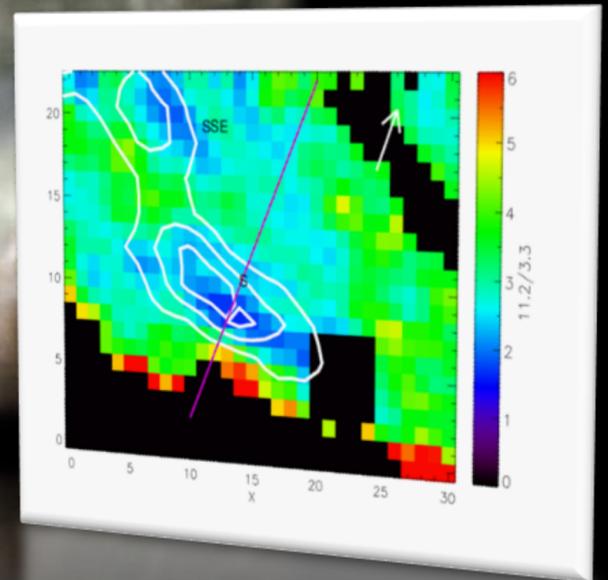
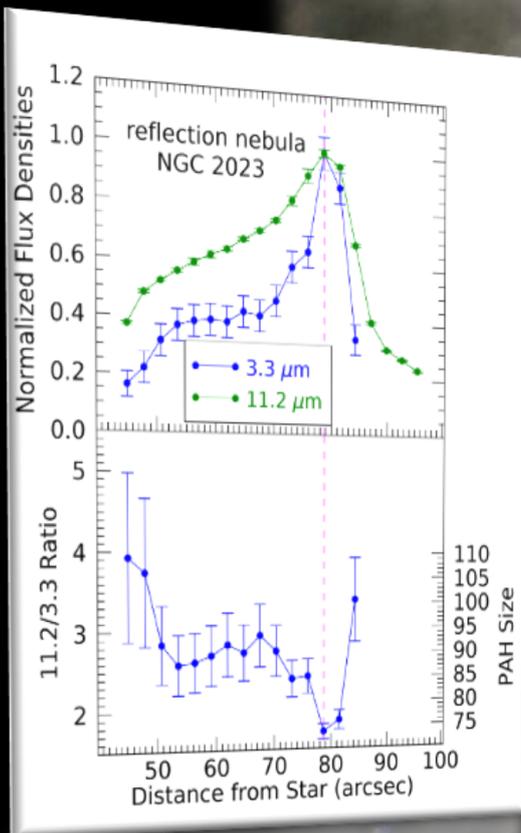


AstropAH

A Newsletter on Astronomical PAHs

Issue 79 • June 2021



Novel trends in PAH size distribution in NGC2023



Editorial

Dear Colleagues,

Welcome to our 79th AstroPAH volume! We hope all of you are healthy and doing well!

The Picture of the Month is about the discovery of novel trends in PAH size in NGC2023. It illustrates how the 11.2/3.3 ratio, and therefore the average PAH size, is highly sensitive to the distance from the star and varies spatially with respect to the Photo-Dissociation Region front and proximity to the star. Make sure you check our abstract section to learn more about it!

Our In Focus this month is an interview with Dr. Amanda Steber who is an expert in microwave spectroscopy and is studying the structure and dynamics of PAHs and their clusters. Amanda was a member of the AstroPAH editorial board until last fall. We are very happy to have her share her experiences with us this month.

In the Abstracts section you will find a great level of diversity with co-authors from all over the globe, with affiliations from 17 different countries, covering almost every continent. This diversity is also reflected in the topics, ranging from observational work showing us the sizes of PAHs, to theoretical work trying to find the next observational candidate; and from theoretical work showing benzene's interactions in water clusters, to experiments showing benzene assembling from acetylene in cold matrices.

You can also go see our new PAH of the Month [on our Instagram page!](#) This month is dedicated to indene (C₉H₈).

We hope you enjoy reading our newsletter, and we thank you for your dedication and your interest in AstroPAH! Please continue sending us your contributions, and if you wish to contact us, feel free to use our [email](#).

Enjoy reading our newsletter!

The Editorial Team

**Next issue: 23 July 2021.
Submission deadline: 9 July 2021.**

AstroPAH Newsletter

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PAH Picture of the Month

Novel trends in PAH size distribution were discovered in NGC2023 by [Knight et al. \(2021\)](#). The bottom panel on the left graph shows how the 11.2/3.3 ratio, and subsequently the average PAH size, is highly sensitive to distance from the star. Similarly, the graph on the right shows how the 11.2/3.3 ratio varies spatially with respect to the PDR front and proximity to the star.

Credits: [Knight et al. 2021](#) (accepted in ApJ). IRAC data by [Fleming et al. 2010](#). IRS SH data by [Peeters et al. 2012](#) and [Peeters et al. 2017](#).



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An Interview with Dr. Amanda Steber

Dr. Amanda Steber works at the Deutsches Elektronen-Synchrotron (DESY) as a research scientist and the astrochemistry sub-group leader in the group of Prof. Melanie Schnell. Her work focuses on using microwave to ultraviolet radiation to probe the structure and dynamics of PAHs and their clusters. She recently stepped down from her role as an editor of AstroPAH due to the birth of her son. She received her bachelor's degree from Eastern Illinois University. During this time, she started her research career in microwave spectroscopy, and she continued it during her PhD with Prof. Brooks H. Pate at the University of Virginia. Here she worked on the development of microwave and millimeter-wave spectrometers, as well as the electrical discharge of astrochemically relevant species. She was then awarded with a Louise Johnson fellowship in Hamburg, Germany, where she joined Prof. Schnell's group as a postdoc and began helping to build up the astrochemistry subgroup activities. In October she will begin a Marie Skłodowska-Curie individual fellowship at the Universidad de Valladolid, Spain, with Prof. Alberto Lesarri where she will be looking into the astrochemistry of sulfur.



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

My foray into PAH-related research started when I started in Melanie Schnell's group. She had just been awarded an ERC starting grant on astrochemistry, and within the grant, she had proposed to look for corannulene, which she had studied earlier in her career. Some experiments were started in which the isotopes and a water complex were identified via microwave spectroscopy. The research line sort of grew from there, and we became interested in not only complexing PAHs with water, but also investigating them with a discharge source and free-electron lasers. I have several ongoing projects that I will continue to collaborate on after my move, but the most exciting project for me is the results that we have been getting by discharging PAHs both by themselves and with other astrochemically relevant species.

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

When I was first asked to be a part of the AstroPAH team, I was thrilled. I had met several of the editors at a PAH event in the Netherlands a few months before that, and I enjoyed getting to know them. The camaraderie that they shared and ease with which they worked with each other was a nice breath of fresh air so when they invited me, I, of course, said yes. From the very beginning they were all very kind, energetic, and full of love for the AstroPAH newsletter. It was such a great working environment and a great group of individuals to get to know. As time went on, the board gained and lost a few members. With each development, the board changed slightly, but it never lost that “family” feel. I think that was my favorite part of working on the newsletter, the second family that I had. In close second was the ability to contact and interact with some very interesting individuals in the field. As one of the editors of the In Focus section, I was able to “meet” some researchers that I might not have otherwise had the opportunity to meet. While I miss being a part of the editorial board, I know it is in good hands and will continue to thrive.

What, in your opinion, is the most important advancement in PAH research that was accomplished during your time on the AstroPAH board?

I know that this happened a little bit after I left the board, but I have to say that one of the most important advancements was the discovery of the two isomers of cyanonaphthalene in TMC-1. While this is not a pure PAH in the sense that it has the cyano group attached, I think we now have a pretty solid foundation to say that PAHs are presently in the ISM.

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

The biggest difficulty that I have faced to stay in the field has been a problem that many deal with - the two body problem. My husband is also a microwave spectroscopist, albeit one that works on a slightly different subject matter, but a microwave spectroscopist all the same. It has been difficult figuring out how we will both be able to advance our careers together. We have decided to take it one step at a time, and we have both been very fortunate to work with people who have helped promote our careers independently of one another. I think the thing that has guided us the most has been establishing our expectations with one another and helping the other to achieve those expectations.

What was the most important advice somebody gave you?

I have been very blessed by the people that have touched my life. I have had many great mentors along the way, and they have all imparted some nuggets of wisdom. However, I would have to say that my undergraduate research advisors, Sean and Rebecca Peebles, really set an example for me to follow as opposed to giving me a spoken piece of advice. What I came away with from working with them was that I should always remain true to

myself. Regardless of what others think and the self-doubts that I may sometimes possess, I should stay true to who I am at my core. This has guided me well and helped me both personally and professionally.

How do you balance your professional and personal life?

This is actually a very interesting question, which I am not sure that I have an answer for yet. My son was just born in November, so I have been on parental leave ever since. I am worried about the changes this will bring when I do go back to work, but I am hoping that by setting my priorities, I will be able to stay above water. In the past, I have found hobbies to engage in, and I tried to make sure that I did not spend too much time in the lab as we really do need time to decompress and take care of ourselves.

What do you do outside of work?

Currently my activities include taking care of my son and packing for my family's relocation to Spain. I am hoping that after the move and once the Covid numbers look even better to again take up racquetball or some other equally physical activity. I also enjoy baking, but many Europeans find my desserts to be too sweet. :)



Abstracts

PAHs as possible catalysts in the formation of Prebiotic molecules in the Horsehead nebula

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Theoretical studies are essential in exploring the mechanisms of the formation and destruction of molecules in the interstellar medium. One key question is about the abundance of molecules with a prebiotic role in environments like the Horsehead nebula, in view of issues such as the origin of life on Earth and other places in the Universe. The Horsehead nebula is an archetype of photodissociation region (PDR), with physical and chemical parameters well-known in the literature. Thus, we could model this region using the PDR Meudon code which is widely used since it can simulate PDR regions accurately considering the physical and chemical properties of a given system. We have shown that long-lived PAHs, such as circumcoronene, can be used as catalysts in the production of prebiotic N-heterocyclics, such as pyridine (C_5H_5N). Thus, we developed a network of reactions considering that PAHs are hardly destroyed, but they can be dehydrogenated. With the insertion of circumcoronene ($C_{54}H_{18}$) in the pyridine formation network, it was found that the abundance of that molecule increased from $\sim 10^{-25}$ to 10^{-15} particles of C_5H_5N (relative to H_2), and the column densities, in the cloud core, reached values above 10^{13} cm^{-2} . Such values are within the current observation limit. Thus, after verifying that the model is in accordance with the observational data for the region, the present simulations demonstrate how the exploration of some possible routes for the production of N-heterocycles resulted in significant abundances for these species. Thus, the exploration of a variety of production paths should reveal more species to be the target of astrophysical observations.

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Theoretical investigation of benzo(a)pyrene formation

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Polycyclic aromatic hydrocarbons (PAH) are harmful chemicals emitted to the environment by incomplete combustion. As the aromatic structure grows, the carcinogenic effect increases, and thus, to understand their formation mechanisms is crucial. In this work, new reaction pathways leading to benzo(a)pyrene, a PAH with well-known carcinogenic effects, were explored by using DFT methods. Starting from chrysene or benzo(a) anthracene, three types of reaction mechanism were studied: hydrogen abstraction acetylene addition (HACA), hydrogen abstraction ethynyl radical addition (HAERA) and Diels-Alder (DA) processes. HAERA was the most and DA was the least exergonic. A deeper understanding of benzo(a)pyrene formation achieved.

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Impacts of the PAH size and the radiation intensity on the IR features of illuminated dust within the reflection nebulae

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Interstellar dust grains are illuminated in the reflection nebulae. Under conditions of the PAH size and the intensity of the interstellar radiation field, we follow their impact on the PAH aromatic infrared bands using the numerical DustEM code. For a dust model consisting of PAH, amorphous C and amorphous silicate, the PAH size varies in a range from 0.31 to 4.9 nm while the radiation intensity varies by a scale factor from 0.1 to 10^4 . Various trends of the results show the effect of varying both the PAH size and the radiation intensity on the strength of the aromatic mid-IR bands. Through small PAH sizes less than 0.7 nm, the grain temperature distribution of PAHs shows a small variation within 2–3 K at low radiation intensity while it increases to 15 and 8 K for PAH⁰ and PAH⁺, respectively, at higher radiation intensity. In final the variability in these results reveals the evolution of the dust grains under the physical space conditions of the reflection nebulae. In the mid-IR region, the contributions of PAH⁰ and PAH⁺ in the total SED intensity agree with the proportions of these PAHs observed in some reflection nebulae having higher radiation intensities.

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Advances in Space Research, Volume 67, 4222–4237 (2021)

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Gas-phase synthesis of benzene via the propargyl radical self-reaction

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Polycyclic aromatic hydrocarbons (PAHs) have been invoked in fundamental molecular mass growth processes in our galaxy. We provide compelling evidence of the formation of the very first ringed aromatic and building block of PAHs – benzene – via the self-recombination of two resonantly stabilized propargyl (C₃H₃) radicals in dilute environments using isomer-selective synchrotron-based mass spectrometry coupled to theoretical calculations. Along with benzene, three other structural isomers (1,5-hexadiyne, fulvene, and 2-ethynyl-1,3-butadiene) and o-benzyne are detected, and their branching ratios are quantified experimentally and verified with the aid of computational fluid dynamics and kinetic simulations. These results uncover molecular growth pathways not only in interstellar, circumstellar, and solar systems environments but also in combustion systems, which help us gain a better understanding of the hydrocarbon chemistry of our universe.

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Science Advances, Volume 7, no. 21, eabf0360 (2021)

<https://advances.sciencemag.org/content/7/21/eabf0360.abstract>

Hydrogenation of small aromatic heterocycles at low temperatures

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The recent wave of detections of interstellar aromatic molecules has sparked interest in the chemical behavior of aromatic molecules under astrophysical conditions. In most cases, these detections have been made through chemically related molecules, called proxies, that implicitly indicate the presence of a parent molecule. In this study, we present the results of the theoretical evaluation of the hydrogenation reactions of different aromatic molecules (benzene, pyridine, pyrrole, furan, thiophene, silabenzene, and phosphorine). The viability of these reactions allows us to evaluate the resilience of these molecules to the most important reducing agent in the interstellar medium, the hydrogen atom (H). All significant reactions are exothermic and most of them present activation barriers, which are, in several cases, overcome by quantum tunneling. Instanton reaction rate constants are provided between 50 K and 500 K. For the most efficiently formed radicals, a second hydrogenation step has been studied. We propose that hydrogenated derivatives of furan, pyrrole, and specially 2,3-dihydropyrrole, 2,5-dihydropyrrole, 2,3-dihydrofuran, and 2,5-dihydrofuran are promising candidates for future interstellar detections.

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<https://arxiv.org/abs/2105.11175>

Tracing PAH Size in Prominent Nearby Mid-Infrared Environments.

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We present observations from the First Light Infrared TEST CAMERA (FLITECAM) on-board the Stratospheric Observatory for Infrared Astronomy (SOFIA), the Spitzer Infrared Array Camera (IRAC) and the Spitzer Infrared Spectrograph (IRS) SH mode in three well-known Photodissociation Regions (PDRs), the reflection nebulae (RNe) NGC 7023 and NGC 2023 and to the southeast of the Orion Bar, which are well suited to probe emission from Polycyclic Aromatic Hydrocarbon molecules (PAHs). We investigate the spatial behaviour of the FLITECAM 3.3 μm filter as a proxy for the 3.3 μm PAH band, the integrated 11.2 μm PAH band, and the IRAC 8.0 μm filter as a proxy for the sum of the 7.7 and 8.6 μm PAH bands. The resulting ratios of 11.2/3.3 and IRAC 8.0/11.2 provide an approximate measure of the average PAH size and PAH ionization respectively. In both RNe, we find that the relative PAH ionization and the average PAH size increases with decreasing distance to the illuminating source. The average PAH sizes derived for NGC 2023 are greater than those found for NGC 7023 at all points. Both results indicate that PAH size is dependent on the radiation field intensity. These results provide additional evidence of a rich carbon-based chemistry driven by the photo-chemical evolution of the omnipresent PAH molecules within the interstellar medium. In contrast, we did not detect a significant variation in the average PAH size found in the region southeast of the Orion Bar and report a peculiar PAH ionization radial profile.

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Non Long-Range Corrected Density Functionals incorrectly describe the intensity of the C-H stretching band in Polycyclic Aromatic Hydrocarbons

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We present a comprehensive study of the most relevant numerical aspects influencing frequencies and intensities in the infrared spectrum of isolated Polycyclic Aromatic Hydrocarbons (PAHs) regarding the overestimate of the IR CH-stretching bands. We use naphthalene as benchmark and show the validity of our results to different members of the PAH family. Our analysis relies on widely employed Density Functional Theory methods and Second Order Vibrational Perturbational Theory for the computation of vibrational eigenstates. We have focused on the elucidation of the origin of the systematic overestimate of the intensities in the CH-stretching region. To rule out non-fundamental numerical errors, we have initially considered the influence of the electronic basis set and various other parameters on the different stages of the vibrational analysis. In a second stage, we have benchmarked the results of different Density Functional Theory functionals with respect to the aforementioned overestimate taken as the ratio between the most prominent features of the spectrum, the CH-bending and the CH-stretching bands. Our results unambiguously indicate that the long-range correction plays a major role in this spurious numerical issue. More specifically, this phenomenon is due to an incorrect description of the charge distribution (and hence dipole) within the symmetrically relevant C–H bonds. Long-Range correction specifically remedies this issue. It improves the description of the intensities in the stretching region while at the same time it does not perturb significantly the rest of the spectrum. With respect to the frequencies, we have observed an overall improvement when compared to non-corrected functionals.

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Physics and Chemistry on the Surface of Cosmic Dust Grains: A Laboratory View

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Dust grains play a central role in the physics and chemistry of cosmic environments. They influence the optical and thermal properties of the medium due to their interaction with stellar radiation; provide surfaces for the chemical reactions that are responsible for the synthesis of a significant fraction of key astronomical molecules; and they are building blocks of pebbles, comets, asteroids, planetesimals, and planets. In this paper, we review experimental studies of physical and chemical processes, such as adsorption, desorption, diffusion, and reactions forming molecules, on the surface of reliable cosmic dust grain analogues as related to processes in diffuse, translucent, and dense interstellar clouds, protostellar envelopes, planet-forming disks, and planetary atmospheres. The information that such experiments reveal should be flexible enough to be used in many different environments. In addition, we provide a forward look discussing new ideas, experimental approaches, and research directions.

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A radiolytic origin of organic matter in primitive chondrites and trans-neptunian objects? New clues from ion irradiation experiments

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We question here the radiolytic origin of (i) polyaromatic insoluble organic matter (IOM) recovered from primitive chondrites, and (ii) organics at the surface of reddish Trans-Neptunian Objects (TNOs), some minor planets and icy satellites. Organic synthesis by ion irradiation was investigated through experiments on a variety of targets: Polyethylene glycol 1450, lignin, cellulose and sucrose, exposed to low (C 40 keV and Ne 170 keV) and high energy (C 12 MeV, Ni 17 MeV, ^{78}Kr 59_{-2}^{+10} MeV) ions. These experiments show that all carbonaceous precursors evolve towards a sp-rich amorphous carbon (a-C) above a critical nuclear dose of 10_{-7}^{+10} eV·atom⁻¹. A thorough review of the literature shows that this value applies for a large range of carbonaceous materials, including C-rich simple ices. Below this critical dose, irradiated targets are carbonized and transformed into cross-linked polymeric disordered solids, with abundant olefinic and acetylenic bonds, but devoid of aromatic or polyaromatic species. Ion irradiation of simple compounds, e.g. ices, is thereby not a viable process to synthesize IOM. However, in the case of aromatic-rich precursors, swift heavy ions irradiation leads to polyaromatic materials, by bridging existing aromatic or polyaromatic units. In the context of Early Solar System, i.e. Galactic Cosmic Rays (GCR) irradiation during 10–20 Myr, the formation of chondritic IOM from simple ices mixed with interstellar Polycyclic Aromatic Hydrocarbons (PAHs) appears as a plausible mechanism. This scenario, based on the recycling of existing carbonaceous interstellar grains under low-temperature conditions, would account for the heterogeneity of the D, ¹⁵N and ¹³C isotopic fractionations at the molecular scale, and the preservation of deuterium hot spots that are highly sensitive to high-temperature conditions (> 300 °C). At the surface of TNOs, sp²-rich amorphous carbons are formed by the implantation of GCRs and Solar wind ions. The electronic dose is also very high for an irradiation time of several Gyr (> 100 eV·atom⁻¹, leading to the formation of reddish disordered solids, provided that the surface contains a minimum abundance of carbonaceous species. Finally, sp²-rich amorphous carbons produced in the laboratory (e.g. the ACAR compound from Zubko et al., 1996) are fair analogues of the darkening agent produced by radiolysis.

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The properties of Polycyclic Aromatic Hydrocarbons in galaxies: constraints on PAH sizes, charge and radiation fields

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Based on theoretical spectra computed using Density Functional Theory we study the properties of Polycyclic Aromatic Hydrocarbons (PAH). In particular using bin-average spectra of PAH molecules with varying number of carbons we investigate how the intensity of the mid-infrared emission bands, 3.3, 6.2, 7.7 and 11.3 μm , respond to changes in the number of carbons, charge of the molecule, and the hardness of the radiation field that impinges the molecule. We confirm that the 6.2/7.7 band ratio is a good predictor for the size of the PAH molecule (based on the number of carbons present). We also investigate the efficacy of the 11.3/3.3 ratio to trace the size of PAH molecules and note the dependence of this ratio on the hardness of the radiation field. While the ratio can potentially also be used to trace PAH molecular size, a better understanding of the impact of the underlying radiation field on the 3.3 μm feature and the effect of the extinction on the ratio should be evaluated.

The newly developed diagnostics are compared to band ratios measured in a variety of galaxies observed with the Infrared Spectrograph on board the Spitzer Space Telescope. We demonstrate that the band ratios can be used to probe the conditions of the interstellar medium in galaxies and differentiate between environments encountered in normal star forming galaxies and Active Galactic Nuclei. Our work highlights the immense potential that PAH observations with the James Webb Space Telescope will have on our understanding of the PAH emission itself and of the physical conditions in galaxies near and far.

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Pyrene adsorption on a Ag(111) surface

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This work describes the adsorption of pyrene molecules on a Ag(111) surface. We first demonstrate that despite its high vapor pressure, pyrene molecules can form ordered films under ultrahigh vacuum conditions, presenting a well-contrasted diffraction pattern. Studies using high-resolution electron energy loss spectroscopy and ultraviolet photoelectron spectroscopy provide compelling evidence of a physisorbed system where the molecules only weakly interact with the substrate underneath. Comparisons with theoretical calculations, as well as with data obtained from optical spectroscopies, clearly demonstrate that the vibrational and electronic properties of the adsorbed molecules are similar to the expected ones for pristine pyrene. Finally, we used temperature-programmed X-rays photoelectron spectroscopy to study the desorption process of pyrene on the Ag(111) surface and estimate its activation energy to desorption.

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Molecular dynamics approach for predicting release temperatures of noble gases in pre-solar nanodiamonds

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Pre-solar meteoritic nanodiamond grains carry an array of isotopically distinct noble gas components and provide information on the history of nucleosynthesis, galactic mixing and the formation of the Solar system. In this paper, we develop a molecular dynamics approach to predict thermal release pattern of implanted noble gases (He and Xe) in nanodiamonds. We provide atomistic details of the unimodal temperature release distribution for He and a bimodal behavior for Xe. Intriguingly, our model shows that the thermal release process of noble gases is highly sensitive to the impact and annealing parameters as well as to position of the implanted ion in crystal lattice and morphology of the nanograin. In addition, the model elegantly explains the unimodal and bimodal patterns of noble gas release via the interstitial and substitutional types of defects formed. In summary, our simulations confirm that low-energy ion-implantation is a viable way for the incorporation of noble gases into nanodiamonds and we provide explanation of experimentally observed peculiarities of gas release.

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Electronic excited states of benzene in interaction with water clusters: influence of structure and size

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This work is dedicated to the theoretical investigation of the influence of water clusters' organisation and size on the electronic spectrum of an interacting benzene (Bz) molecule using both TD-DFT and CASPT2 approaches. Two series of geometries, namely Geo_{IEI} and Geo_{IED} were extracted from two Bz-hexagonal ice configurations leading to maximum and minimum ionization energies respectively. An appropriate basis set containing atomic diffuse and polarisation orbitals and describing the Rydberg states of Bz was determined. The TD-DFT approach was carefully benchmarked against CASPT2 results for the smallest systems. Despite some discrepancies, the trends were found to be similar at both levels of theory: the positions and intensities of the main $\pi \rightarrow \pi^*$ transitions were found slightly split due to symmetry breaking. For the smallest systems, our results clearly show the dependence of the electronic transitions on the clusters' structures. Of particular interest, low energy transitions of non negligible oscillator strength from a Bz π orbital to a virtual orbital of Rydberg character, also involving atomic diffuse functions and partially expanded on the water cluster, were found for the Geo_{IED} series. The energies of such transitions were determined to be more than 2 eV below the ionization potential of Bz. When the cluster's size increases, similar transitions were found for all structures, the virtual orbitals becoming mainly developed on the H atoms of the water molecules at the edge of the cluster. Given their nature and energy, such transitions could play a role in the photochemistry of aromatic species in interaction with water clusters or ice, such processes being of astrophysical interest.

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Competitive Dehydrogenation and Backbone Fragmentation of Super-Hydrogenated PAHs: A Laboratory Study

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Super-hydrogenated Polycyclic Aromatic Hydrocarbons (PAHs) have been suggested to catalyze the formation of H₂ in certain regions of space, but it remains unclear under which circumstances this mechanism is viable given the reduced carbon backbone stability of super-hydrogenated PAHs. We report a laboratory study on the stability of the smallest pericondensed PAH, pyrene (C₁₆H_{10+N}, with N=4, 6, and 16 additional H atoms), against photodestruction by single vacuum ultraviolet photons using the Photo-Electron Photo-Ion Coincidence technique. For N=4, we observe a protective effect of hydrogenation against the loss of native hydrogens, in the form of an increase in the appearance energies of the C₁₆H₉⁺ and C₁₆H₈⁺ daughter ions compared to those reported for pristine pyrene (C₁₆H₁₀). No such effect is seen for N=6 or 16, where the weakening effect of replacing aromatic bonds with aliphatic ones outweighs the buffering effect of the additional hydrogen atoms. The onset of fragmentation occurs at similar internal energies for N=4 and 6, but is significantly lower for N=16. In all three cases, H-loss and C_mH_n-loss ($m \geq 1$, carbon backbone fragmentation) channels open at approximately the same energy. The branching fractions of the primary channels favor H-loss for N=4, C_mH_n-loss for N=16, and are roughly equal for the intermediate N=6. We conclude that super-hydrogenated pyrene is probably too small to support catalytic H₂-formation, while trends in the current and previously reported data suggest that larger PAHs may serve as catalysts up to a certain level of hydrogenation.

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Direct evidence for a single-step radiation-induced assembling of benzene ring from acetylene trimer at cryogenic temperatures

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The discovery of carbon-rich species, including polycyclic aromatic hydrocarbons (PAH) and fullerenes, in the space environment is among the most intriguing findings in molecular astrophysics and astrochemistry of the recent decades. The mechanism of their formation remains unclear and the one of the key issues is related to making “first ring”, i.e., formation of benzene from simple small molecules abundant in the outer space. Different routes involving C₂, C₃ and C₄ hydrocarbons are considered in literature. Here we report the first direct evidence for a single-step radiation-induced formation of benzene from pre-existing isolated acetylene trimer occurring in frozen inert environment at very low temperature (6 K). The finding is based on the correlation between trimer decay and build-up of benzene as monitored by FTIR spectroscopy. This concerted pathway may be applicable to acetylene aggregates trapped in the bulky ices or in the grain pores and it emphasizes the importance of concept of molecular organization in the chemical history of the Universe.

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