

# AstroPAH

A Newsletter on Astronomical PAHs

Issue 76 • March 2021

**Catalysis of COMs on  
interstellar dust grains**



# Editorial

## Dear Colleagues,

Welcome to our 76<sup>th</sup> AstroPAH volume! We hope all of you are healthy and doing well.

The Picture of the Month is a depiction of complex organic molecules formation on interstellar dust grains. This is a topic which you can read more about in our In Focus!

Our In Focus this month, presented by Dr. Liv Hornekær, covers the Center for Interstellar Catalysis, a recent initiative by the Danish National Research Foundation aiming to investigate the role of dust grain surfaces as catalysts in the formation of complex organic molecules in the universe.

As always, we have many new tantalizing abstracts to share with you this month. Thanks to everyone for your contributions! We are also happy to announce the recent release of two new PhD theses, by Dr. Carla Martinez Canelo and Dr. Sandra Wiersma, on the cosmic distribution of aromatics and the spectroscopy of gas phase PAHs, respectively. Congratulations to both! A book titled *Molecular Astrophysics* written by our Editor-in-Chief Prof. Alexander Tielens has been published by Cambridge University Press, and is presented in the Announcements section.

We would also like to draw your attention to two job opportunities in the Announcement section: an associate professor or tenure-track assistant professor position in experimental surface science and/or laboratory astrochemistry at Aarhus University, Denmark; and a PhD Position in Energetic ion processing of polycyclic aromatic hydrocarbons in the solid phase at the Normandie University and Centre de recherche sur les ions, les matériaux et la photonique (CIMAP) in Caen, France.

Our [new Instagram page](#) is live! Check it out!

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, feel free to use our [email](#).

Enjoy reading our newsletter!

**The Editorial Team**

**Next issue: 22 April 2021.  
Submission deadline: 9 April 2021.**

# AstroPAH Newsletter

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## PAH Picture of the Month

Depiction of complex organic molecules (COMs) catalysis on interstellar dust grains. The figure also illustrates the aim of the Center for Interstellar Catalysis (InterCat): discover the origin of the molecular building blocks of life in space. More information about InterCat can be found in the In Focus.

**Credits:** Background image of the Eagle Nebula by T.A. Rector (NRAO/AUI/NSF and NOIRLab/NSF/AURA) and B.A. Wolpa (NOIRLab/NSF/AURA). Composition by the Center for Interstellar Catalysis.



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# In Focus

## InterCat Center for Interstellar Catalysis

by Liv Hornekær  
InterCat Center Leader, Aarhus University

The Center for Interstellar Catalysis - InterCat - is a 10M€ center of excellence funded by the Danish National Research Foundation. The Center kicked off in July 2020 and is presently funded until the end of 2026. The center has nodes at Aarhus University, Denmark (Liv Hornekær and Bjørk Hammer) and at Leiden University, Netherlands (Ewine van Dishoeck and Harold Linnartz) – and welcomes collaborators (see <http://intercat.au.dk>). The center aims to investigate whether interstellar dust grain surfaces and nanograins play a role as catalysts in the formation of complex, biologically relevant, organic molecules in the interstellar medium and circumstellar disks – with specific focus on the formation of the molecular building blocks of life – amino acids, DNA bases, sugars and Fatty Acids.

### Symposium on “The Life Cycle of Cosmic PAHs”

InterCat is a co-sponsor of the Symposium on “The Life Cycle of Cosmic PAHs” to be held at Aarhus University, 20th - 24th of June 2022.  
(See: <https://conferences.au.dk/cosmicpah2022/>)

Researchers under InterCat combine state-of-the-art surface science techniques with laboratory astrochemistry setups and new machine learning methods to follow catalytic reactions at low temperatures and pressures on interstellar, dust grain analogue surfaces and nanoparticles. While much attention presently focuses on reactions in solid state ices, InterCat aims to also investigate the catalytic effect of silicate and carbonaceous nanograins, both as bare grains and as substrates for ice clusters and icy layers. Hence, we will follow the changes to catalytic activity as we go from bare carbonaceous and silicate surfaces, with nanostructures, defects and single adatom impurities acting as catalysts, all the way up to thick solid ices. We will investigate how ice clusters (water, CO, methanol) nucleate and grow on silicate and carbonaceous, dust grain analogue surfaces; and consider how these structures impact catalytic activity and how this changes as we transition to few-layer ices and thick icy layers. The catalytic and photocatalytic effects of nanograins embedded in solid ices will also be studied. The experimental and theoretical efforts will be guided by and will guide observations from *ALMA* and - in the coming years - *JWST*.

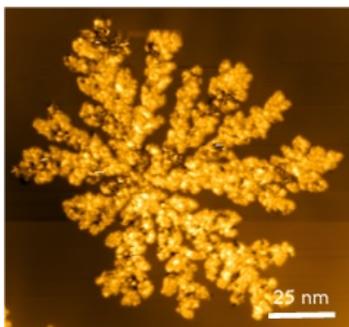


Figure 1: STM image of an Ice cluster on a graphite surface. InterCat Post Doctoral researcher Frederik Doktor Simonsen investigates low-temperature, water-ice clusters on a graphite surface. Scanning Tunneling Microscopy (STM) images obtained at cryogenic temperatures, using liquid helium cooling, show fractal-like structures that indicate a diffusion-limited growth process. These studies were conducted in collaboration with Karina Morgenstern, Ruhr-University Bochum.

## INTERCAT WEBINARS

We invite you to attend the InterCat webinars. These webinars take place on the first Tuesday of each month at 11 am CET. Topics include astrochemistry and surface science. You can see a list of upcoming webinars, and sign up for information and zoom links to future webinars at: <http://intercat.au.dk>.

Several of the past webinars are available as video recordings. Upcoming webinars include talks by Jose Angel Martin Gago, on results from the Nanocosmos Stardust Machine (6th April 2021) and by Stefan Bromley, on Nanoscale Silicate Stardust: Astrochemical Relevance and Observational Signatures (4th May 2021).

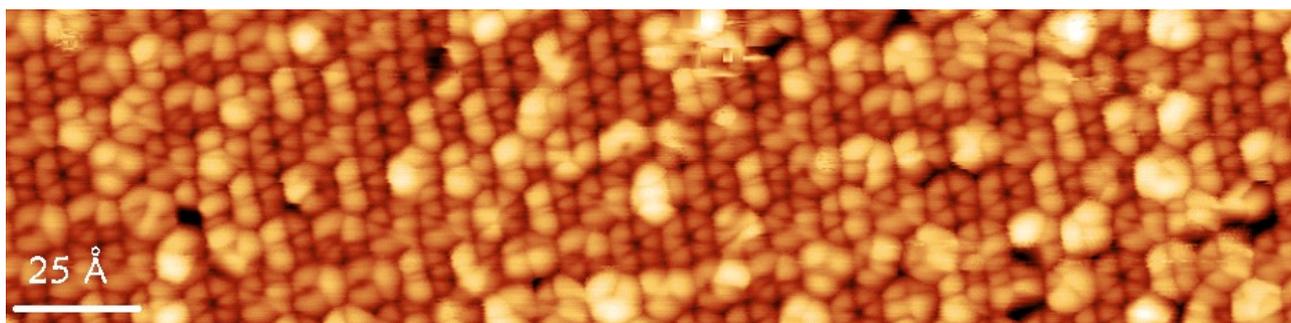


Figure 2: Hydrogen-functionalized coronene molecules on graphite. InterCat Post Doctoral researcher Rijutha Jaganathan investigates whether PAHs are a precursor to the formation of more complex, biologically relevant molecules. She exposes PAH molecules to atomic beams and follows the reaction products using Temperature Programmed Desorption (TPD), X-ray Photoemission Spectroscopy (XPS) and STM. The image shows an STM measurement of hydrogen-functionalized coronene molecules on a graphite surface. Unfunctionalized coronene molecules appear as 6 reddish lobes, while functionalized PAHs show irregular bright features that reflect the change in molecular orbitals imposed by the addition of hydrogen atoms. TPD measurements show break-up of functionalized PAHs, resulting in the formation of a range of smaller, hydrocarbons. The STM image was recorded by Jakob Jørgensen, Frederik Doktor Simonsen and Richard Balog.

## Unique instrumentation

InterCat hosts unique instrumentation. At Aarhus University, InterCat boasts several Scanning Probe Microscopy (SPM) setups, including helium cryogenic (5 K) STM and Atomic Force Microscope (AFM) setups, equipped with a full suite of surface science instrumentation including lab-source XPS and instrumentation for TPD measurements. The SPM setups are equipped with atomic and molecular beam sources, and evaporators that

allow for in-situ synthesis of carbonaceous, silicate and oxide surfaces and nano-particles, as well as atomic and molecular deposition of reaction partners (H, O, N, C), single atom catalysts (Fe, Al, Mg) and ice-cluster components on the surfaces. InterCat researchers also utilize the ASTRID2 Synchrotron Source, which is placed in the basement below the Dept. of Physics and Astronomy at Aarhus University.

### New surface/solid state UV beamline at the ASTRID2 Synchrotron Source in Aarhus

Under InterCat, a new endstation will be set up on one of the UV beamlines on ASTRID2 with the aim of **studying low temperature reactions of interstellar relevance on surfaces and in ices. The end station will be open to external users via beam time applications.** We are presently in the early design phase and invite input from interested parties and potential future users. **Please send an email to [InterCat@phys.au.dk](mailto:InterCat@phys.au.dk) to express your interest.**

At Leiden University, InterCat researchers will use three different UHV setups. CRYOPAD2 — CRYOgenic Photoproducts Analysis Device — is a new, state-of-the-art, low-temperature (10 K), UHV setup, designed to study photo-induced ice processes upon VUV irradiation, simulating the interstellar radiation field. It is equipped with a microwave-discharge, hydrogen flow lamp and a gas mixing system that allows for ice layer growth with monolayer precision. The photo-processed ices are studied in situ using Fourier transform reflection absorption/transmission IR spectroscopy (FT-RAIRS) and by TPD. MATRI2CES — Mass Analytical Tool for Reactions in Interstellar ICES — is similar to CRYOPAD2, but with different diagnostics based on laser-ablation, time-of-flight mass spectrometry. As a result, the molecular complexity in the ice can be lifted beyond what is possible with CRYOPAD2. However, unlike traditional ex-situ experiments, much lower radiation doses can be used and ice components are studied in situ avoiding thermal heating or air exposure of the UV irradiated ice sample. CRYOPAD2 and MATRI2CES allow for the study of UV-induced ice chemistry, typical of the processes in translucent clouds and proto-planetary disks. SURFRESIDE3 — SURFace Reactions Simulation Device — simulates the conditions in dense and cold dark clouds. It incorporates three independent atomic beam lines that allow for the study of chemical processes triggered by H, D, O, N, and C-atoms on interstellar ice analogues. FT-RAIRS and TPD are available to characterize solid state pathways towards molecular complexity.

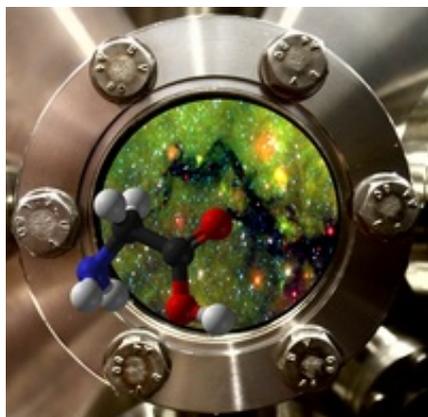


Figure 3: Glycine in Space produced by Dark Chemistry. An international team of laboratory astrophysicists, in part active within INTERCAT used SURFRESIDE 3 to show that glycine, the simplest amino acid and an important building block of life, can form under the harsh conditions that govern chemistry in space. The results have been published in *Nature Astronomy* (S. Ioppolo et al., *Nature Astronomy* 5, pp. 197–205, 2021) and show that glycine and very likely other amino acids are formed in dense interstellar clouds, well before these transform into new stars and planets.

## Astrochemical observations

InterCat researchers are involved in ALMA programs probing molecular complexity in the interstellar medium and in upcoming observing programmes on JWST — including the Ice Age Early Release Science program, searching for molecular complexity in ices in space. Theory activities under InterCat: InterCat researchers employ density functional theory (DFT), machine learning (e.g. evolutionary algorithms and compressed sensing), molecular dynamics and kinetic Monte Carlo simulations to identify molecular and surface structures, catalytic sites and reaction pathways, and molecular break-up under UV-, thermal- or chemical-processing. Methods are also developed to perform automated vibrational spectra calculations for identified products and intermediates, and compare them to observational spectra.

### Open Theory PhD position

InterCat presently has an open PhD position in Theoretical Surface Catalysis with focus on density functional theory, machine learning and compressed sensing approaches to unravel interstellar catalytic reaction pathways on interstellar dust grain analogue surfaces. See <http://intercat.au.dk> for more information.

If you are interested in collaborating with InterCat then browse the InterCat website: <http://intercat.au.dk> and send an email to [InterCat@phys.au.dk](mailto:InterCat@phys.au.dk).



**Liv Hornekær** is the InterCat Center leader and professor in the department of physics and astronomy at the University of Aarhus, Denmark. She is also head of the Surface Dynamics Group at the Interdisciplinary Nanoscience Center.

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# Abstracts

## Electronically Excited States of Closed-Shell, Cyano-Functionalized Polycyclic Aromatic Hydrocarbons Anions

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Few anions exhibit electronically excited states, and, if they do, the one or two possible excitations typically transpire beyond the visible spectrum into the near-infrared. These few, red-shifted electronic absorption features make anions tantalizing candidates as carriers of the diffuse interstellar bands (DIBs), a series of mostly unknown, astronomically ubiquitous absorption features documented for over a century. The recent interstellar detection of benzonitrile implies that cyano-functionalized polycyclic aromatic hydrocarbon (PAH) anions may be present in space. The presently reported quantum chemical work explores the electronic properties of deprotonated benzene, naphthalene, and anthracene anions functionalized with a single cyano group. Both the absorption and emission properties of the electronically excited states are explored. The findings show that the larger anions absorption and emission energies possess both valence and dipole bound excitations in the 450–900 nm range with oscillator strengths for both types of  $>1 \times 10^{-4}$ . The valence and dipole bound excited state transitions will produce slightly altered substructure from one another making them appear to originate with different molecules. The known interstellar presence of related molecules, the two differing natures of the excited states for each, and the wavelength range of peaks for these cyano-functionalized PAH anions are coincident with DIB properties. Finally, the methods utilized appear to be able to predict the presence of dipole-bound excited states to within a 1.0 meV window relative to the electron binding energy.

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Chemistry, 3, 296-313 (2021)

<https://www.mdpi.com/2624-8549/3/1/22>

# Assessment of the Presence of PAHs and Hydrogenated PAHs in the Young Stellar Object Mon R2 and the Taurus Cloud Toward Elias 16

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This study assesses the contribution of neutral polycyclic aromatic hydrocarbons (PAHs) and hydrogenated PAHs ( $H_n$ -PAHs) in  $H_2O$ -ices to the 3  $\mu\text{m}$  and 5–8  $\mu\text{m}$  regions of the infrared absorption spectrum of the Young Stellar Object, Mon R2 IRS 3, and the Taurus dense cloud in the direction of Elias 16. We compare the astronomical spectra to the previously published laboratory data of matrix-isolated PAHs and  $H_n$ -PAHs in  $H_2O$ -ices. For the molecules in this study, the band positions, FWHMs, and integrated band strengths have been measured. For the PAHs considered here, the ratio of the experimental A(C–H) stretch (in  $H_2O$  ices) to the theoretical A(C–H) stretch (in the gas phase) is consistently about 0.10, meaning that the trove of theoretical data can be reliably scaled to compare to the astronomical spectra. We find that the fractional percentage contribution to the 5–8  $\mu\text{m}$  region for Mon R2 IRS 3 ranges between 2.7 and 3.9 for neutral PAHs and 0.25–1.2 for  $H_n$ -PAHs. The best match to the observed 3.25  $\mu\text{m}$  profile in the Mon R2 IRS 3 spectrum is accomplished with the laboratory-measured coronene: $H_2O$  spectrum. Using this spectrum we estimate that neutral PAHs contribute up to 12.0% of the cosmic carbon budget for Mon R2 IRS 3 and <14.5% for Elias 16. Neutral hydrogenated PAHs contribute mainly to the 3.47  $\mu\text{m}$  absorption and very little to the 5 to 8  $\mu\text{m}$  region. For neutral  $H_n$ -PAHs, we estimate that they contribute up to 0.6% of the cosmic carbon budget for Mon R2 IRS 3 and <1% for Elias 16.

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# Five Birds with One Stone: Photoelectron Photoion Coincidence Unveils Rich Phthalide Pyrolysis Chemistry

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Phthalide pyrolysis has been assumed to be a clean fulvenallene source. We show that this is only true at low temperatures, and the C<sub>7</sub>H<sub>6</sub> isomers 1-, 2- and 5-ethynylcyclopentadiene are also formed at high pyrolysis temperatures. Photoion mass-selected threshold photoelectron spectra are analyzed with the help of (time-dependent) density functional theory, (TD-)DFT, and equation-of-motion ionization potential coupled cluster, EOM-IP-CCSD, calculations to assign ionization energies with the help of Franck–Condon simulations of partly overlapping bands. The fulvenallene ionization energy is confirmed at 8.23±0.01 eV, and the ionization energies of 1-, 2 and 5-ethynylcyclopentadiene are newly determined at 8.27±0.01, 8.49±0.01 and 8.76±0.02 eV, respectively. Excited state features in the photoelectron spectrum, in particular the  $\tilde{A}^+ 2A'$  band of 1-ethynylcyclopentadiene, are shown to be practical to isomer-selectively detect species when the ground-state band is congested. At high pyrolysis temperatures, the C<sub>7</sub>H<sub>6</sub> isomers may lose a hydrogen atom and yield the fulvenallenyl radical. Its ionization energy is confirmed at 8.20±0.01 eV. The vibrational fingerprint of the first triplet fulvenallenyl cation state is also revealed and yields an ionization energy of 8.33±0.02 eV. Further triplet cation states are identified and modeled in the 10–11 eV range. A reaction mechanism is proposed based on potential energy surface calculations. Based on a simplified reactor model, we show that the C<sub>7</sub>H<sub>6</sub> isomer distribution is far from thermal equilibrium in the reactor, presumably because irreversible H loss competes efficiently with isomerization.

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<https://pubs.acs.org/doi/full/10.1021/acs.jpca.1c00149>

# Observing Carbon and Oxygen Carriers in Protoplanetary Disks at Mid-infrared Wavelengths

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Infrared observations probe the warm gas in the inner regions of planet-forming disks around young sun-like, T Tauri stars. In these systems, H<sub>2</sub>O, OH, CO, CO<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>, and HCN have been widely observed. However, the potentially abundant carbon carrier CH<sub>4</sub> remains largely unconstrained. The James Webb Space Telescope (JWST) will be able to characterize mid-infrared fluxes of CH<sub>4</sub> along with several other carriers of carbon and oxygen. In anticipation of the JWST mission, we model the physical and chemical structure of a T Tauri disk to predict the abundances and mid-infrared fluxes of observable molecules. A range of compositional scenarios are explored involving the destruction of refractory carbon materials and alterations to the total elemental (volatile and refractory) C/O ratio. Photon-driven chemistry in the inner disk surface layers largely destroys the initial carbon and oxygen carriers. This causes models with the same physical structure and C/O ratio to have similar steady state surface compositions, regardless of the initial chemical abundances. Initial disk compositions are better preserved in the shielded inner disk midplane. The degree of similarity between the surface and midplane compositions in the inner disk will depend on the characteristics of vertical mixing at these radii. Our modeled fluxes of observable molecules respond sensitively to changes in the disk gas temperature, inner radius, and the total elemental C/O ratio. As a result, mid-infrared observations of disks will be useful probes of these fundamental disk parameters, including the C/O ratio, which can be compared to values determined for planetary atmospheres.

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# The infrared spectrum of protonated C<sub>70</sub>

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With the detection of C<sub>60</sub>, C<sub>70</sub> and C<sub>60</sub><sup>+</sup> in the interstellar medium, fullerenes are currently the largest molecules identified in space. The relatively high proton affinities of C<sub>60</sub> and C<sub>70</sub> support the hypothesis that protonated fullerenes may also be abundant in the ISM. Here, we present the first experimental vibrational spectrum of C<sub>70</sub>H<sup>+</sup>, recorded in the gas phase. The attachment of a proton to C<sub>70</sub> causes a drastic symmetry lowering, which results in a rich vibrational spectrum. As compared to C<sub>60</sub>, where all C-atoms are equivalent due to the icosahedral symmetry, C<sub>70</sub> belongs to the D<sub>5h</sub> point group and has five non-equivalent C-atoms, which are available as protonation sites. Combined analysis of the experimental spectrum and spectra computed at the density functional theory level enables us to evaluate the protonation isomers being formed. We compare the IR spectra of C<sub>60</sub>H<sup>+</sup> and C<sub>70</sub>H<sup>+</sup> to IR emission spectra from planetary nebulae, which suggests that a mixture of these fullerene analogues could contribute to their IR emission.

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<https://iopscience.iop.org/article/10.3847/2041-8213/abe874>

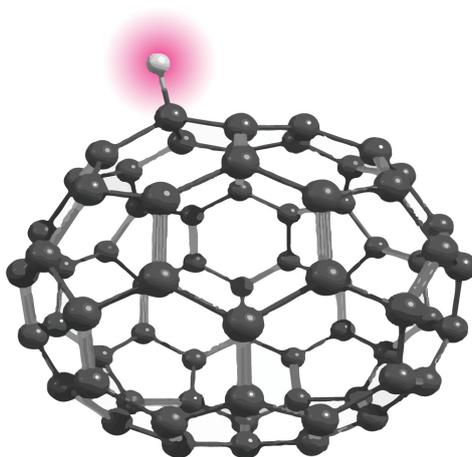


Figure 1: The IR spectrum of C<sub>70</sub>H<sup>+</sup> has been recorded for the first time and identifies the site of protonation on this fullerene.

# Infrared action spectroscopy of doubly charged PAHs and their contribution to the aromatic infrared bands

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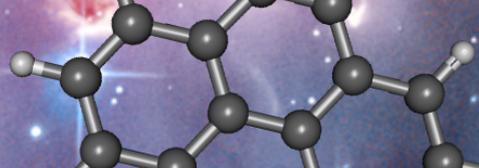
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The so-called aromatic infrared bands (AIBs) are attributed to emission of polycyclic aromatic hydrocarbons (PAHs). The observed variations towards different regions in space are believed to be caused by contributions of different classes of PAH molecules, i.e. with respect to their size, structure, and charge state. Laboratory spectra of members of these classes are needed to compare to observations and to benchmark quantum-chemically computed spectra of these species. In this paper we present the experimental infrared spectra of three different PAH dications, naphthalene<sup>2+</sup>, anthracene<sup>2+</sup> and phenanthrene<sup>2+</sup>, in the vibrational fingerprint region 500–1700 cm<sup>-1</sup>. The dications were produced by electron impact ionization of the vapors with 70 eV electrons, and remained stable against dissociation and Coulomb explosion. The vibrational spectra were obtained by infrared pre-dissociation of the PAH<sup>2+</sup> complexed with neon in a 22-pole cryogenic ion trap setup coupled to a free-electron infrared laser at the FELIX Laboratory. We performed anharmonic DFT calculations for both singly and doubly charged states of the three molecules. The experimental band positions showed excellent agreement with the calculated band positions of the singlet electronic ground state for all three doubly charged species, indicating its higher stability over the triplet state. The presence of several strong combination bands and additional weaker features in the recorded spectra, especially in the 10–15 μm region of the mid-IR spectrum, required anharmonic calculations to understand their effects on the total integrated intensity for the different charge states. These measurements, in tandem with theoretical calculations, will help in the identification of this specific class of doubly-charged PAHs as carriers of AIBs.

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<https://www.aanda.org/component/article?access=doi&doi=10.1051/0004-6361/202039744>



# Meetings

## Symposium

# The Life Cycle of Cosmic PAHs

**Aarhus University**

**20-24 June 2022**

<https://conferences.au.dk/cosmicpah2022/>

More information on the symposium website above. Communicated by Liv Hornekær.



# Announcements

## Job opening

### Associate professor or tenure-track assistant professor in experimental surface science and/or laboratory astrochemistry

The Department of Physics and Astronomy, Aarhus  
University, Denmark

Advertised by Ulrik I. Uggerhøj

The Department of Physics and Astronomy, Aarhus University, Denmark ([www.phys.au.dk](http://www.phys.au.dk)) invites applications for a permanent associate professor or tenure-track assistant professor position in experimental surface science and/or laboratory astrochemistry, complementing and strengthening existing activities. The position is open from 1 November 2021 or as soon as possible thereafter.

**Profile:** The candidate is expected to establish an independent research activity and to develop and strengthen experimental surface science and/or laboratory astrochemistry across the Department, possibly in collaboration with other departments and/or interdisciplinary materials science centers at Aarhus University, e.g. iNano and iMat. It is an advantage if applicants can strengthen the ongoing activities at the ASTRID2 synchrotron source and/or the astrochemical research activities under Center for Interstellar Catalysis. We are looking for applicants with a prior record of developing novel approaches and techniques in their respective fields, who have demonstrated the ability to conduct collaborative research. The successful candidate is expected to be a team player and to contribute to the development of the research fields within the Department.

Applicants must have a satisfactory record of original scientific research at a high international level and they are invited to document examples of collaborative research and external funding. Applicants must hold a PhD in physics or similar, and be able to teach physics at all levels of the University curriculum. The assessment of applicants (in particular for the associate professor level) will include an evaluation of their teaching statement, expressing clear thoughts connected to teaching strategies, and documenting experience and qualifications. Applicants should therefore provide a teaching portfolio, which documents their experience with all facets of university teaching, including the

supervision of MSc and PhD students, depending on the level of application. It should be clearly stated if the application targets the associate professor or the tenure-track assistant professor level.

**Contact:** Further information can be obtained from the Head of Department Ulrik I. Uggerhøj.

**E-mail for contact:** [ulrik@phys.au.dk](mailto:ulrik@phys.au.dk)

**Deadline for Application:** 1 July 2021.

# PhD Position in Energetic ion processing of polycyclic aromatic hydrocarbons in the solid phase

Normandie University and Centre de recherche sur les ions,  
les matériaux et la photonique (CIMAP, Caen, France)

Advertised by Alicja Domaracka

A PhD position in experimental physics is available at Normandie University and Centre de recherche sur les ions, les matériaux et la photonique (CIMAP, Caen, France) with a nominal starting date of September/October 2021, under the joint supervision of Drs. Alicja Domaracka and Philippe Boduch.

**Project description:** Polycyclic Aromatic Hydrocarbons (PAHs) are a ubiquitous component of organic matter in space. Their contributions invoked in a broad spectrum of astronomical observations that range from the ultra-violet to the far-infrared and cover a wide variety of objects and environments from interplanetary dust particles to outer Solar System bodies to the interstellar medium in the local Milky Way and in other galaxies. PAH molecules can represent up to 2% of the interstellar carbon mass, therefore, they have profound implications for the complex chemistry in space. It is important to understand how energetic processing affects the formation, survival, and destruction of PAHs. Another key question concerns the role of a surrounding environment (e.g. mixed PAH-water mantels) in these processes and formation of new species (e.g. complex organic molecules - like nucleobases). The goal of this project is to mimic energetic ion processing of PAH molecules (pure PAH and water-PAH mixed ices) due to interaction with cosmic rays/solar wind (fragmentation, sputtering and formation of new species). To perform experiments in keV-MeV ion energy range, we will use large ion facilities like GANIL (Caen, France), GSI (Darmstadt, Germany) and ATOMKI (Debrecen, Hungary).

**Requirements:** A M.Sc. degree or equivalent in Physics, Chemistry or related fields, with a background in experimental physics (e.g. vacuum techniques, FTIR, mass spectrometry, ...)

**Contact:** Interested candidates are encouraged to contact Dr. Alicja Domaracka as soon as practical for more information regarding the application process.

**E-mail for contact:** [domaracka@ganil.fr](mailto:domaracka@ganil.fr)

**Deadline for Application:** Jun 15, 2021.

# PHD THESIS

## Cosmic distribution of aromatics and other species of biotic interest

**Carla Martinez Canelo**

**Adviser:** Prof. Dr. Amâncio C. S. Friaça

**Institution:** Departamento de Astronomia, Instituto de Astronomia, Geofísica e Ciências Atmosféricas, Universidade de São Paulo, São Paulo, Brazil

This thesis presents an astrobiological and astrochemical study of the molecular complexity in the Universe, through distinct spectral regions. Polycyclic aromatic hydrocarbons (PAHs) and polycyclic aromatic nitrogen heterocycles (PANHs), which have the potential to form prebiotic molecules, were studied for a sample of 126 to 155 starburst-dominated galaxies, extracted from the Spitzer/IRS ATLAS project. These objects have their 6.2, 7.7 and 8.6  $\mu\text{m}$  mid-infrared (MIR) PAH bands fitted and separated into the Peeters' A, B and C classes. For the first time in literature, a study of PAHs and Peeters classes is performed with robust statistics for a large number of galaxies. The blueshift of the 6.2  $\mu\text{m}$  band, typical for a class A object, was attributed to PANH molecules and seems to dominate this spectral feature. Analyses of these bands also indicate that the distribution of the PAH profile variations along the redshift of the galaxies could suggest a possible PAH evolutionary timescale. In addition, precursors of PAHs and PANHs such as HNCO,  $\text{HC}_3\text{N}$  and  $\text{NH}_2\text{CHO}$ , can be observed at radio wavelengths. Spectral line surveys revealed rich molecular reservoirs in G331.512–0.103, a compact radio source in the center of an energetic molecular outflow. The observations were carried out with the APEX antenna in the interval frequency of 160–355 GHz. In particular, 42 transitions of HNCO were detected with an excitation temperature about 60 K. The abundance and chemical evolution of HNCO were modeled with the astrochemical code NAUTILUS, which simulates grain and gas phase reactions in molecular cores. Finally, the code was also used to simulate the abundances of  $^{13}\text{CS}$ , OCS,  $\text{CH}_3\text{CHO}$  and  $\text{CH}_3\text{OCHO}$  in the infrared cold core called as IRDC-C9 Main.

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Download: <https://www.teses.usp.br/teses/disponiveis/14/14131/tde-03022021-131439/>

# PHD THESIS

## The hidden life of cosmic carbon: Infrared fingerprint spectroscopy and fragmentation chemistry of gas-phase polycyclic aromatic hydrocarbons

Sandra D. Wiersma<sup>1,2</sup>

**Promotor:** Wybren Jan Buma<sup>1,2</sup>

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This thesis aims to improve our understanding of how polycyclic aromatic hydrocarbons (PAHs) in astronomical environments interact react to harsh photonic conditions, and how these excited molecules express signatures of their shapes and sizes in their (far-)infrared spectra. Using both mass spectrometry and infrared spectroscopy at the Free Electron Laser for Infrared eXperiments (FELIX) in Nijmegen, we are able to measure the infrared signatures and dissociation characteristics of different types of PAHs, resulting in various astronomically relevant conclusions. In Chapter 4, we showed that that PAHs show a much stronger than expected tendency to retain deuterium than hydrogen under the influence of both UV and IR light, which has important implications for the isotopic balance interstellar environments. In Chapter 5, we showed that phenylium, an important precursor molecule for PAHs, dominantly exists in singlet ground state, and that from there, it is subjected to a facile ring-opening mechanism. In Chapter 6, we presented the first far-infrared spectra of three, small PAHs, providing essential benchmarking opportunities for spectra which were only theoretically available. Trends extrapolated from these far-infrared bands can be used for guided searches for molecule-specific PAH signatures in both the interstellar medium and extraterrestrial atmospheres. Finally, in Chapter 7, we present the IR spectrum and fragmentation of a highly asymmetric, non-planar PAH. We believe that it is likely that similar molecules play a role in the formation of molecular hydrogen in an astronomical context, but that finding specific signatures of irregular species requires a wider experimental survey.

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# BOOK

## Molecular Astrophysics

Alexander G. G. M. Tielens

Cambridge University Press

Focusing on the organic inventory of regions of star and planet formation in the interstellar medium of galaxies, this comprehensive overview of the molecular universe is an invaluable reference source for advanced undergraduates through to entry-level researchers. It includes an extensive discussion of microscopic physical and chemical processes in the universe; these play a role in the excitation, spectral characteristics, formation, and evolution of molecules in the gas phase and on grain surfaces. In addition, the latest developments in this area of molecular astrophysics provide a firm foundation for an in-depth understanding of the molecular phases of the interstellar medium. The physical and chemical properties of gaseous molecules, mixed molecular ices, and large polycyclic aromatic hydrocarbon molecules and fullerenes and their role in the interstellar medium are highlighted. For those with an interest in the molecular universe, this advanced textbook bridges the gap between molecular physics, astronomy, and physical chemistry.

<https://doi.org/10.1017/9781316718490>

### AstroPAH Newsletter

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

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