

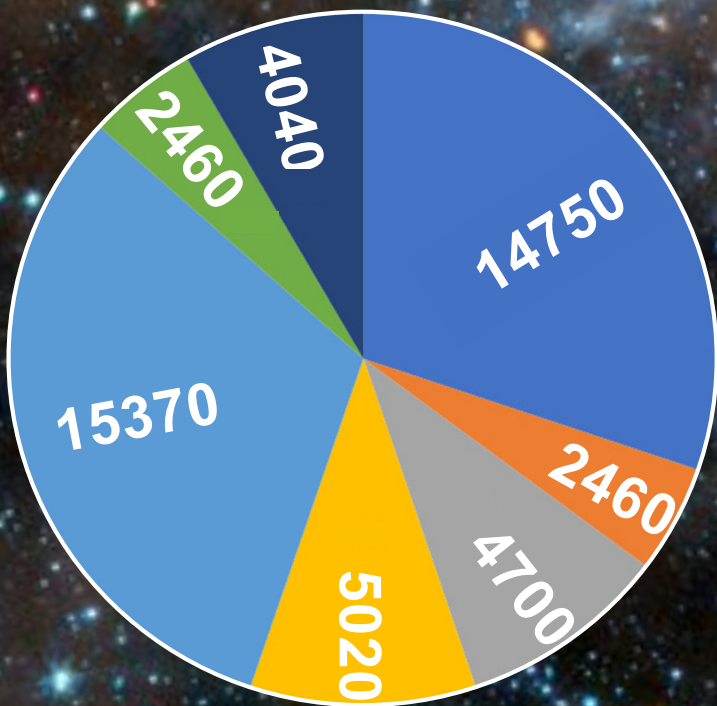
AstropAH

A Newsletter on Astronomical PAHs

Issue 103 • November 2023

Cycle 3 hours

- ExoPlanets
- Solar System
- Stellar Physics and Stellar Types
- Stellar Populations and the ISM
- Galaxies and IGM
- Large Scale Structure
- Super Massive Black Holes and Active Galaxies



Setting a Record: 1931 Proposals Submitted for the JWST Cycle 3!



Editorial

Dear Colleagues,

Welcome to our 103rd AstroPAH volume! We hope all of you are healthy and doing well as we are approaching the end of the year! Once again, we are very grateful to all of you who have contributed to our newsletter.

Our Picture of the Month shows NGC 6822 as observed by the JWST MIRI instrument, with the bright blue colours indicating PAHs emission. The pie chart shows the distribution of the nearly 45,000 hours of observations proposed in Cycle 3!

In the In Focus section, Vincent Esposito from NASA Ames Research Center presents "Anharmonicity in the 1 – 5 μm Region of PAH IR Spectra". Vincent's research primarily focuses on computing anharmonic IR absorption and emission PAH spectra in support of JWST data analysis. The In Focus provides information on this effort and on the associated improvement of the NASA Ames PAH Infrared spectroscopic database PAHdb.

In the Abstract section, you can read about newly published papers on DFT calculations of biomolecules, photoionization of benzonitrile, anharmonic spectral computations, and the detection of ethynylbenzene in TMC-1.

The Meetings section draws your attention to a 4-month online course (Jan–Apr 2024), titled "Astrochemistry: From the Big Bang to Life" part of the Global Astrochemistry Lecture Series (GLAS), and a meeting on "Processing, reactivity and relaxation pathways of nC" hosted by the NanoSpace Working Group 2 in Edinburgh in February 2024.

In our Announcements section, Otto Dopfer is advertising a 5-year senior postdoctoral position opening in the laser molecular spectroscopy group at the Berlin Institute of Technology, Germany (application deadline: December 15, 2023) and Ugo Jacovella is advertising a postdoctoral position on the experimental study of ion mobility, mass spectrometry, and laser spectroscopy of large carbon-rich molecular gas phase ions in the context of astrochemistry and astrophysics (application deadline: December 5, 2023).

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](#).

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**Next issue: 21 December 2023.
Submission deadline: 8 December 2023.**

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PAH Picture of the Month

By the Cycle 3 deadline, a groundbreaking number of proposals (1,931) were submitted for the JWST, totaling 44,980 hours of proposed observations! This remarkable achievement establishes a new world record for astronomical proposal submissions. More information can be found [here](#).

The background picture features NGC 6822 as observed by the Mid-Infrared Instrument (MIRI) on the James Webb Space Telescope. The bright blue colours indicate emission by PAHs.

Credits: Background image: ESA/Webb, NASA & CSA, M. Meixner. The image is available [here](#).

Anharmonicity in the 1-5 μm Region of PAH IR Spectra

by Vincent J. Esposito

Introduction

The commissioning of capable infrared space telescopes, e.g., the Infrared Space Observatory (ISO) and the Spitzer Space Telescope, elucidated the presence of broad emission features in the mid-infrared (mid-IR) spectra of various astronomical environments such as planetary nebulae, reflection nebulae, asymptotic giant branch stars, and distant galaxies (Tielens, 2008). Such spectra show strong, broad features in the 3-20 μm region that are now commonly attributed to IR emissions of polycyclic aromatic hydrocarbons (PAHs) and are termed the PAH bands. These astronomical IR emission spectra include major features at 3.3, 6.2, 7.7, 8.6, 11.2, 12.7 and 16.4 μm as illustrated in Figure 1, which are mainly attributed to fundamental C-H and C=C stretching and bending vibrational normal modes of PAHs (Chown et al., 2023). Additionally, weaker features are interspersed throughout this wavelength region (Tielens, 2008). Many of these minor features, which can have intensities nearly as large as the major features, are currently unassigned.

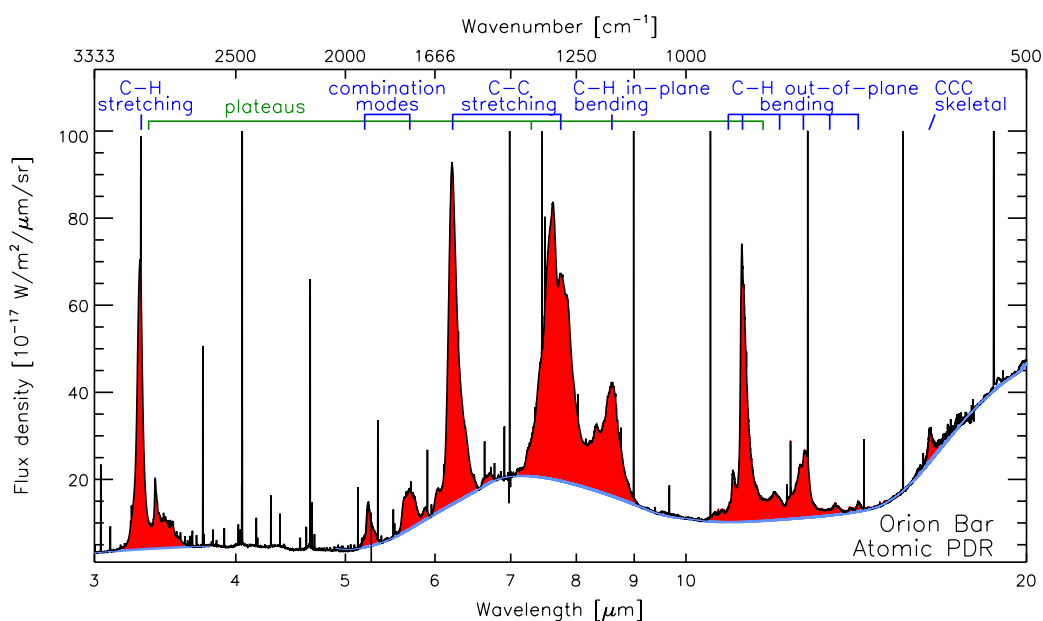


Figure 1 – Mid-IR JWST emission spectrum of the Orion Bar Atomic PDR showing the major and minor features and labeled with the vibrational normal modes of PAHs. Reproduced from Chown et al. (2023).

Except for the PAH aromatic and aliphatic CH stretch fundamentals, the 1-5 μm region is relatively unexplored by both observational and theoretical means because of the limited capabilities of earlier telescopes (e.g., ISO and Akari) along with the low intrinsic intensity of the transitions in this region. The PAH model predicts many important, weak features in the 1-5 μm region that could solve long-lived quandaries related to PAHs (Allamandola et al., 2021). The strong 3-20 μm bands seen in Figure 1 mainly originate from fundamental transitions ($\nu = 1 \rightarrow 0$) in PAHs, with the aliphatic and aromatic CH stretch fundamentals occurring in the 3.3-3.4 μm region. The overtone ($\nu = 2 \rightarrow 0, 3 \rightarrow 0, 4 \rightarrow 0$, etc.) and combination band transitions involving the CH stretching modes fall exclusively in the 1-3 μm range.

This region has been overlooked despite its fundamental importance to our understanding of PAHs in the Universe, and the recent launch of JWST is allowing astronomers to observe the 1-5 μm region with unprecedented spatial and spectral resolution. The influx of these important, high-resolution data sets in the 1-5 μm spectral range from the NIRSpec instrument onboard JWST requires an increased theoretical effort, without which spectral analysis and quantification will be severely hampered.

Photophysics of PAH Emission

In space, PAHs often exist in low density, low temperature radiation fields. Such an environment leads to non-thermal equilibrium dynamics during photochemical processes. Electronic excitation via the absorption of a UV photon is modeled to occur approximately once per day, which is of the same order as collision reactions (Tielens 2008; Mackie et al. 2018). The large, hyper-conjugated system of PAHs creates a continuum of electronic states, leading to the absorption of a UV photon in a large range of energies (6-12 eV).

Following electronic excitation, a PAH molecule undergoes fast (hundreds of femtoseconds), emission-less internal conversion to the ground electronic state. Once in the ground electronic state, due to the collision-free environment, the original energy supplied by the UV photon is partitioned into many vibrational degrees of freedom through rapid intramolecular vibrational energy redistribution (IVR). The molecule then radiatively relaxes to the vibrational ground state by emitting single IR photons. Because vibrational normal modes are coupled by anharmonicities, the emission of an IR photon changes the total vibrational temperature of the molecule, affecting subsequent IR photon emissions by shifting the frequency to lower energy. This process produces what is termed an IR 'cascade' spectrum. Band profiles in cascade spectra are asymmetric by nature, with a sharp high frequency side and long tail on the low frequency side as shown in Figure 2.

The Role of Computational Chemistry in Modeling the Anharmonic Emission Spectra of PAHs

Large observational datasets exist for the IR emission spectra of PAHs in the 3-20 μm region. Accurate predictions for these spectra are needed because IR telescopes (such as the JWST) detect the fluorescence emission from PAHs as cascade spectra. Only recently has computation and modeling of the emission spectra begun to catch up. Detected emission is routinely characterized by fitting models that are based on theoretical IR absorption spectra contained in the NASA Ames PAH IR Spectroscopic

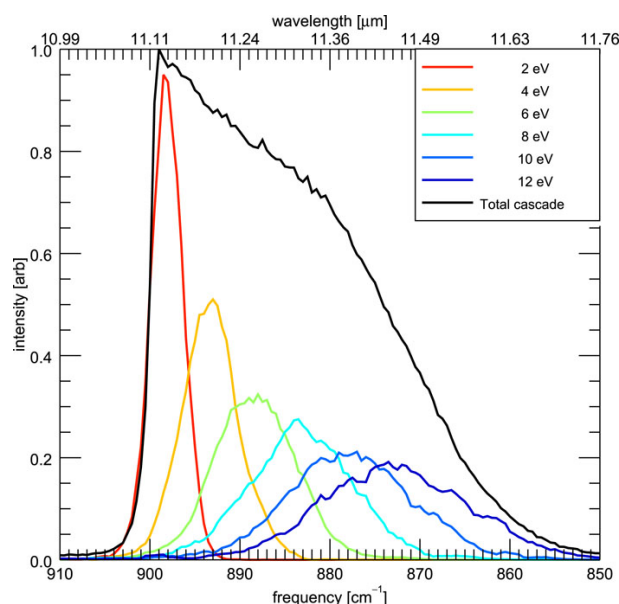


Figure 2 – Representative IR cascade spectrum (black) with individual contributions from electronic excitations at different energies. Reproduced from [Mackie et al. \(2018\)](#).

Database (PAHdb; [Bauschlicher et al. 2018](#)). Those data are broadly based on semi-empirical density functional theory (DFT) calculations using small basis sets under the double harmonic approximation because of the otherwise high computational cost, and scaling factors are often used to approximate the anharmonic contributions and presence of resonances. However, molecular vibrations are anharmonic in nature, namely they deviate from the harmonic oscillator model, which allows for bond breaking. Unfortunately, the harmonic DFT approach misses important anharmonic coupling effects such as Fermi resonances and mischaracterizes anharmonic transitions such as overtones and combination bands ([C. J. Mackie 2015](#); [Mackie et al. 2018](#)). Additionally, the inclusion of a standard scaling factor was recently shown to be in error ([Mackie et al., 2018](#)). Figure 3 compares the harmonic and anharmonic calculated IR spectrum for anthracene with its experimentally determined counterparts ([C. J. Mackie 2015](#)). The harmonic calculation misses over 10 important overtone and combination bands (labeled p-E in Figure 3) that are realized once anharmonicity is taken into account. Additionally, and very importantly, many of these overtone and combination features occur in the 1-5 μm region of the spectrum.

Recently, anharmonicity has been introduced to the IR cascade emission spectra simulations via second-order vibrational perturbation theory (VPT2) for realistic PAHs (up to 30 carbon atoms) using quantum chemistry ([Esposito et al.](#); [C. J. Mackie 2015](#); [Mackie et al. 2018](#); [Chen et al. 2019](#); [Mackie et al. 2021](#); [Joblin et al. 2011](#); [Basire et al. 2011](#); [Calvo et al. 2011](#); [Mulas et al. 2018](#); [Chakraborty et al. 2021](#); [Banhatti et al. 2022](#); [Panchagnula et al. 2020](#) and molecular dynamics ([Joalland et al. 2010](#); [Simon et al. 2011](#)) approaches. Experimental efforts have been made ([Lacinbala et al., 2022](#)) but are difficult due to the need for extreme high-vacuum, a collision-free environment, and quenched rotations, among other conditions. IR experiments often take the form of high temperature gas-phase absorption experiments or matrix isolation experiments that are difficult to connect with astronomical observations. This leaves theoretical predictions as the sole guidance for observational analysis and interpretation, and achieving high chemical accuracy is integral to doing this successfully.

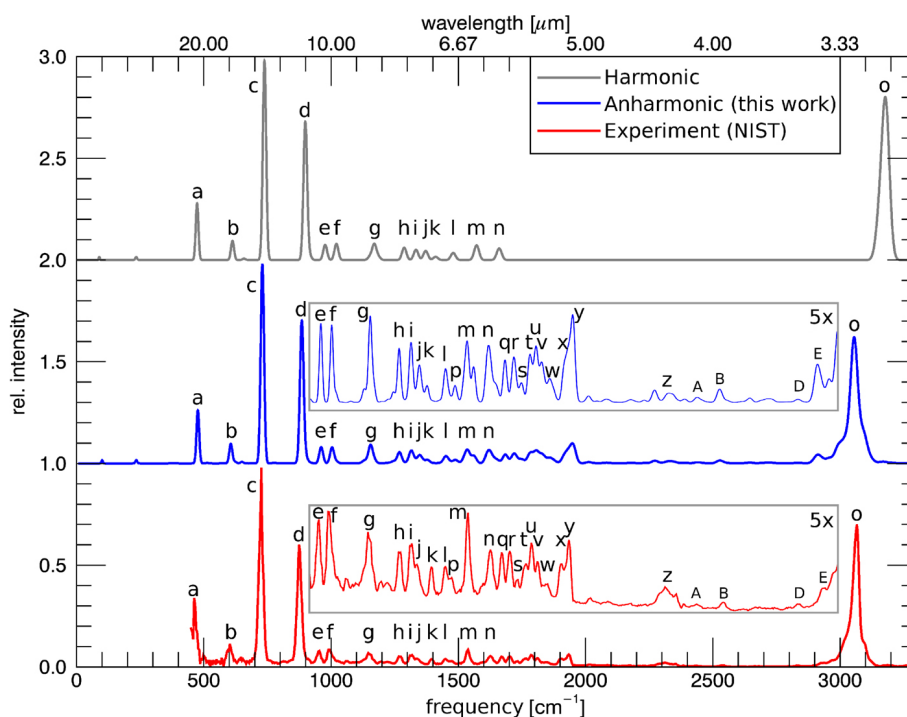


Figure 3 – Full IR absorption spectrum for anthracene computed using harmonic (top) and anharmonic (middle) methods compared to its gas-phase experimental spectrum at 300 K (bottom). Reproduced from *C. J. Mackie (2015)*.

The PAH Continuum

The IR spectrum observed towards most astronomical sources exhibits a jump in the baseline that occurs around 3 μm and plateaus from 3.5-5 μm (Boersma et al., 2023) before increasing again past 5 μm as illustrated in Figure 4. Based on new anharmonic calculations recently published in the Tim Lee memorial issue of *Molecular Physics* (Esposito et al., 2023), combination band and overtone transitions of PAH cations may be the possible source of this broad emission. In this study, we looked at three small, prototypical PAHs containing between 14 to 22 carbon atoms, relatively small molecules within the overall PAH family. As previously noted in the literature, fundamental modes of neutral PAH molecules are the likely source for the major features at 3.3 (aromatic CH stretches) and 11.2 μm (CH out-of-plane bends), among many others. Upon ionization, IR intensity shifts away from these regions towards the 6.2, 7.8, and 8.6 μm (CH in-plane bends and C=C skeletal deformations) features.

Due to this shift in intensity for the cations, combination bands and overtones stemming from the strong fundamental modes at 6.2, 7.8, and 8.6 μm fall in the 3-5 μm range, which is illustrated in Figure 5. This figure shows hundreds of weak, but significant bands that produce a quasi-continuum, especially when the bands of each molecule are combined. This is the region where the underlying baseline continuum is seen in the observations, and the intensity from the PAH cation features may explain some, if not all, of the excess emission in the observed spectra. The amazing fact is that the three PAHs considered in this study are but a small subset of the overall PAH population, and only contain 66, 72, and 102 vibrational modes, respectively. PAHs with 80 or more carbons will have a huge number of vibrational modes (>300) and exponentially more combination bands in the 3-5 μm region. Our results show that the buildup of intensity in this region from ever-larger, positively charged PAHs is potentially responsible for the continuum observed from 3-5 μm .

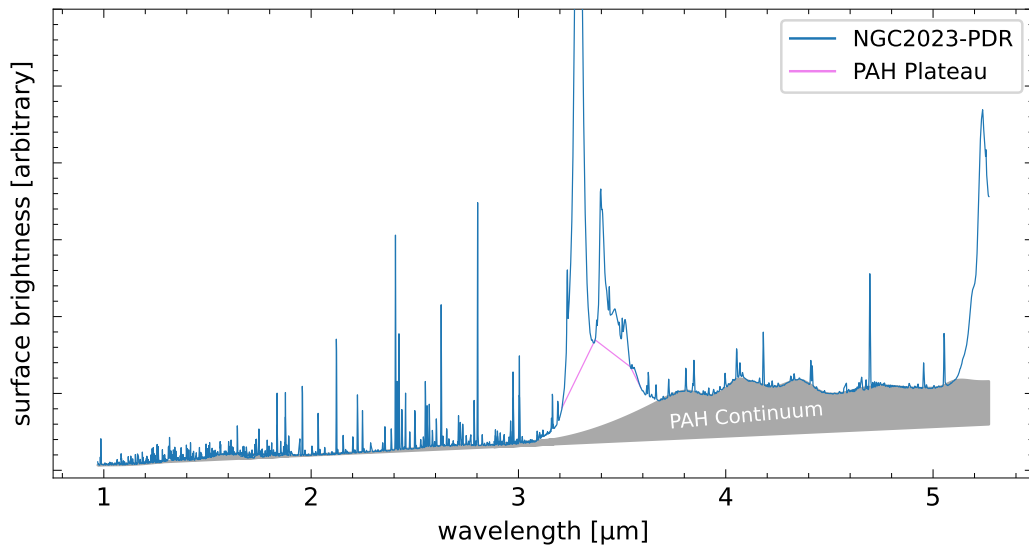


Figure 4 – 1-5 μm JWST spectrum of the reflection nebula NGC2023-PDR indicating the PAH-continuum (dark grey). The triangular shaped region below the 3.3/3.4 μm band complex (violet line segments) designates emission associated with the 3 μm band complex. Adapted from *Boersma et al. (2023)*.

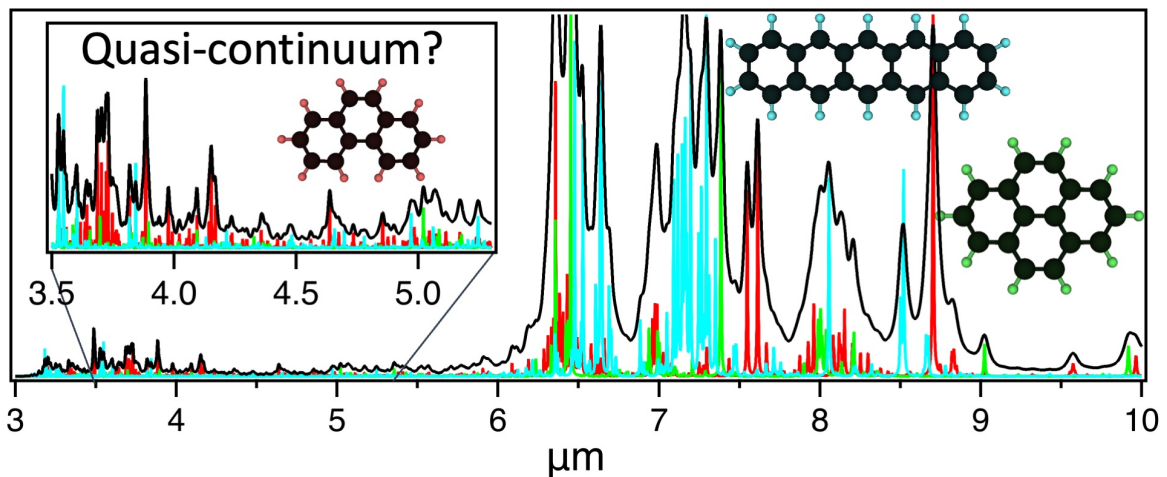


Figure 5 – The anharmonic computational IR absorption spectra of phenanthrene (red), pyrene (green), and pentacene (blue) and their composite spectrum (black). Reproduced from *Esposito et al. (2023)*.

Looking Ahead

As more and more JWST observations are released from their proprietary period, huge amounts of data are going to become available, many of which will include broad spectrum, high-resolution IR emission observations, emission most likely from PAHs. Some scientists, like the ones reading this newsletter, are interested in the PAH emissions themselves; however, others would prefer to have some insight into what is *hidden* by the PAH emission. This is one reason why the work we as a community do is so important beyond our own interests. We not only service the PAH field, but the whole of astrophysics and astronomy gains from the insights provided through these studies.

On that note, the overarching goal of my group of collaborators and myself is to continue improving PAHdb (www.astrochemistry.org/pahdb) for use by the whole scientific community. This includes adding anharmonic absorption and emission spectra to the database, as well as the forthcoming release of PAHdb version 4.00 that includes over 6,000 new spectra of large PAHs (Ricca et al. in preparation). I strongly believe that anharmonicity plays a more important role in understanding the astrophysical impact that PAHs have in space than is currently recognized. One small example of which is the many features in the 3-5 μm range in PAH cations that would have gone unnoticed if not for the inclusion of anharmonicity in the calculations (Esposito et al., 2023). We have only scratched the surface of the possible implications that anharmonicity might reveal about PAHs and their impact on the Universe. Computations that include anharmonicity can help reveal PAH growth and fragmentation pathways; determine the key stages within the PAH formation and destruction cycle in different environments; and decipher PAH structure, size, and charge ambiguities throughout various space environments via the 1-5 μm region that is not accurate without anharmonicity. Additionally, JWST's NIRSPEC instrument and the forthcoming Nancy Grace Roman Space Telescope will continue to expand our view of the Universe in the Near-IR, and anharmonicity will form a foundation for the study of PAHs to ensure the maximum science return from these missions.

Dedication to Tim Lee

Finally, even though I never had the pleasure of actually meeting him in person, I want to thank my NASA Postdoctoral Program (NPP) advisor Dr. Timothy J. Lee. He sponsored my NPP application and ensured I had the support infrastructure around me to succeed here at Ames before his untimely passing. For that, I will forever be grateful. I have heard he was an incredible scientist and mentor, and I lament that I did not get the opportunity to work with him directly. When I run into trouble, I try to think "WWTD?" (what would Tim do?). I believe that one of the markers of a great person is how they impact people even after they are gone. And from what I have heard and seen, I think that Tim will stay with many of us for years to come.



Dr. Vincent J. Esposito earned his Ph.D. in chemistry from the University of Pennsylvania under the mentorship of Dr. Joseph Francisco and Dr. Marsha Lester. His dissertation was on the spectroscopic properties and photochemistry of small, astrochemical aluminum-bearing molecules as well as Criegee intermediates. He is currently a NASA Postdoctoral Fellow at the NASA Ames Research Center in the Astrophysics branch. His research focuses on computing the anharmonic IR absorption and emission spectra of PAHs working toward the goal of populating the PAHdb with spectral data for use in the analysis and interpretation of new JWST data.

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Abstracts

Density Functional Theory Calculations on the Interstellar Formation of Biomolecules

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Density functional theory (DFT) is the most versatile electronic structure method used in quantum chemical calculations, and is increasingly applied in astrochemical research. This mini-review provides an overview of the applications of DFT calculations in understanding the chemistry that occurs in star-forming regions. We survey investigations into the formation of biologically-relevant compounds such as nucleobases, and also covers the formation of both achiral and chiral amino acids, as well as biologically-relevant molecules such as sugars, and nitrogen-containing polycyclic aromatic hydrocarbons.

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Threshold Photoelectron Spectrum and Dissociative Photoionization of Benzonitrile

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The threshold photoionization and dissociative ionization of benzonitrile (C_6H_5CN) were studied using double imaging photoelectron photoion coincidence (i^2 PEPICO) spectroscopy at the Vacuum Ultraviolet (VUV) beamline of the Swiss Light Source (SLS). The threshold photoelectron spectrum was recorded from 9.6 to 12.7 eV and Franck–Condon simulations of ionization into the ionic ground state, \tilde{X}^+ , as well as the \tilde{B}^+ and \tilde{C}^+ states were made to assign the observed vibronic structures. The adiabatic ionization energy of the \tilde{X}^+ , \tilde{B}^+ and \tilde{C}^+ states are determined at (9.72 ± 0.02) , (11.85 ± 0.03) and, tentatively, (12.07 ± 0.04) eV, respectively. Threshold ionization mass spectra were recorded from 13.75 to 19.75 eV and the breakdown diagram was constructed by plotting the fractional abundances of the parent ion and ionic dissociation products as a function of photon energy. The seven lowest energy dissociative photoionization channels of benzonitrile are found to yield $CN^\bullet + c-C_6H_5^+$, $HCN + C_6H_4^{\bullet+}$, $C_2H_4 + HC_5N^{\bullet+}$, $HC_3N + C_4H_4^{\bullet+}$, $H_2C_3N^\bullet + C_4H_3^+$, $CH_2CHCN + C_4H_2^{\bullet+}$ and $H_2C_4N^\bullet + c-C_3H_3^+$. HCN loss from the benzonitrile cation is the dominant dissociation channel from the dissociation onset up to 18.1 eV and CH_2CHCN loss becomes dominant from 18.1 eV and up. We present extensive potential energy surface calculations on the $C_6H_5CN^{\bullet+}$ surface to rationalize the detected products. The breakdown diagram and time-of-flight mass spectra are fitted using a Rice–Ramsperger–Kassel–Marcus statistical model. Anchoring the fit to the CBS-QB3 result (3.42 eV) for the barrier to HCN loss, we obtained experimental dissociation barriers for the products of 4.30 eV (CN loss), 5.53 eV (C_2H_4 loss), 4.33 eV (HC_3N loss), 5.15 eV (H_2C_3N loss), 4.93 eV (CH_2CHCN loss) and 4.41 eV (H_2C_4N loss). We compare our work to studies of the electron-induced dissociative ionization of benzonitrile and isoelectronic phenylacetylene (C_8H_6), as well as the VUV-induced dissociation of protonated benzonitrile ($C_6H_5CNH^+$). Also, we discuss the potential role of barrierless association reactions found for some of the identified fragments as a source of benzonitrile^($\bullet+$) in interstellar chemistry and in Titan’s atmosphere.

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High Throughput Anharmonic Vibrational and Rotational Spectral Computations

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Theoretical spectroscopy is a powerful tool in the chemist's toolbox, providing insight into experimental investigations here on Earth and into the observations of telescopes like the recently-operational JWST. This work presents recent developments in our group focused on extending the application of highly-accurate, theoretical spectroscopic techniques to large molecules. By leveraging composite and hybrid methods based on coupled cluster theory, molecules of study can increase in size from three to five atoms to upwards of ten atoms. In turn, using such results as a training set lays the foundation for methods capable of treating dozens, or potentially hundreds, of atoms in the future.

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Taming Semi-Empirical Methods for PAHs and Vibrational Spectra

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Semi-empirical methods offer a cost-effective means of computing explicit, anharmonic vibrational frequencies for large molecules, such as polycyclic aromatic hydrocarbons (PAHs), but their default parameters produce insufficiently accurate results for comparison to experiment, especially in the hydride stretching region where the NIRSpec instrument on JWST is most effective. This work delivers several reparameterized variants of the PM6 semi-empirical method trained to reproduce the experimental vibrational frequencies of 5 small hydrocarbon molecules. When benchmarked on the experimental frequencies of benzene and naphthalene, these reparameterized methods match the empirical values to within 38.7 cm^{-1} on average. Combining these values with the default PM6 frequencies below 3000 cm^{-1} brings the average deviation below 2 cm^{-1} for naphthalene, comparing favorably with the existing state of the art in B3LYP/4-31G, for a two order of magnitude decrease in the computational cost. As such, the present work offers a promising means of extending the computation of explicit, anharmonic vibrational frequencies to PAHs larger than those that can be examined anharmonically via B3LYP. Such large and accurate data sets are necessary to disentangle the unidentified spectral features observed around myriad astronomical bodies and the influx of observational data from JWST.

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Detection of ethynylbenzene in TMC-1 and the interstellar search for 1,2-diethynylbenzene

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Aims. We investigate the outcome of an electrical discharge of naphthalene and search for the resulting products in the Taurus Molecular Cloud (TMC-1).

Methods. Using chirped pulse Fourier transform microwave spectroscopy paired with an electric discharge source, we investigated products resulting from the naphthalene discharge. Quantum chemical calculations were used to help assign species and investigate potential reaction pathways relevant to the interstellar medium. These products were searched for in TMC-1 using the QUIJOTE line survey, covering 31.0-50.3 GHz.

Results. We confirm the detection of ethynylbenzene in TMC-1, and we also present a new molecular species, 1,2-diethynylbenzene, which could play an important role in the formation of naphthalene. Over ten products have been identified as resulting from the discharge, with only one of these species found in a previous IR-UV discharge study of naphthalene.

Conclusions. Ethynylbenzene has definitively been detected in TMC-1, and while we have identified a potentially important species for the formation of naphthalene and an exothermic reaction pathway, there is no current indication of its presence in TMC-1.

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Meetings

Global Astrochemistry Lecture Series (GALS)

“Astrochemistry: From the Big Bang to Life”

**Online Course
January – April, 2024**

<https://www.astrochemistry.de/online-course/>

Our universe is full of molecules, from the simplest – molecular hydrogen – all the way up to the complex molecular structures essential to the chemistry of life on Earth. A large and diverse array of chemical species has been detected not only on planets but in interstellar clouds, in regions of star formation, in protoplanetary disks, and in comets and meteorites within the solar system. But how and when was all this material formed, and how does it evolve over time? How much molecular content is inherited from one stage of star and planet formation to the next? What role does the chemistry of the universe through cosmic time play in the origins of life? A major unanswered question remains whether the molecules essential to life were produced on the early Earth (endogenous origin), or whether they were produced in the parent interstellar medium or planet-forming disk and delivered to Earth via asteroids, comets and their meteoritic remains (exogenous origin).

This lecture course will be devoted to astrochemistry and the exploration of topics related to the chemical origins of life. In 18 lectures from the world-leading experts, we will discuss the history of the early molecular universe starting from the Big Bang; environmental conditions and key physico-chemical processes in space; astronomical observations (from ground to space) of objects of astrochemical interest; chemical models describing astrophysical environments and their reaction networks; key laboratory techniques and approaches for studying astrochemical processes; chemistry in specific environments, such as the interstellar medium, protoplanetary disks, and atmospheres of (exo)planets; exogenous synthesis and delivery of biomolecule precursors; and, finally, evolution of these precursors on the early Earth.

GALS is aimed at providing a broad overview of scientific issues, problems, achievements, and open questions in astrochemistry; and at helping senior undergraduate and postgraduate students as well as early career scientists to expand their interests and develop a firm understanding of this area, sufficient to choose an appropriate direction for their future career. The course is open to students and scientists from all over the world.

GALS is an annual event. The first round took place in summer semester 2023 and was organized by Robin Garrod, Wolf Geppert, Martin McCoustra, and Alexey Potapov. GALS in summer semester 2024 is organized by Robin Garrod, Wolf Geppert, Serge Krasnokutski, Martin McCoustra, and Alexey Potapov, is supported by the COST Action "Nanospace" (CA21126), and is accredited by the Faculty of Sciences, University of La Laguna (ULL, Spain). The course carries a credit weighting of 3 ECTS.

Registration: December 01 2023 - January 21 2024

**Global Astrochemistry Lecture Series
(GALS)**

**Astrochemistry:
From the Big Bang to Life**

January 30 – April 11 2024

**Register Now at
<https://www.astrochemistry.de/online-course/>**

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Prebiotic synthesis

Edwin Bergin
Dieter Braun
Paola Caselli
Robin Garrod
Wolf Geppert
Eric Herbst
Laura Kreidberg
Martin McCoustra
Alessandro Morbidelli
Hans Olofsson
Alexey Potapov
Sean Raymond
Barbara Ryden
Dima Semenov
Alexander Tielens
Catherine Walsh
Rens Waters

The poster features a dark space background with various astronomical and chemical illustrations. At the top, there are images of a nebula and a galaxy. In the center, a bright blue and white nebula is shown. Below it, there are images of a protoplanetary disk, a molecular structure, and a planet. The text is arranged in a central column with a list of topics on the left and a list of speakers on the right.

NanoSpace Working Group 2 Meeting: Processing, reactivity and relaxation pathways of nC

**Edinburgh, Scotland
February 20 – 23, 2024**

<https://nanospacewg2.sciencesconf.org/>

The 1st Meeting of working group 2 of the COST Action CA21126 (Carbon Molecular Nanostructures in Space) network will be held in Edinburgh in February, 2024.

Working group 2 focuses on the formation, excitation, relaxation and destruction pathways of nanocarbon species along with their chemical reactivity and role in carbon transport throughout space (<https://research.iac.es/proyecto/nanospace/>).

The meeting will bring together experts in laboratory experiments, theory and observations to discuss recent advances in understanding the role of nanocarbons in space. It will include 25 invited talks, along with contributed talks and poster presentations. One of the sessions will be dedicated to short presentations by young researchers (PhD students/early postdoc). A selection of short oral presentations will be made based on received abstracts. Early registration is encouraged as spaces are limited.





Announcements

5 Year Postdoc in Molecular Physics / Physical Chemistry Laboratory Astrophysics

Advertised by Otto Dopfer

A (senior) postdoctoral position for five years is available in the laser molecular spectroscopy group of Otto Dopfer at Berlin Institute of Technology (Technical University 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. More details of our research activities and a list of publications are available at: <https://www.tu.berlin/en/lmsu>

Available state-of-the-art equipment includes a variety of pulsed and tuneable IR and UV lasers, several ion sources and cryogenic rf-traps, as well as several types of tandem mass spectrometers. The group is also strongly involved in international collaborations with groups in Japan, France, Italy, UK, Netherlands, and has been a regular user of the IR free electron laser facilities CLIO (France), FELIX (Netherlands), and more recently the FHI-FEL (Berlin).

Qualified candidates hold a PhD in Physics, Physical Chemistry, or related fields with a strong publication record and have ideally already some initial postdoctoral experience (all in experimental science) which is not substantially longer than 5 years.

The successful candidate will be involved in supervising PhD and undergraduate students, will take high responsibility for several existing research projects, and will be strongly involved in developing new research directions (i.e. writing proposals). The position is ideal for candidates who are pursuing an academic career (with possibility for Habilitation) by developing also their own research interests. The position is funded by TU Berlin and thus involves also teaching duties in the area of Experimental Physics (mostly Molecular Physics) either in German or in English.

1. laser spectroscopy, mass spectrometry, ion sources and traps, cluster science
2. vacuum techniques, optics, data acquisition, construction of apparatus
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 December 15 (2023) and will continue until the position is filled. The desired starting date is as soon as possible but this is negotiable to some extent.

Berlin is an international city and offers an exciting scientific and cultural environment.

Deadline: 15 December 2023

E-mail for contact: dopfer@physik.tu-berlin.de

Webpage: <https://www.tu.berlin/en/lmsu>

Postdoctoral Position in Molecular Physics Applied to Astrophysics / Astrochemistry (M/W)

Advertised by Ugo Jacovella

The experimental research involves ion mobility, mass spectrometric, and laser spectroscopic investigations of large carbon-rich molecular ions in the gas phase in the context of astrochemistry and astrophysics.

Available equipment includes pulsed dye lasers and OPO laser systems, a CRDS coupled to a discharge source mounted at the exit of a molecular beam, an ablation laser source and a drift-tube mobility spectrometer. A cryo-ion trap coupled to a TOF is under construction. The group is also strongly involved in international collaborations with groups in the US, Italy, UK, Australia, and is a regular user of the SOLEIL synchrotron facility (France).

Qualified candidates for the postdoc position hold a PhD in Physics, Physical Chemistry, or related fields. The successful candidate will be involved in co-supervising PhD and undergraduate students. The position is 1 + 1 years if less than 2 years of experience since PhD defense or 13 months if more than 2 years of experience (support will be provided to apply for external grant such as Marie Skłodowska-Curie Actions).

Experience in several of the following fields is mandatory:

1. laser spectroscopy, ion mobility, mass spectrometry, ion traps,
2. vacuum, optics, data acquisition (Python preferred), construction of apparatus
3. writing of publications
4. strong communication and presentation skills

Please provide a detailed CV (including a list of publications), a cover letter, and the names and contact details of two potential references. The assessment of applications will commence immediately and continue until the position is filled. The starting date for the position can fall between January 1st, 2024 and September 1st, 2024. For further information, please feel free to contact us.

Paris-Saclay is an expanding campus situated just a 30-minute drive or public transportation ride from Paris, offering an enriching blend of scientific and cultural experiences.

Deadline: 5 December 2023

E-mail for contact: ugo.jacovella@universite-paris-saclay.fr

Webpage: <https://emploi.cnrs.fr/Offres/CDD/UMR8214-UGOJAC-001/Default.aspx?lang=EN>

AstroPAH Newsletter

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

astropah@strw.leidenuniv.nl

Next issue: 21 December 2023

Submission deadline: 8 December 2023