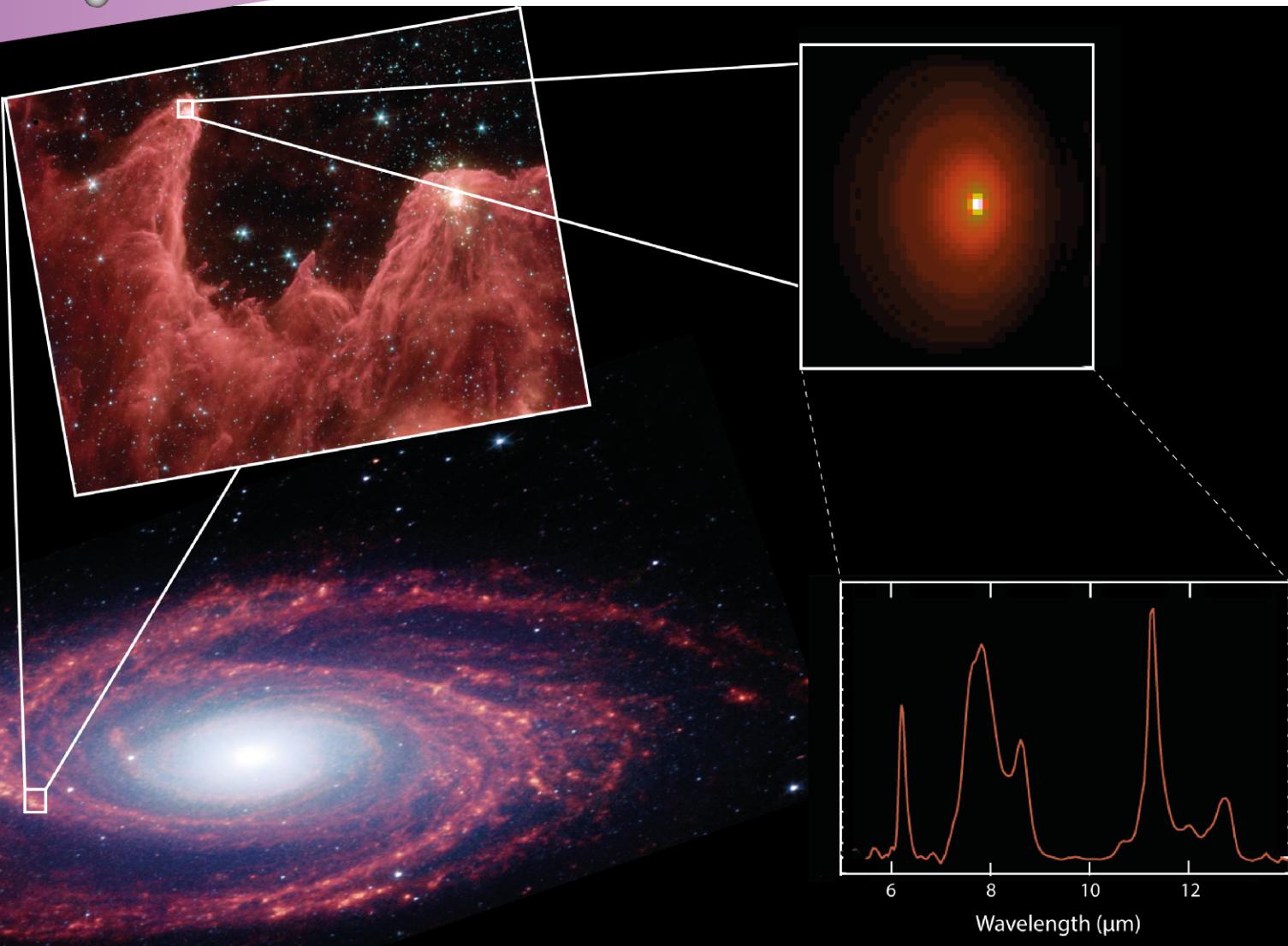


AstroPAH

A Newsletter on Astronomical PAHs

Issue 54 | December 2018



UBIQUITY

Editorial

Dear Colleagues,

In this last issue of 2018, the Picture of the Month reminds us of the ubiquity of PAHs in our Universe, in celebration of all the topics covered by the contributions you all sent to AstroPAH this year.

Anharmonicity is *In Focus!* Dr. Cameron Mackie, who recently graduated from the University of Leiden, discusses the effects of considering anharmonicity in the theoretical simulations of the PAH infrared spectrum, the subject of his PhD thesis.

Interesting subjects are covered in our Abstracts section including anharmonicity, differences between PAH and PANH formation, VUV photoprocessing of PAHs, the 7.7 μm band, and PAHs as probes for galaxies. Do not skip any!

For information on how to contribute to AstroPAH, visit our webpage (<http://astropah-news.strw.leidenuniv.nl>) or contact us by email (astropah@strw.leidenuniv.nl).

AstroPAH will have its usual January break, but we will be back in February (see the deadlines below). For those taking a break too, we wish you happy holidays!

Enjoy reading our newsletter!

The Editorial Team

**Next issue: 21 February 2018.
Submission deadline: 8 February 2018.**

AstroPAH Newsletter

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PAH Picture of the Month

The ubiquity of PAH emission in the Universe. Starting from the left lower corner and going clockwise: Spitzer composite image of Messier 81 where the color red corresponds to the $8.0 \mu\text{m}$ emission from PAHs; the iconic star forming region Mountains of Creation in the Eagle Nebula in the $8.0 \mu\text{m}$ Spitzer filter; the protoplanetary disk around the young star HD 97048 observed in the PAH filter of the Very Large Telescope (VLT) (image adapted from C. Doucet et al., *Astron. Astrophys.* 470, 625 (2007)); PAH spectrum of HD 97048 (image adapted from C. Boersma et al., *Astron. Astrophys.*, 484, 241 (2008)).

Credits: M81, Mountains of Creation:NASA/JPL/Caltech/Harvard-Smithsonian Center for Astrophysics; Image composition: A. Canadian.

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The Anharmonic Infrared Spectra of Polycyclic Aromatic Hydrocarbons

A Thesis

by Cameron J. Mackie

The majority of our knowledge of interstellar PAHs has been gained through the interpretation of their infrared emissions. The majority of our knowledge of their infrared emissions has been gained through laboratory and theoretical studies of a handful of representative species. However, these laboratory and theoretical studies – while very successful in expanding our understanding of PAHs – have a number of shortcomings when applied to the spectra of interstellar PAHs.

The processes which lead to the infrared emissions of interstellar PAHs, known as the infrared cascade spectra, is complex. A PAH will absorb a UV photon from a nearby stellar object, become electronically excited, then quickly undergo (hundreds of femtoseconds) an emission-less inter-conversion from an excited electronic state to the electronic ground state, transferring the absorbed energy into highly excited vibrational states. The PAHs then cool slowly (seconds) through the emission of IR photons before repeating this process over again (days). This non-equilibrium stochastic heating and cooling processes are difficult to reproduce both in the lab^[1,2,3] and theoretically^[4,5].

Laboratory studies have been limited largely to high-temperature gas-phase^[6] or "low-temperature" matrix isolation spectroscopic (MIS) techniques^[7,8,9]. Recent efforts in the last few years have also produced high-resolution low-temperature gas-phase infrared spectra of a handful of small (up to 4 rings) PAHs^[10,11,12]. Temperature effects (band shifts and broadenings), matrix interactions (unpredictable band shifts and intensity suppression) and species size restrictions (low volatility) have all impeded and complicated the translation to realistic cascade models. Additionally, the laboratory spectra is taken dominantly in absorption under thermal equilibrium conditions, whereas the interstellar PAHs are dominantly in emission under non-thermal equilibrium conditions. Only a handful of studies have investigated PAHs under "true" interstellar IR cascade conditions^[1,2,3].

Theoretical studies have been limited largely to the double harmonic approximation through the use of density functional theory (DFT) methods. Databases containing the harmonic spectra of thousands of PAHs are available online^[13,14]. While successful in reproducing the large picture of the overall IR spectra of PAHs, again a number of limitations have impeded and complicated the translation to realistic cascade models. Due to the nature of the harmonic approximation a number of corrections need to be applied to the resulting spectra in order to obtain agreement with experiments. Scaling factor(s) need to be applied to the band positions in order to account for the anharmonic relaxation of the vibrational modes, band profiles need to be added ad-hoc through convolutions with Gaussian or Lorentzian (or Voigt) functions in order to account for temperature effects, and band shifts need to be empirically derived from experiment and applied, again in order to account for temperature effects. The harmonic models also cannot take into account combination bands, overtones, or resonances (the perturbation of band positions and sharing of intensities between closely spaced features); all of which play important roles in the IR spectra of PAHs, especially in the 5 and 3 μm regions where they dominate.

On March 29, 2018, I successfully defended my thesis entitled “The Anharmonic Infrared Spectra of Polycyclic Aromatic Hydrocarbons” at the University of Leiden in the Netherlands. This work was accomplished through a Dutch Astrochemistry Network (DAN) collaboration of four institutes: the University of Leiden, NASA Ames Research Center, the University of Amsterdam, and Radboud University. The collaborations included theorists: Alessandra Candian, Timothy J. Lee, Xinchuan Huang, and Tao Chen; experimentalists: Elena Maltseva, Annemieke Petrignani, Wybren Jan Buma, Jos Oomens, Andrew L. Mattioda, and Scott Sandford; and astronomers: Alexander Tielens (as well as many of the previously mentioned collaborators who consider themselves of two worlds).

The aim of this thesis was to use theoretical methods to reproduce and understand the IR spectra of PAHs at the anharmonic level. Including anharmonicities in theoretical calculations alleviates a number of issues seen with the harmonic calculations: scaling factors are no longer required; combination bands, overtones, and resonances can be accounted for; band profiles can be calculated (not convolved); and temperature effects such as band shifts, broadenings, and changes to intensities can be calculated. However, accounting for anharmonicities comes at an extreme computational cost (weeks worth of computations for even the smallest PAHs), therefore the studies were limited to a handful of species with less than 18 carbon atoms, as well as some methylated and hydrogenated species. These PAHs are far from the hundreds-of-carbon-atom PAHs thought to dominate the interstellar population, but the goal was to understand how and why a spectrum changes when moving from a harmonic to a more realistic anharmonic model, which is equally valid for both small and large species. The work in this thesis led to a better understanding of the experimental PAH spectra through fundamental band identifications, identifications of combination bands and overtones which litter the spectra, as well as explaining the appearance of moderately strong bands which occur through resonances. The work also led to a better understanding of the harmonic spectra, and why and how it fails in some regions (3 and 5 μm in particular) due to the neglect of combination bands and resonances.

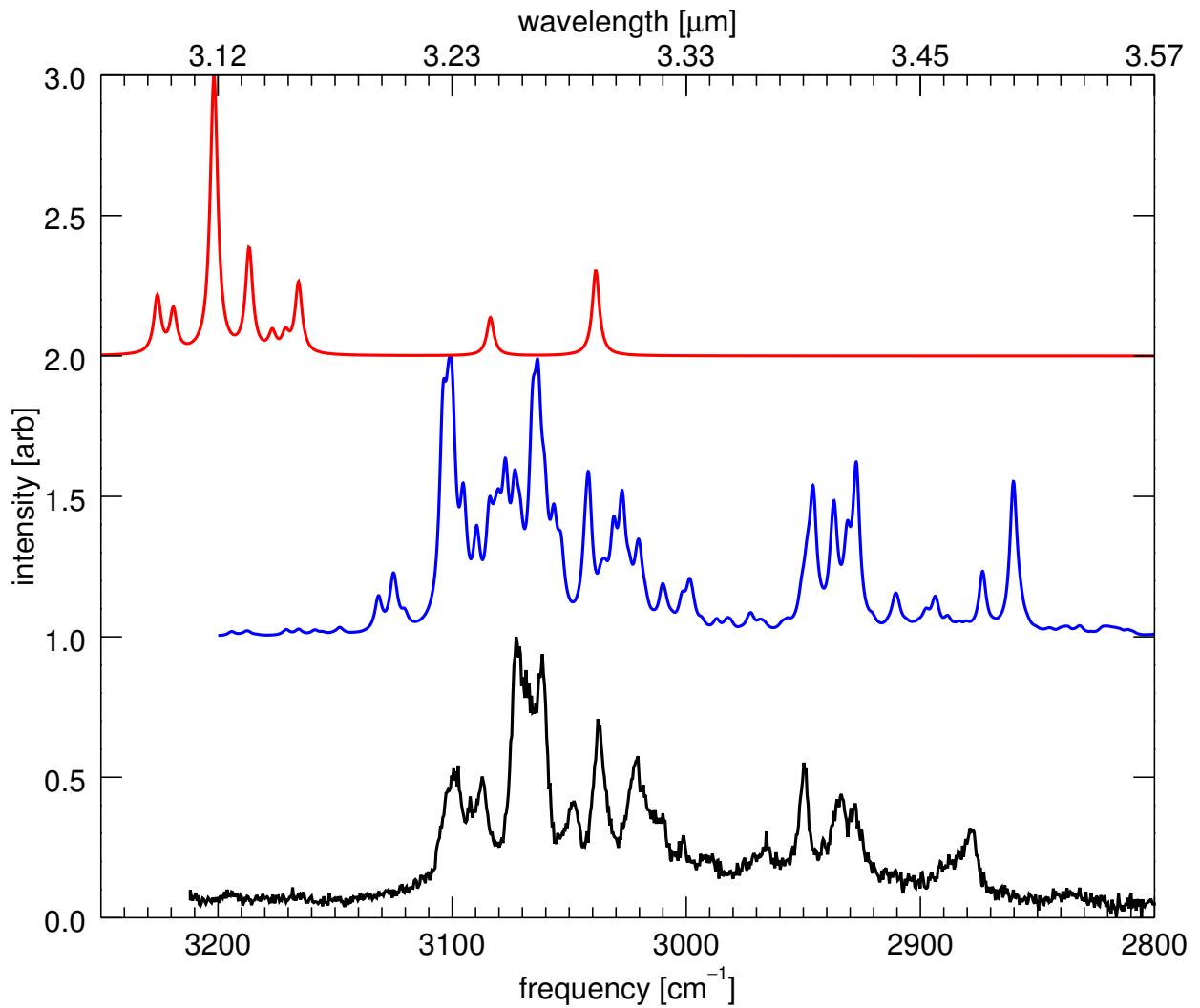


Figure 1: The infrared spectra of the C–H stretching region of 9–methylanthracene: The harmonic spectrum (red), anharmonic spectrum (this work) (blue), and the high–resolution experimental spectrum (black).

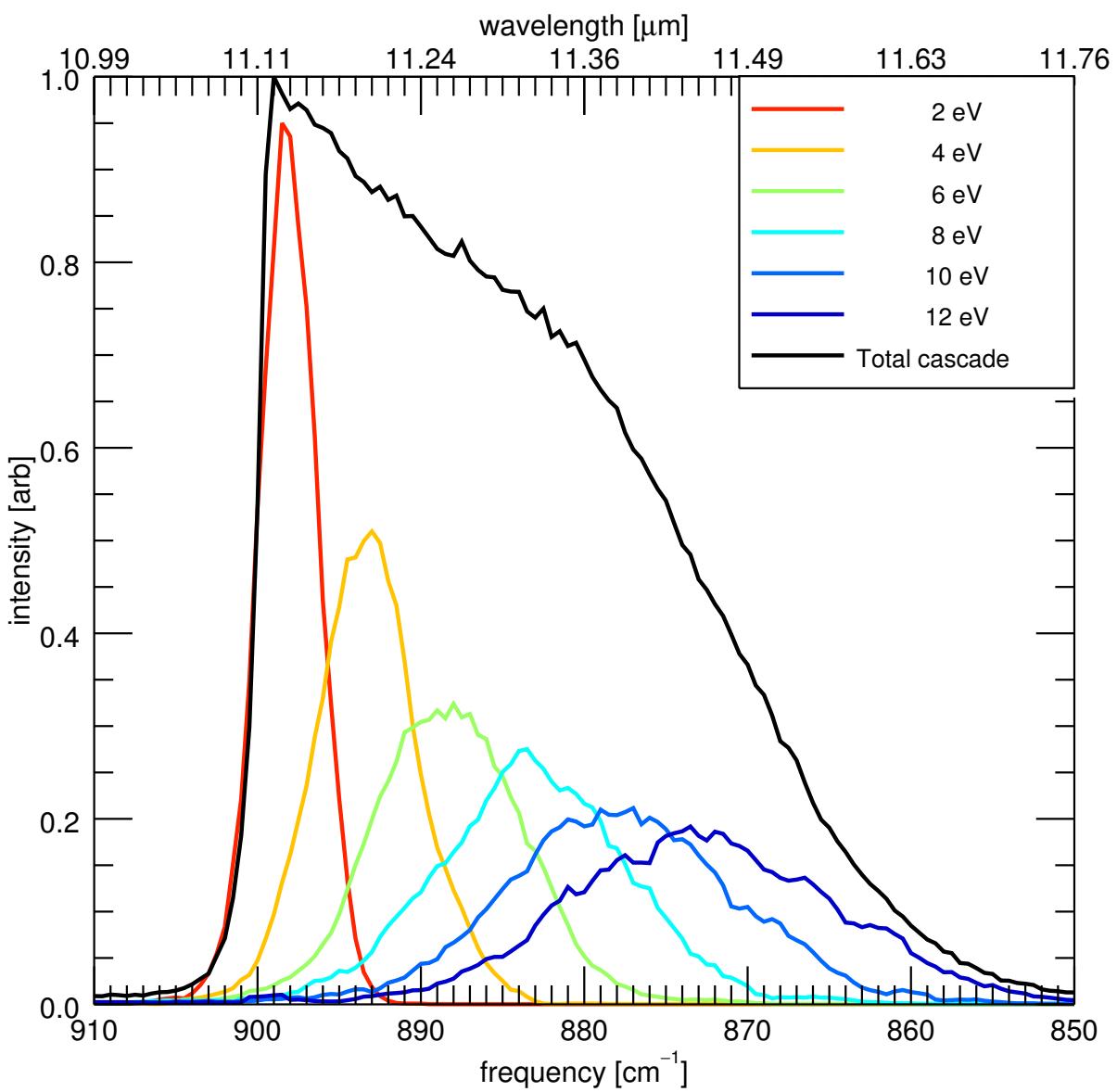


Figure 2: Snapshots of a PAH IR cascade process at various internal energies (colors) as the PAH cools; leading to the overall cascade feature (black).

We also took these calculations to their logical conclusion and used them to produce theoretical anharmonic infrared cascade spectra, equivalent to an interstellar PAH IR cascade (albeit with species much too small to reproduce observations). This however, allowed for a deeper understanding of the processes involved in an interstellar PAH cascade spectrum, and the origin of both the asymmetric profiles and the appearance of “pseudoshifts”.

The take-home messages from this thesis can be summarized as follows:

- The $3 \mu\text{m}$ region of PAH spectra is dominated by resonances. The spectra cannot be reproduced at the harmonic level; anharmonicities need to be taken into account. See figure 1.
- The $5 \mu\text{m}$ region of PAH spectra is dominated by combination bands. The spectra cannot be reproduced at the harmonic level; anharmonicities need to be taken into account.
- Resonances, combination bands, and overtones may explain some plateau features.
- Resonances continue to play a dominant role even at high temperatures and during the IR cascade.
- IR cascade features do NOT shift in peak position with temperature (as we are used to seeing under thermal equilibrium conditions). See figure 2.
- The steep high energy wall of IR cascade features are stable in position at their zero Kelvin position regardless of the energy of the exciting UV photon.
- Experimental low-temperature gas-phase *absorption* spectra or zero Kelvin theoretical anharmonic spectra can be used or accurately predict the high energy wall of the IR cascade spectra of PAHs.

The last three points are perhaps the most useful to the astronomical PAH community. Since the position of the steep wall of a feature is stable at the zero-Kelvin position then high-quality low-temperature (preferably gas-phase) *absorption* spectra can be used to pin down the exact astronomical PAH band positions. Likewise, high-quality zero-Kelvin theoretical band positions can also be utilized in the same manner. Temperature effects only manifest themselves as the “growing” of the red wings, out from the steep wall positions. Ironically, the complexity of PAH cascade emissions has led to a simple understanding and explanation of interstellar PAH IR cascade spectral features.

The thesis is available in digital form through:

<https://openaccess.leidenuniv.nl/handle/1887/61203>

Conversely, each paper which comprises the thesis, can be obtained (and cited) through references [15, 16, 17, 18, 19]. (Chapters 6 and 7 are currently on embargo and are only available through reference [19].)

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Cameron Mackie received his PhD in 2018 at the University of Leiden (Prof. Dr. A. G. G. M. Tielens) after completing his undergraduate work in Chemical Physics at the University of Waterloo (Canada), and his Masters in Astronomy at the University of Western Ontario (Canada). He is currently a post-doctoral researcher at the Lawrence Berkeley National Lab studying the development and application of electronic structure theories alongside Prof. Dr. Martin Head-Gordon.

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Abstracts

Anharmonic vibrational spectroscopy of polycyclic aromatic hydrocarbons (PAHs)

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While powerful techniques exist to accurately account for anharmonicity in vibrational molecular spectroscopy, they are computationally very expensive and cannot be routinely employed for large species and/or at non-zero vibrational temperatures. Motivated by the study of Polycyclic Aromatic Hydrocarbon (PAH) emission in space, we developed a new code, which takes into account all modes and can describe all infrared transitions including bands becoming active due to resonances as well as overtone, combination, and difference bands. In this article, we describe the methodology that was implemented and discuss how the main difficulties were overcome, so as to keep the problem tractable. Benchmarking with high-level calculations was performed on a small molecule. We carried out specific convergence tests on two prototypical PAHs, pyrene ($C_{16}H_{10}$) and coronene ($C_{24}H_{12}$), aiming at optimising tunable parameters to achieve both acceptable accuracy and computational costs for this class of molecules. We then report the results obtained at 0 K for pyrene and coronene, comparing the calculated spectra with available experimental data. The theoretical band positions were found to be significantly improved compared to harmonic density functional theory calculations. The band intensities are in reasonable agreement with experiments, the main limitation being the accuracy of the underlying calculations of the quartic force field. This is a first step toward calculating moderately high-temperature spectra of PAHs and other similarly rigid molecules using Monte Carlo sampling.

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<http://adsabs.harvard.edu/abs/2018JChPh.149n4102M>

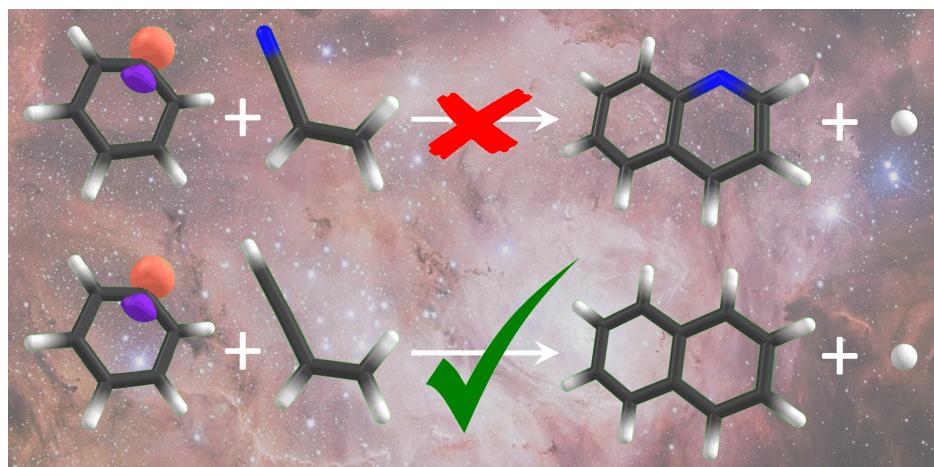
Nitrogen matters: the difference between PANH and PAH formation

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A solid understanding of and a reliable model for the formation pathways of polycyclic aromatic (nitrogen containing) hydrocarbons (PA(N)Hs) is needed to account for their abundance in the interstellar medium and in Titan's atmosphere as well as to mitigate the emission of these carcinogens in our terrestrial environment. We have investigated the phenyl + acrylonitrile reaction mechanism between 600 and 1200 K in a hot microreactor. Radical intermediates ($C_9H_8N^\bullet$), formed by addition, and closed-shell C_9H_7N products, formed by subsequent hydrogen elimination, are isomer-selectively identified using photoion mass-selected threshold photoelectron spectroscopy in conjunction with Franck-Condon simulations. Although quinoline is the most stable product, the calculated potential energy surface and a kinetic model confirm that the reaction is kinetically controlled and yields four open-chain isomers instead. The absence of quinoline is in stark contrast with the isoelectronic phenyl + vinylacetylene reaction that produces naphthalene. Ab initio calculations suggest that this change is brought about by the stability of the nitrile group, which inhibits ring formation. Therefore, it is unlikely that nitrile precursors form nitrogen-containing rings, which calls for alternative pathways by which nitrogen atoms can be incorporated in aromatic systems to explain their presence in the ISM and Titan's atmosphere.



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<https://pubs.rsc.org/en/content/articlelanding/2018/cp/c8cp05830j#!divAbstract>

Study on the dissociation of astro-PAHs

Sarah Rodriguez Castillo

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Thesis conducted at the following institutes:

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This PhD thesis has been defended at Toulouse University on the 30th of October 2018.

Polycyclic Aromatic Hydrocarbons (PAHs) are revealed in astrophysical environments thanks to their characteristic infrared features that are emitted following the absorption of vacuum ultraviolet (VUV) photons from nearby massive stars. This interaction regulates their charge state, stability and dissociation mechanisms, which in turn affect the energy balance and the chemistry of the gas in the interstellar medium. In particular, PAHs could contribute to the formation of the most abundant molecule, H₂, in photodissociation regions (PDRs). This work aims at contributing to these topics by quantifying the VUV photoprocessing of specific medium-sized PAH cations through experimental studies complemented by computational investigations.

The experimental results were gathered from two campaigns at synchrotron facilities: ion trap experiments allowed us to obtain the yields of ionization and fragmentation and the branching ratios between the different photoevents, while from iPEPICO spectroscopy we obtained breakdown curves and dissociation rates from their fitting using an RRKM model. We detail the case of the fragmentation processes of two isomers of dibenzopyrene cation (C₂₄H₁₄⁺) in order to assess the impact of structure on these processes. We present Density Functional Theory calculations and Molecular Dynamics simulations, which evidence the importance of structure and non-planarity in these mechanisms and provide a better view on the dissociation pathways and energetics.

This work brings significant new data for models that describe the chemical evolution of PAHs in astrophysical environments, including the first measurement of the ionization yield of medium-sized PAH cations as well as several dissociation rates. We also report a new mechanism that would need to be considered while evaluating the contribution of PAHs to the formation of H₂ in PDRs. This mechanism involves specific structures with bay areas that would need to be studied on a larger sample of PAHs.

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Examining the class B-to-A shift of the 7.7 μ m PAH band with the NASA Ames PAH IR Spectroscopic Database

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We present insights into the behavior of the astronomical 7.7 μ m polycyclic aromatic hydrocarbon (PAH) emission complex as gleaned from analyzing synthesized spectra, utilizing the data and tools from the NASA Ames PAH IR Spectroscopic Database. We specifically study the influence of PAH size, charge, aliphatic content and nitrogen substitution on the profile and peak position of the 7.7 μ m feature ($\lambda_{7.7}$). The 7.7 μ m band is known to vary significantly from object-to-object in astronomical observations, but the origin of these variations remains highly speculative. Our results indicate that PAH size can accommodate the largest shift in $\lambda_{7.7}$ ($\simeq 0.4 \mu$ m), where relatively small PAHs are consistent with class A spectra ($N_C \leq 60$) while large PAHs are consistent with red/very red class B spectra. Aliphatic PAHs, of which our sample only contains a few, can produce redshifts typically around 0.15 μ m; changes in ionization fraction, depending on the species, produce shifts up to 0.1 μ m; and nitrogen substitution has no effect on $\lambda_{7.7}$. Within the limits of our study, the class B \rightarrow A transition is best explained with a changing PAH size distribution, with a relatively minor role assigned to aliphatic content and varying charge states. The resulting astronomical picture is that the photochemical evolution of PAHs moving from shielded class C/B environments into exposed ISM-like class A environments may be intrinsically different from the reverse class A \rightarrow B transition of interstellar PAHs being incorporated into newly-forming star systems.

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PAHs as tracers of the molecular gas in star-forming galaxies

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We combine new CO(1–0) line observations of 24 intermediate redshift galaxies ($0.03 < z < 0.28$) along with literature data of galaxies at $0 < z < 4$ to explore scaling relations between the dust and gas content using polycyclic aromatic hydrocarbon (PAH) 6.2 μm ($L_{6.2}$), CO (L'_{CO}), and infrared (L_{IR}) luminosities for a wide range of redshifts and physical environments. Our analysis confirms the existence of a universal $L_{6.2}-L'_{\text{CO}}$ correlation followed by normal star-forming galaxies (SFGs) and starbursts (SBs) at all redshifts. This relation is also followed by local ultraluminous infrared galaxies that appear as outliers in the $L_{6.2}-L_{\text{IR}}$ and $L_{\text{IR}}-L'_{\text{CO}}$ relations defined by normal SFGs. The emerging tight ($\sigma \approx 0.26$ dex) and linear ($\alpha = 1.03$) relation between $L_{6.2}$ and L'_{CO} indicates a $L_{6.2}$ to molecular gas (M_{H_2}) conversion factor of $\alpha_{6.2} = M_{\text{H}_2}/L_{6.2} = (2.7 \pm 1.3) \times \alpha_{\text{CO}}$, where α_{CO} is the L'_{CO} to M_{H_2} conversion factor. We also find that on galaxy integrated scales, PAH emission is better correlated with cold rather than with warm dust emission, suggesting that PAHs are associated with the diffuse cold dust, which is another proxy for M_{H_2} . Focusing on normal SFGs among our sample, we employ the dust continuum emission to derive M_{H_2} estimates and find a constant $M_{\text{H}_2}/L_{6.2}$ ratio of $\alpha_{6.2} = 12.3 \text{ M}_{\odot}/L_{\odot}$ ($\sigma \approx 0.3$ dex). This ratio is in excellent agreement with the L'_{CO} -based $M_{\text{H}_2}/L_{6.2}$ values for $\alpha_{\text{CO}} = 4.5 \text{ M}_{\odot}/(\text{K km}^{-1} \text{ s}^{-1} \text{ pc}^2)$ which is typical of normal SFGs. We propose that the presented $L_{6.2}-L'_{\text{CO}}$ and $L_{6.2}-M_{\text{H}_2}$ relations will serve as useful tools for the determination of the physical properties of high- z SFGs, for which PAH emission will be routinely detected by the *James Webb Space Telescope*.

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<https://academic.oup.com/mnras/article-abstract/482/2/1618/5129151>

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meetings

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March 3-6, 2018
Madrid

The evolution of carbonaceous clusters and macromolecules, such as polycyclic aromatic hydrocarbons and fullerenes, in cosmic environments is a highly interdisciplinary field where physicists, physical chemists, astrophysicists, and astronomers mingle. The international meeting, EPoLM, Energetic Processing of Large Molecules was initiated to foster discussions and collaborations between these different disciplines. The EPoLM-1, 2 and 3 meetings were held in Leiden (May 2015), Stockholm (May 2016) and Toulouse (June 2017). EPoLM-4 will maintain the dynamics of exchanges between researchers from the different communities. It will be the occasion to present the most recent results on the structure and dynamics of large molecular species, their evolution under photon irradiation and energetic ion collisions, their spectroscopic characteristics, as well as the formation and processing of clusters and grains. These results comprise quantum chemical studies, molecular dynamics simulations, and laboratory experiments obtained from a variety of techniques, including plasmas, jets, storage rings and ion traps. The workshop will also continue to explore the connection with observational constraints and astronomical models.

For more information, consult the website:

https://nanocosmos.iff.csic.es/?page_id=1959,

which will open up soon.

AstroPAH Newsletter

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