AstroPAH

A Newsletter on Astronomical PAHs

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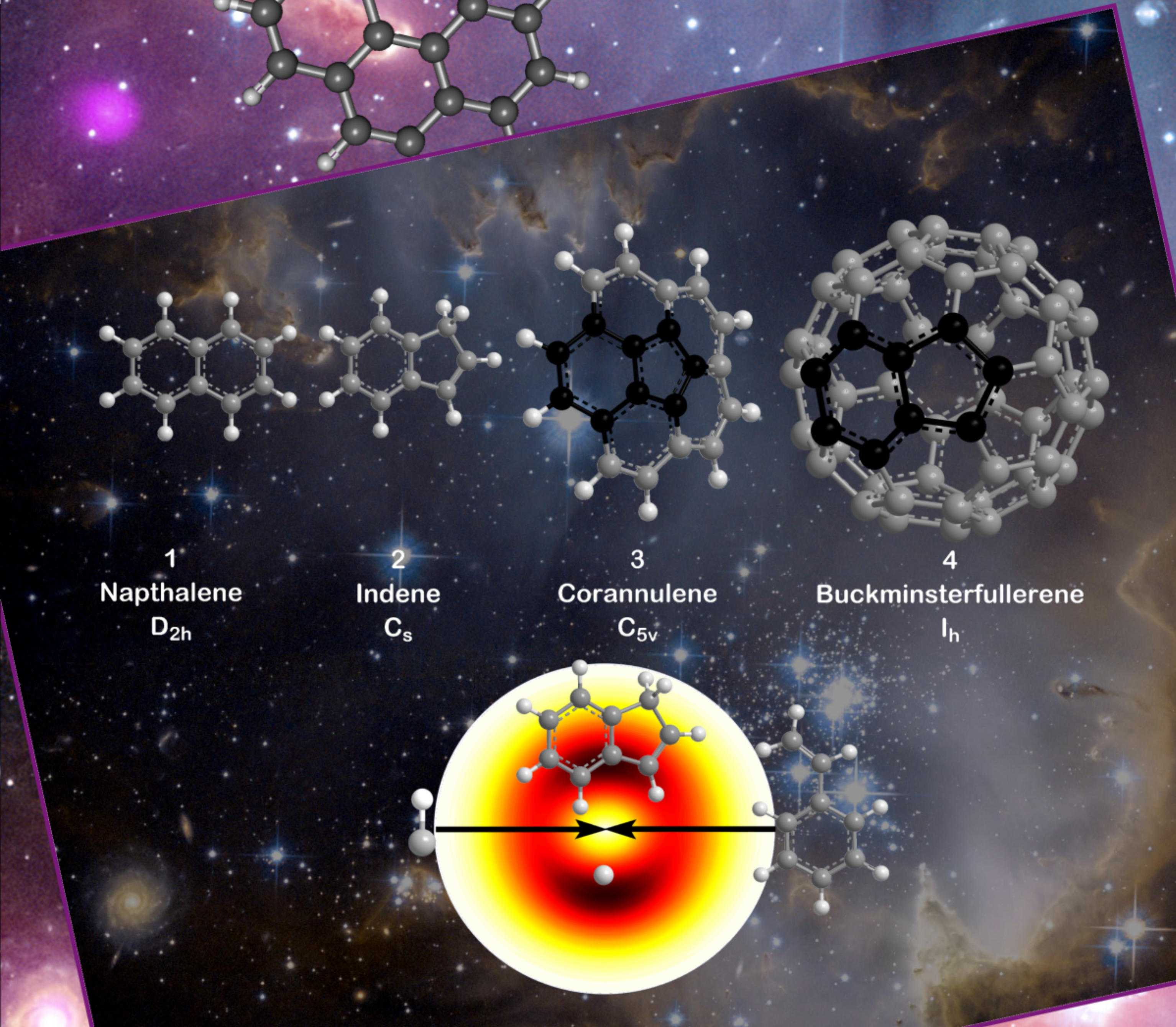

Low-temperature pathway to indene formation

Editorial

Dear Colleagues,

Welcome to our 75^{th} AstroPAH volume, we are back from our January break! We hope all of you are healthy and doing well. Happy belated New Year to all!

Our Picture of the Month relates to a recent study by Doddipatla et al. (2021) about low-temperature pathways to the formation of indene. Make sure to check out our Abstracts section to learn more about pathways leading to the formation of this five-membered ring molecule in the interstellar medium! Do not miss our other contributions on gas phase formation of carbon clusters, PAH emission and cation formation!

We also advertise for two PhD positions: one at Western University (Canada) and one at the GSMA (France), along with a Postdoctoral position at the Southwest Research Institute (USA).

If you are on Instagram, you may want to follow our new page! We will be posting selected PAH molecules of the month and sharing more PAH-related content, showcasing the mesmerizing beauty of PAHs.

Lastly, we hope you enjoyed watching the successful Mars Perseverance rover landing this week. Mars has been getting quite the attention lately with the recent successful Chinese Tianwen-1 mission and the UAE's Hope mission.

We hope you enjoy reading our newsletter, and we thank you for your dedication and interest in AstroPAH! In the meantime, 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: 18 March 2021.
Submission deadline: 5 March 2021.

AstroPAH Newsletter

Contents

PAH Picture of the Month

An unusual low-temperature pathway leading to the formation of indene was revealed using crossed molecular beam experiments and electronic structure calculations by S. Doddipatla et al. (2021). See more about this work in the abstract section.

Credits: S. Doddipatla et al. (2021). Background image by NASA, ESA, and the Hubble Heritage Team (STScI/AURA)-ESA/Hubble Collaboration.

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Abstracts

Low Temperature Gas Phase Formation of Indene in the Interstellar Medium

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Polycyclic aromatic hydrocarbons (PAHs) are fundamental molecular building blocks of fullerenes and carbonaceous nanostructures in the interstellar medium and in combustion systems. However, an understanding of the formation of aromatic molecules carrying five-membered rings — the essential building block of nonplanar PAHs — is still in its infancy. Exploiting crossed molecular beam experiments augmented by electronic structure calculations and astrochemical modeling, we reveal an unusual pathway leading to the formation of indene (C_9H_8 — the prototype aromatic molecule with a five-membered ring — via a barrierless bimolecular reaction involving the simplest organic radical-methylidyne (CH) — and styrene ($C_6H_5C_2H_3$) through the hitherto elusive methylidyne addition-cyclization-aromatization (MACA) mechanism. Through extensive structural reorganization of the carbon backbone, the incorporation of a five-membered ring may eventually lead to three-dimensional PAHs such as corannulene ($C_{20}H_{10}$) along with fullerenes (C_{60}, C_{70}), thus offering a new concept on the low-temperature chemistry of carbon in our galaxy.

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https://advances.sciencemag.org/content/7/1/eabd4044.full

The Helicenes: Potential Carriers of Diffuse Interstellar Bands

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In this work, the helicenes are postulated as potential carriers of the diffuse interstellar bands, DIBs. The helicenes are nonplanar *cata*-condensed molecules structurally related to the polyacenes, and polyacenes have been already proposed as conceivable carriers of the DIBs. In here, the possible identity of the carrier of the DIB at 4502 Å is studied and potentially identified as a *cata*-condensed helicene using spectroscopic, statistical, and stability methods. First, statistic and spectroscopic information allow the fitting of the regression equation that governs the variation of the location of the published absorbance p-bands as a function of the number of fused aromatic rings (nFAR) for planar and helical *cata*-condensed polycyclic aromatic hydrocarbons with 1–14 FAR, and the application of this equation to establish the identity of the possible carrier of the 4502 Å DIB, that is, [26]helicene ($C_{106}H_{56}$). The difference between the calculated location of the *p*-band from the fitted equation and the DIB location under study is equal to 0.21%. Subsequently, an aromaticity argument demonstrates the presence of π-delocalizing benzene effect in helicenes with the general formula $C_{2+4N}H_{2N+4}$, for example, [26]helicene, that would theoretically provide supplementary stability to the molecule to justify its occurrence. Finally, a feasible mechanism of formation of helicenes in the interstellar medium is proposed that involves successive additions of n-butane units to a phenanthrene moiety. To the best of our knowledge, this is the first report about the possible presence of *cata*-condensed helical molecules in the DIBs and the first study that theorizes that [26]helicene is the possible carrier of the DIB at 4502 Å.

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Gas phase formation of carbon cluster (fullerenes and graphenes)/prebiotic sugar complexes

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Among the constituent molecular classes of proteins and nucleic acids, the presence of Ribose and deoxy-Ribose in space remains unclear. Here, we provide experimental evidence of astronomically related sugar derivatives - carbon cluster (fullerenes and graphenes)/prebiotic sugar complexes - and study their formation processes in the gas phase. As the initial molecular precursor, PAH cations (dicoronylene, DC, $C_{48}H_{20}^{+}$)/(2-deoxy-d-Ribose, dR, $C_5H_{10}O_4$, and dehydrated 2-deoxy-d-Ribose, DedR, $C_5H_8O_3$) and fullerene cations (C_{60}^{+})/(dR and DedR), the results show that two series of graphenes-prebiotic sugar cluster cations (graphene/dR and graphene/DedR, e.g., (dR)C_n^{+} and (DedR)C_n^{+}) and two series of fullerenes-prebiotic sugar cluster cations (fullerene/dR and fullerene/DedR, e.g., (dR)(DedR)$_2C_n^{+}$, (DedR)$_3C_n^{+}$, and (dR)$_2$(DedR)C_n^{+}) are formed through an ion-molecule reaction pathway under the influence of a strong radiation field. The structure of newly formed complexes and the binding energy for these formation reactions are initially theoretically calculated. These laboratory studies attest to the importance of ion-molecule reaction synthesis routes for the chemical complexity in space, demonstrated the gas phase interstellar materials could directly lead to the formation of large and complex sugar derivatives in a bottom-up growth process. The chemical evolution in space where single molecules are transformed into complex molecules produces a wide variety of organic compounds (e.g., carbon cluster (fullerenes and graphenes)/prebiotic sugar complexes). For their astrobiological implications, it opens up an aromatic based biogenic chemistry that is available to the parent of PAHs or fullerenes in the interstellar environments.

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Physical Chemistry Chemical Physics, 23, 1424, 2021

https://pubs.rsc.org/en/content/articlelanding/2021/CP/D0CP04366D#!divAbstract

IR photofragmentation of the phenyl cation: spectroscopy and fragmentation pathways

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We present the gas-phase infrared spectra of the phenyl cation, phenylium, in its perprotio ($C_6H_5^+$) and perdeutero ($C_6D_5^+$) forms, in the 260–1925 cm^{-1} (5.2–38 μm) spectral range, and investigate the observed photofragmentation. The spectral and fragmentation data were obtained using Infrared Multiple Photon Dissociation (IRMPD) spectroscopy within a Fourier Transform Ion Cyclotron Resonance Mass Spectrometer (FTICR MS) located inside the cavity of the free electron laser FELICE (Free Electron Laser for Intra-Cavity Experiments). The $^1A_1$ singlet nature of the phenylium ion is ascertained by comparison of the observed IR spectrum with DFT calculations, using both harmonic and anharmonic frequency calculations. To investigate the observed loss of predominantly [2C,nH] (n = 2–4) fragments, we explored the potential energy surface (PES) to unravel possible isomerization and fragmentation reaction pathways. The lowest energy pathways toward fragmentation include direct H elimination, and a combination of facile ring-opening mechanisms ($\leq$2.4 eV), followed by elimination of H or CCH_2. Energetically, all H-loss channels found are more easily accessible than CCH_2-loss. Calculations of the vibrational density of states for the various intermediates show that at high internal energies, ring opening is the thermodynamically the most advantageous, eliminating direct H-loss as a competing process. The observed loss of primarily [2C,2H] can be explained through entropy calculations that show favored loss of [2C,2H] at higher internal energies.

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Extended Red Emission: Observational Constraints For Models

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Extended Red Emission (ERE) is a widely observed optical emission process, present in a wide range of circumstellar and interstellar environments in the Milky Way galaxy as well as other galaxies. Definitive identifications of the ERE carriers and the ERE process are still a matter of debate. Numerous models have been proposed in recent decades, often developed without consideration of the growing body of observational constraints, which by now invalidate many of these models. This review focuses on the most well-established observational constraints which should help to delineate the way toward a generally accepted explanation of the ERE and an understanding of its place in the radiation physics of the interstellar medium.

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Astrophysics and Space Science. 365, 58 (2020)

https://arxiv.org/pdf/2003.06453.pdf
https://link.springer.com/article/10.1007/s10509-020-03766-w

Production of PAH cations with narrow internal energy distribution using single nanosecond pulsed laser

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The internal energy dynamics of three examples of PAHs are probed using a high resolution energy time of flight spectrometer. The measured H-loss rates are converted to internal energy values fora range of UV photon wavelengths. Multi step multi photon absorption scheme is proposed to estimate the possible internal energy values with reasonable accuracies. This was possible because of the ultrafast radiationless internal conversion process in PAHs and their structural rigidity. Thus, a method is proposed to produce PAH cations with narrow and known internal energy distribution using a single nanosecond pulsed laser, paving a way to study statistical unimolecular decay in PAHs very efficiently.

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The European Physical Journal D, 74, 217, 2020

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Isomerization and dehydrogenation of highly vibrationally excited azulene$^+$ produced via S_2 vibrational manifold

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High resolution energy-ToF correlation spectrometer and a nanosecond laser is employed to extract H loss rate in hot azulene cations in UV region. Correlation between the photon wavelength and H-loss rate is obtained for 3-photon process and it is explained by a two-step mechanism: (i) 1 + 1 ionization with ultrafast internal conversion to the long-lived S_2 state (ii) the increase of internal energy by absorption of the third photon and isomerization. The work uncovers the role of S_2 state dynamics in azulene in controlling the internal energy to a very narrow range.

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Role of Polycyclic Aromatic Hydrocarbons on the Cosmic-Ray ionization rate in the Galaxy

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The cosmic-ray ionization rate (ζ, s^{-16}) plays an important role in the interstellar medium. It controls ion-molecular chemistry and provides a source of heating. Here we perform a grid of calculations using the spectral synthesis code CLOUDY along nine sightlines towards, HD 169454, HD 110432, HD 204827, λ Cep, X Per, HD 73882, HD 154368, Cyg OB2 5, Cyg OB2 12. The value of ζ is determined by matching the observed column densities of H_3^+ and H_2. The presence of polycyclic aromatic hydrocarbons (PAHs) affects the free electron density, which changes the H_3^+ density and the derived ionization rate. PAHs are ubiquitous in the Galaxy, but there are also regions where PAHs do not exist. Hence, we consider clouds with a range of PAH abundances and show their effects on the H_3^+ abundance. We predict an average cosmic-ray ionization rate for H_2 ($\zeta(H_2)$)= (7.88 $\pm$ 2.89) $\times$ 10^{-16} s^{-1} for models with average Galactic PAHs abundances, (PAH/H =$10^{-6.25}$), except Cyg OB2 5 and Cyg OB2 12. The value of ζ is nearly 1 dex smaller for sightlines toward Cyg OB2 12. We estimate the average value of $\zeta(H_2)$= (95.69 $\pm$ 46.56) $\times$ 10^{-16} s^{-1} for models without PAHs.

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Observational Constraints on the Physical Properties of Interstellar Dust in the Post-Planck Era

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We present a synthesis of the astronomical observations constraining the wavelength-dependent extinction, emission, and polarization from interstellar dust from UV to microwave wavelengths on diffuse Galactic sightlines. Representative solid phase abundances for those sightlines are also derived. Given the sensitive new observations of polarized dust emission provided by the *Planck* satellite, we place particular emphasis on dust polarimetry, including continuum polarized extinction, polarization in the carbonaceous and silicate spectroscopic features, the wavelength-dependent polarization fraction of the dust emission, and the connection between optical polarized extinction and far-infrared polarized emission. Together, these constitute a set of constraints that should be reproduced by models of dust in the diffuse interstellar medium.

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The Astrophysical Journal, 906, 73, 2021

https://ui.adsabs.harvard.edu/abs/2021ApJ...906...73H

Regulating Star Formation in Nearby Dusty Galaxies: Low Photoelectric Efficiencies in the Most Compact Systems

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Star formation in galaxies is regulated by the heating and cooling in the interstellar medium (ISM). In particular, the processing of molecular gas into stars will depend strongly on the ratio of gas heating to gas cooling in the neutral gas around sites of recent star-formation. In this work, we combine mid-infrared (mid-IR) observations of polycyclic aromatic hydrocarbons (PAHs), the dominant heating mechanism of gas in the ISM, with [C II], [O I], and [Si II] fine-structure emission, the strongest cooling channels in dense, neutral gas. The ratio of IR cooling line emission to PAH emission measures the photoelectric efficiency, a property of the ISM which dictates how much energy carried by ultraviolet photons gets transferred into the gas. We find that star-forming, IR-luminous galaxies in the Great Observatories All-Sky LIRG Survey (GOALS) with high IR surface densities have low photoelectric efficiencies. These systems also have, on average, higher ratios of radiation field strength to gas densities, and larger average dust grain size distributions. The data support a scenario in which the most compact galaxies have more young star-forming regions per unit area that exhibit less efficient gas heating. These conditions may be more common at high z, and may help explain the higher star-formation rates at cosmic noon. We make predictions on how this can be investigated with the James Webb Space Telescope.

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A Method to Extract Spatially Resolved Polycyclic Aromatic Hydrocarbon Emission from Spitzer Spectra: Application to M51

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The mid-infrared spectrum contains rich diagnostics to probe the physical properties of galaxies, among which the pervasive emission features from polycyclic aromatic hydrocarbons (PAHs) offer a promising means of estimating the star formation rate (SFR) relatively immune from dust extinction. This paper investigates the effectiveness of PAH emission as a SFR indicator on sub-kpc scales by studying the Spitzer/IRS mapping-mode observations of the nearby grand-design spiral galaxy M51. We present a new approach of analyzing the spatial elements of the spectral datacube that simultaneously maximizes spatial resolution and spatial coverage, while yielding reliable measurements of the total, integrated 5–20 μm PAH emission. We devise a strategy of extracting robust PAH emission using spectra with only partial spectral coverage, complementing missing spectral regions with properly combined mid-infrared photometry. We find that in M51 the PAH emission correlates tightly with the extinction-corrected far-ultraviolet, near-ultraviolet, and Hα emission, from scales $\sim$ 0.4 kpc close to the nucleus to 6 kpc out in the disk of the galaxy, indicating that PAH serves as an excellent tracer of SFR over a wide range of galactic environments. But regional differences exist. Close to the active nucleus of M51 the 6.2 μm feature is weaker, and the overall level of PAH emission is suppressed. The spiral arms and the central star-forming region of the galaxy emit stronger 7.7 and 8.6 μm PAH features than the inter-arm regions.

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https://ui.adsabs.harvard.edu/abs/2021AJ....161...29Z

Lyman-α irradiation of superhydrogenated coronene films: implications for H_2 formation

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We present the results of an experimental study of the interaction of Ly-α photons with superhydrogenated coronene films. The effects of UV irradiation have been analyzed with infrared spectroscopy. The spectral changes provide evidence for UV photodestruction of the C-D bonds of the superhydrogenated coronene with a cross-section of $8 \pm 2 \times 10^{-20}$ cm^2. The comparison of our experimental result with the prediction from theoretical modeling suggests an extension of the region inside PDRs where superhydrogenated coronene can survive and contribute to H_2 formation. H_2 formation through abstraction in superhydrogenated coronene dominates over direct H_2 loss induced by UV photodestruction.

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An investigation of spectral line stacking techniques and application to the detection of $HC_{11}N$

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As the inventory of interstellar molecules continues to grow, the gulf between small species, whose individual rotational lines can be observed with radio telescopes, and large ones, such as polycyclic aromatic hydrocarbons best studied in bulk via infrared and optical observations, is slowly being bridged. Understanding the connection between these two molecular reservoirs is critical to understanding the interstellar carbon cycle, but will require pushing the boundaries of how far we can probe molecular complexity while still retaining observational specificity. Towards this end, we present a method for detecting and characterizing new molecular species in single-dish observations towards sources with sparse line spectra. We have applied this method to data from the ongoing GOTHAM (GBT Observations of TMC-1: Hunting Aromatic Molecules) Green Bank Telescope large programme, discovering six new interstellar species. Here we highlight the detection of $HC_{11}N$, the largest cyanopolyyne in the interstellar medium.

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Nature Astronomy, 5, 188–196, 2021

https://www.nature.com/articles/s41550-020-01261-4

Ph.D. Position in Astrochemistry

Advertised by: Prof. Els Peeters

A Ph.D. position in computational astrochemistry is available at Western University (Canada) with a nominal starting date of September 2021, under the joint supervision of Prof. Viktor N. Staroverov (Department of Chemistry) and Profs. Jan Cami and Els Peeters (Department of Physics & Astronomy).

Project description: The Universe is aglow with the infrared emission of large carbonaceous molecules such as polycyclic aromatic hydrocarbons (PAHs) and fullerenes. Their emission encodes a large amount of information about the physical and chemical environments in which they reside and is a powerful messenger which can be used to study large-scale astrophysical processes such as star and planet formation, as well as galaxy evolution. The interpretation of these astronomical observations requires theoretically generated PAH spectra in conjunction with astronomical models of PAH evolution. This is particularly important and timely, given that the world is eagerly awaiting the launch of the James Webb Space Telescope (JWST) in October 2021. Hailed as the bigger and vastly more sensitive successor to the Hubble Space Telescope, JWST will allow researchers to process and analyze observations of unprecedented quality in order to study the Universe both near and far. Many JWST observations will be dominated by this emission due to large molecules. The goal of this project is to devise and carry out systematic theoretical simulations of PAH spectra relevant to the interpretation of JWST observations of diverse astronomical objects.

Requirements: A M.Sc. degree or equivalent in Chemistry, Astronomy, Astrophysics, or related fields, with a background in computational chemistry and/or quantum physics, and demonstrated experience in scientific programming.

Contact: Interested candidates are encouraged to contact Prof. Els Peeters as soon as practical for more information regarding the application process.

E-mail for contact: epeeters@uwo.ca

Deadline for Application: position will remain open until filled.

CNES PhD position
Methane cycle: from *Cassini* observations to *Dragonfly* exploration

Groupe de Spectrometrie Moléculaire et Atmosphérique
Reims, France

Advertised by Dr. Pascal Rannou

Duration: 36 months
Education level: Masters Degree MA/MS/Msc

Motivation and objectives: The main motivation of this work is to significantly improve the Institut Pierre-Simon Laplace (IPSL) Titan Global Climate Model (GCM) in order to better understand Cassini and Huygens results, but also to better characterise the expected climate in Dragonfly's landing region. The goal of this thesis is to implement the IPSL GCM with missing processes. Some, like the cloud microphysics, are partly ready for implementation and need to be completed, and other still need to be developed like the interaction between surface, atmosphere and liquid bodies. Once this development is done, the purpose of the project is to explore the different processes characterizing the methane cycle in the troposphere and all interactions with the surface of Titan. This will allow, at the end, to interpret the observed structures (distribution and composition of lakes, equatorial dunes, seasonal cycle, clouds and precipitation) and make prediction for Dragonfly.

Proposed schedule:
- *1st year*: Technical developments to introduce all the missing processes.
- *2nd year*: Definition of simulations of interest and related boundary conditions. Simulations and tests of several parameters. Comparison with observations and with other GCMs.
- *3rd year*: Exploration of new scientific questions such as the distribution of clouds and equinox precipitation, their link with dunes, surface winds, conditions around the polar lakes and the formation of evaporites.

Deadline: April 2, 2021

For more information and to apply: follow **this link**

Contact: pascal.rannou@univ-reims.fr

Postdoctoral Researcher in Solar System Science

Southwest Research Institute
Boulder, Colorado

Advertised by Dr. Silvia Protopapa

Objectives of this Role: Analysis of ground- and space-based data of Pluto to quantify the spatial distribution and long-term evolution of Pluto's ices; the main goal is to further understand the mechanisms of interaction between Pluto's surface and its atmosphere. Be involved in the development of an optical constants database for quantitative spectral analysis of small bodies in the Solar System; this will be achieved through the synergy between laboratory measurements and computational analysis.

Daily and Monthly Responsibilities: Radiative transfer model of Pluto's spectroscopic measurements acquired from ground (e.g., IRTF) and space (New Horizons). Laboratory measurements of small bodies analog materials and software development to compute optical constants. Meet weekly with the project team/lead to discuss progress and develop project pathways. Assist with scientific publications, presentations at scientific meetings, PDS archiving, proposal writing to secure observing time and/or funding.

Deadline: Wednesday, February 24, 2021

Applications via: https://resapp.swri.org/ResApp/Job_Details.aspx?JOB_CD=15-01487

Email for Contact: silvia.protopapa@swri.org

AstroPAH Newsletter

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

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Submission deadline: 5 March 2021