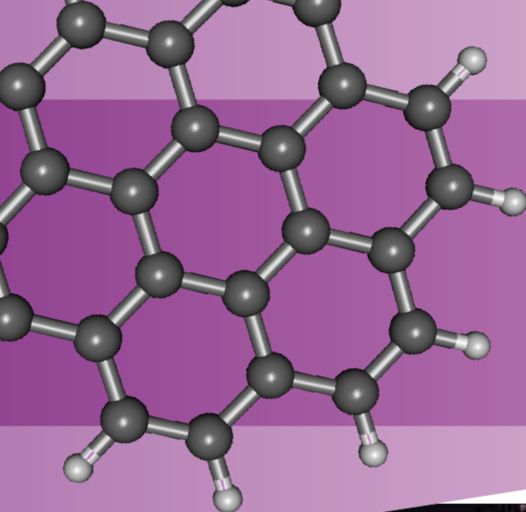
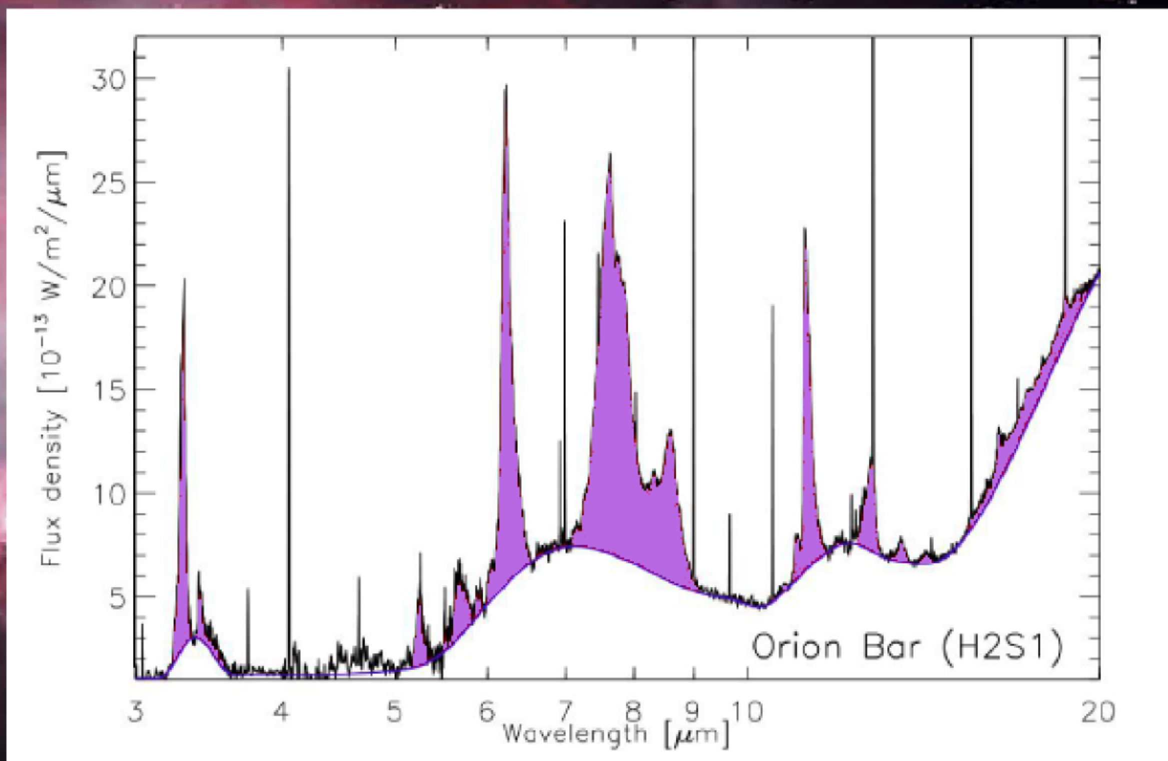


AstroPAH

A Newsletter on Astronomical PAHs

Issue 34 | December 2016

The Spectrum



Editorial

Dear Colleagues,

Welcome to the last AstroPAH of 2016! Our cover features the PAH emission bands in the Orion star-forming region as seen by the Infrared Space Observatory (ISO). This spectrum is one of the most significant legacy of ISO on astronomical PAHs, and with the JWST so close to be launched, one may wonder which spectrum will take its place in the post-JWST era

At the beginning of November a workshop took place in the Netherlands to delineate the future of astronomical PAH research with a major focus on the JWST capabilities. You can find a summary of the workshop together with a call to subscribe to news updates on the PAH-JWST science consortium in our *In Focus* section.

As a nice wrap up of the research year, this month you can read about many different topics: PAH charge in reflection nebulae, irradiation on aliphatic PAHs and interstellar dust analogs, fullerenes in circumstellar envelopes, molecular emission in dusty bubbles, PAHs as catalyzing surfaces for noble gas molecules and spectroscopy of radical hydrocarbons as potential DIBs carriers.

Also check out the 1st Faraday Joint Interest Group Conference in our *Announcement* section.

AstroPAH takes a well deserved holiday break in January, but you can send us your contributions anytime as usual. The next AstroPAH will be published in February 2017.

We would like to thank you for the amazing contributions we received during the year and wish you a very productive and happy 2017.

The Editorial Team

Next issue: 21 February 2017.
Submission deadline: 7 February 2017.

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Contents

PAH Picture of the Month

The rich spectrum of the PAH emission bands in the Orion Bar region (adapted) as seen by the Infrared Space Observatory (ISO, on the left). Background image: The Orion Nebula nebula (M42).

Credits: E. Peeters (Spectrum); Copyright ©2006 by Daniel McCauley, Website (Background).

Newsletter Design: Isabel Aleman
Background image: NASA, ESA, and the Hubble Heritage Team (STScI/AURA)

The Past and Future of AstroPAH Research Workshop Summary

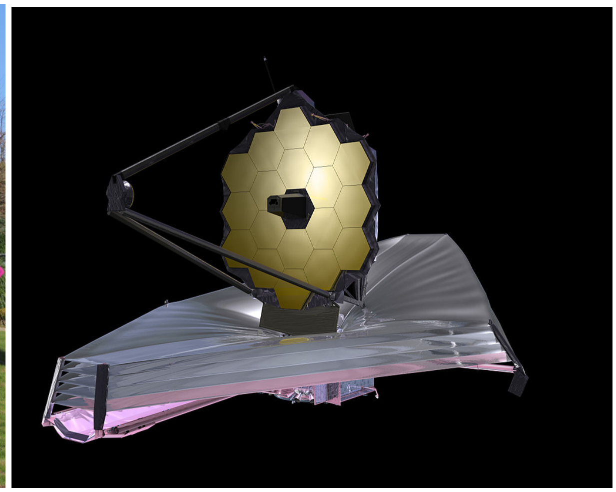
by
Annemieke Petrignani
Alessandra Candian
Els Peeters

Spurred by the imminent launch of the James Webb Space Telescope (JWST) and its immense potential to push Astronomical Polycyclic Aromatic Hydrocarbon (AstroPAH) research to the next level, "The Past and Future of AstroPAH Research" workshop was held in Noordwijk, The Netherlands from October 30 to November 4, 2016. The aim of the workshop was to assess the state-of-the-art research and key questions of today and evaluate the advances made since the successful PAH workshop in 2013. Additionally, the aim was to chart the future of astronomical PAH research with a major focus on the potential contributions of JWST to PAH research. Indeed, JWST will revolutionize the PAH research field ... but only if we prepare well! Last but not least, the aim was to foster the existing international and interdisciplinary collaborations and also to form possible new collaborations.

The workshop was very successful and brought together experts from fields involved in observational, theoretical, and experimental research on PAH research in astronomy and chemistry. A total of 60 people from 13 different countries all over the world participated in the workshop. There were 25 invited and 20 contributed talks, 8 contributed posters, and 6 discussion sessions covering the multidisciplinary aspects of the field and PAH research with JWST. You can find the detailed program, abstracts, talks, and photos on the workshop website.

The workshop science program started on Monday with three review talks on astroPAH research, followed by a session solely dedicated to JWST highlighting the telescope, the science themes, instruments, time lines, and proposal categories. The day ended with a fruitful discussion on the opportunities of PAH research with JWST during the Q&A session and, in a more informal setting, during the poster session. The following days, sessions were focused on "PAH emission features in space", "PAH Spectroscopy and the Search for Signatures", "Formation and Processing of PAHs", and "Relationship between PAHs and Fullerenes". During these days, the observational, theoretical, and experimental state-of-the-art research and the key questions of

AstroPAH research were highlighted as each day ended with a discussion session on the respective topics. The workshop further provided an all included and dedicated environment to facilitate informal discussions during coffee breaks, breakfasts, lunches, and dinners. It ended on Friday with two overarching discussion sessions, one to address the key questions for all AstroPAH research and one to address the key questions for AstroPAH research with JWST. The focus on JWST is meant to best prepare for the upcoming calls for proposals for JWST and fully exploit the capabilities of JWST, making sure all important (PAH) science will be done by JWST and that it is done well. If you're interested to be kept in the loop about the cycle 1 JWST-ERS proposal round, please keep on reading and sign up!



The James Webb Space Telescope

The James Webb Space Telescope (JWST) is a large infrared (IR) space observatory with a primary mirror of 6.5 meter diameter. It is an international collaboration of 17 countries led by NASA, with significant contributions of the European Space Agency (ESA) and Canadian Space Agency (CSA). The telescope is scheduled to be launched in October 2018. After a commissioning of 6 months, scientific observations are expected to start in April 2019. The scientific mission is focused on four science themes: ”First Light and Reionization”, ”Assembly of Galaxies”, ”Birth of Stars and Protoplanetary Systems”, and ”Planets and the Origins of Life”.

JWST has an impressive instruments suite: the Near-Infrared Camera (NIRCAM), the Near-Infrared Spectrograph (NIRSpec), the Mid-Infrared Instrument (MIRI) and the Fine Guidance Sensor / Near Infrared Imager and Slitless Spectrograph (FGS/NIRISS). Together, these instruments cover the full wavelength range from 0.6 to 28.8 μm with an improvement on sensitivity of a factor $\sim$100 and on resolution of a factor $\sim$ 10 with respect to previous instruments. This offers a unique opportunity and completely novel approaches to key astronomical questions, including those related to PAH research (see below). Indeed, the wavelength range is well matched with that of the PAH features, its sensitivity and spectral resolution allow for detailed studies of the spectral variability in the band profiles and the relative intensities of the PAH bands, including the weaker bands. Combined with the superb spatial resolution, this allows for the full exploration of the interplay between the PAH population and the local physical conditions. Clearly, JWST is made for PAH research and PAH research is made for JWST (even the primary mirror has the shape of a PAH molecule).

Key Questions in Astronomical PAH Research

The particpants highlighted key questions for each of the discussion sessions: "PAH emission features in space", "PAH Spectroscopy and the Search for Signatures", "Formation and Processing of PAHs", "Relationship between PAHs and Fullerenes", "Open key science questions on PAHs", and topped it with key questions to "step into the Future with JWST". We collected all formulated key questions and summarized them here into overarching key questions.

Is the **Holy grail** within reach?

Will we be able to identify individual PAHs with JWST or otherwise? If the Diffuse Interstellar Bands (DIBs) are linked to PAHs, this may lead to identification. JWST enables observations of the near infrared DIBs in conjunction with the aromatic infrared emission bands (AIBs). These observations allow for possible correlation studies, which will, together with laboratory and theoretical studies of the electronic spectra, bring us closer to the holy grail.

What is the **Inventory** of interstellar hydrocarbons?

Given the anticipated groundbreaking observations, it will become possible, together with laboratory and theoretical studies, to extract any possible molecule specific information embedded in the AIBs.

- What is the inventory of PAHs and related species?
  What are the mass, size, shape, and charge distributions of PAHs? What are the contributions of N/O/H-PAHs, fullerene derivatives (smaller cages, fulleranes, and metal-complexes). Observationally, deconvolution of the subcomponents of the AIBs will represent a huge step forward. At the same time, theoretical and experimental spectra of PAH species currently lacking are required. These include large PAHs, different types of charged PAHs (open/closed shell), large (cationic) clusters, N/O/H/methylated-PAHs, radical PAHs, and deuterated PAHs.
- GrandPAHs or MultiPAH?
  Are there GrandPAHs, a single end-population of a limited number of large symmetric PAHs or are there numerous PAHs of various classes?
- What is the nature of PAH clusters and Very Small Grains (VSGs)/nano-particles?
  What is the contribution of the different types of clusters, such as cationic PAH clusters? And what is the composition of VSGs?
- Where are PAHs and alike present and absent?
  Where are PAHs observed, are they expected, and why are they sometimes absent? PAHs are observed in astronomical objects from (low metallicity) PDRs, evolved stars, and proto planetary disks to galaxies. Are PAHs present on Earth-like planets?

What are the **signatures** of PAHs?

- The infrared: what are the (sub)components of the AIBs?
  Observationally, how do you decompose an AIB spectrum? What is the exact nature of the subcomponents (including the plateaus) and to what extent can they be deconvolved with JWST? Together with the anticipated ground-breaking JWST observations, a good theoretical and experimental understanding of anharmonicity and size/structure dependencies that affect the line profile and position as well as of the overtones and combination bands, may lead to the identification of these subcomponents.

- Beyond the infrared
  What are the electronic structures of PAHs and related species? What are the rotational spectra of N/O/H/methylated-PAHs? Can it lead to their identification?

- PAH precursors and products as identifiers of PAH subclasses
  Are there specific precursors and products of PAHs related to specific PAH classes? If so, these can guide future observational studies using JWST in combination with e.g. submm- and radio instruments.

What is the **Entanglement** of PAHs in the cosmic carbon chemistry network?

- How are PAHs formed?
  What are the circumstellar and interstellar formation processes? Top-down or bottom-up? Are free-flying grains precursors of PAHs?

- How do PAHs evolve?
  What are the isomerisation and fragmentation rates and patterns upon UV photolysis for PAHs and alike, such as large PAHs, PAH clusters, VSGs, neutrals, ions, deuterated PAHs, fullerenes. What is the UV photolysis and processing of PAHs in ices? How do PAHs coagulate and form VSG/dust? Can we learn from the far-IR dust/mid-IR PAH ratios?

- What is variation in chemistry of PAHs?
  What chemistry occurs in which regions? What are the different mechanisms involved, such as dissociation, collision, electron recombination, and competition between relaxation channels? What are the different species involved, including radicals and silicates.

What is the extent of the **Probing powers** of PAHs?

- Quantitative relationships between PAHs and the local conditions
  JWST observations can extend empirical relationships between PAHs and the local physical conditions. Taking this to the next level requires laboratory and theoretical studies of temperature dependency and of the kinetic parameters involved in photolysis, fragmentation, and collision. This data serves as critical input for astronomical PAH models.

- PAHs and the star formation rate (SFR)
  JWST has the potential to extend the SFR probing power of PAHs through a better understanding of their dependence on e.g. metallicity and radiation hardness.

- What can we learn from the isotopic fractionation?
  Deuterated PAHs may shed light of the D/H ratio (the first PAHs) and the ^{13}C-PAHs on the $^{13}C/^{12}C$ ratio.

JWST proposals & PAH research

JWST will have yearly call for proposals (and thus proposal cycles) and has three different types of observer programs:

- the Guaranteed Time Observers program (GTO): A total of 4020 hours are allocated over first 30 months (i.e. Cycles 1 through 3) to e.g. the different instrument teams.
- the General Observers program (GO): this program is accessibility to the entire astronomical community and corresponds to ∼80% of the total observing hours in Cycles 1 to 5.
- the Director's Discretionary Time programs (DDT): A total of up to 10% per cycle (i.e. ≤877 hours) is allocated to rapid response observations and targeted science programs, such as the Early Release Science program (ERS).

The ERS program is unique to JWST and aims to "accelerate the diffusion of JWST know-how, expand early opportunities for the community to gain experience with JWST data and scientific analysis" and to demonstrate the science capabilities of JWST. Hence, it is designed to help with the preparation of Cycle 2 GO proposals, which will be submitted seven months after end of commissioning – at a time when the general community would have very limited access to JWST data in the absence of the ERS program. Data taken in the ERS program will become immediately public to the community. Consequently, the selection criteria for ERS proposals are distinct from those for GO proposals and will be selected spanning the science themes of JWST. Projects are expected to i) provide representative data of broad interest to researchers in major astrophysical sub-disciplines, ii) provide products to the community to observe effectively with JWST and to analyze the data, and iii) represent a range in expertise and demographics. A total of ∼ 500 hours is available for ERS, allocated to up to 15 teams. The first (open) calls for proposals are **August 18, 2017 for ERS proposals** and **November 30, 2017 for GO cycle 1 proposals.**

Clearly, many of the key questions addressed above are ideally suited for the GO program. Of these, the following questions/topics were mentioned for a PAH/ISM ERS program: PAHs and Carbon Inventory, PAHs as precursors of the building blocks of life, Impact of PAHs on COM formation in interstellar chemistry, Effect of PAHs on Physical Parameters, Tools for astronomical community, Chemical Composition of PAHs, PAH evolution, Signatures of precursors of PAHs, Signatures of products of PAHs, and Broadening mechanisms. To increase the success rate of the ERS program, those most attractive to a broader community and best aligned with the four JWST science themes will be further pursued. To appeal to a broad community, the PAH ERS effort has been merged with a similar PDR ERS effort into "the infrared ISM" ERS to best adhere to the guidelines and requirements. In addition, several PAH researchers who attended the workshop, are also involved in the ERS team on evolved stars that includes PAH research in its science goals. If you're interested to be kept informed on these ERS programs, please visit the ISM team website for the ISM ERS program or contact Jeronimo Bernard-Salas for the evolved stars ERS program. Those who signed up at the PAH workshop do not need to express interest again for the ISM ERS program but need to do so, if interested, for the evolved stars ERS program. More information will come when the call for proposals is released in January.

Acknowledgments

The authors would like to thank Pierre Ferruit, Karl Gordon, Karl Misselt, and Alain Abergel for their insight on JWST and JWST science, Xander Tielens for his advisory role, the Local Organising Committee (Wim Roeterdink, Cameron Mackie, Matt Shannon, Collin Knight, Sandra Wiersma) for their hard work, and all participants for turning this workshop into a great success.

AstroPAH Workshop Details

A detailed program, photos, abstracts, and online talks can be found on the workshop website.
Your talk missing? Please send your talk to the workshop organisers.

Do you want to stay informed about the ISM-ERS? Sign up here.

CO observations and investigation of triggered star formation towards N10 infrared bubble and surroundings

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We studied the environment of the dust bubble N10 in molecular emission. Infrared bubbles, first detected by the GLIMPSE survey at 8.0 µm, are ideal regions to investigate the effect of the expansion of the HII region on its surroundings and the eventual triggered star formation at its borders. In this work, we present a multi-wavelength study of N10. This bubble is especially interesting as infrared studies of the young stellar content suggest a scenario of ongoing star formation, possibly triggered on the edge of the HII region. We carried out observations of ^{12}CO(1-0) and ^{13}CO(1-0) emission at PMO 13.7 m towards N10. We also analyzed the IR and sub-millimeter emission on this region and compare those different tracers to obtain a detailed view of the interaction between the expanding HII region and the molecular gas. We also estimated the parameters of the denser cold dust condensation and of the ionized gas inside the shell. Bright CO emission was detected and two molecular clumps were identified from which we have derived physical parameters. We also estimate the parameters for the densest cold dust condensation and for the ionized gas inside the shell. The comparison between the dynamical age of this region and the fragmentation timescale favors the "Radiation-Driven Implosion" mechanism of star formation. N10 is a case of particular interest with gas structures in a narrow frontier between HII region and surrounding molecular material, and with a range of ages of YSOs situated in region, indicating triggered star formation.

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http://iopscience.iop.org/article/10.3847/0004-637X/830/2/57/pdf

Photo-stability of super-hydrogenated PAHs determined by action spectroscopy experiments

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We have investigated the photo-stability of pristine and super-hydrogenated pyrene cations ($C_{16}H^{+}_{10+m}, m = 0, 6, \text{ or } 16$) by means of gas-phase action spectroscopy. Optical absorption spectra and photo-induced dissociation mass spectra are presented. By measuring the yield of mass-selected photo-fragment ions as a function of laser pulse intensity, the number of photons (and hence the energy) needed for fragmentation of the carbon backbone was determined. Backbone fragmentation of pristine pyrene ions ($C_{16}H^{+}_{10}$) requires absorption of three photons of energy just below 3 eV, whereas super-hydrogenated hexahydropyrene ($C_{16}H^{+}_{16}$) must absorb two such photons and fully hydrogenated hexadecahydropyrene ($C_{16}H^{+}_{26}$) only a single photon. These results are consistent with previously reported dissociation energies for these ions. Our experiments clearly demonstrate that the increased heat capacity from the additional hydrogen atoms does not compensate for the weakening of the carbon backbone when pyrene is hydrogenated. In photodissociation regions, super-hydrogenated Polycyclic Aromatic Hydrocarbons (PAHs) have been proposed to serve as catalysts for H_2 formation. Our results indicate that carbon backbone fragmentation may be a serious competitor to H_2 formation at least for small hydrogenated PAHs like pyrene.

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Astrophys. J. 832, 24 (2016)

http://dx.doi.org/10.3847/0004-637X/832/1/24

The Formation of Potential Interstellar Noble Gas Molecules in Gas and Adsorbed Phases

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The discovery of naturally-occurring ArH^{+} in various regions of the interstellar medium (ISM) has shown the need for more understanding of the reactions that lead to covalently-bonded noble gas molecules. The test comes with trying to predict the formation of other small noble gas molecules. Many molecules have been observed in various interstellar environments which possess the possibility of bonding with noble gases. This work explores how both argon and neon can form bonds to ligands made of these species through quantum chemical computations. Argon and neon are chosen since they are among the most abundant atoms in the universe but are more polarizable than the more common but smaller helium atom. Reactions leading to noble gas molecules are modeled in the gas phase as well as through the adsorbed phase by catalysis with a polycyclic aromatic hydrocarbon (PAH) surface. The adsorption energy of the neutral noble gas atoms to the surface increases as the size of the PAH also increases, but this is still less than 10 kcal/mol. It is proposed and supported herein that an incoming molecule can bond with the noble gas atom adsorbed onto the PAH, form a stable structure, and have the PAH function as the leaving group. This work shows that the noble gas molecules $ArCCH^+$, $ArOH^+$, $ArNH^+$, and $NeCCH^+$ are not only stable minima on their respective potential energy surfaces but can also be formed in either the gas phase or through PAH adsorption with known or hypothesized interstellar molecules. Most notably, $NeCCH^+$ does not appear to form in the gas phase, but could be catalyzed on PAH surfaces. Hence, the interstellar detection of such molecules could also serve as a probe for the observation of interstellar PAHs.

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ACS Omega, 1, 765 (2016)

http://pubs.acs.org/doi/abs/10.1021/acsomega.6b00249

The Charge State of Polycyclic Aromatic Hydrocarbons Across Reflection Nebulae: PAH Charge Balance and Calibration

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Low-resolution Spitzer spectral map data (>1700 spectra) of ten reflection nebulae (RNe) fields are analyzed using the data and tools available through the NASA Ames PAH IR Spectroscopic Database. The PAH emission is broken down into PAH charge state using a database fitting approach. Here, the physics of the PAH emission process is taken into account and uses target appropriate parameters, e.g., a stellar radiation model for the exciting star. The breakdown results are combined with results derived using the traditional PAH band strength approach, which interprets particular PAH band strength ratios as proxies for the PAH charge state, e.g., the 6.2/11.2 µm PAH band strength ratio. These are successfully calibrated against their database equivalent; the PAH ionized fraction (f_i). The PAH ionized fraction is converted into the PAH ionization parameter, which relates the PAH ionized fraction to the strength of the radiation field, gas temperature and electron density. The behavior of the 12.7 µm PAH band is evaluated as a tracer for PAH ionization and erosion. The plot of the 8.6 versus 11.2 µm PAH band strength for the northwest photo-dominated region (PDR) in NGC 7023 is shown to be a robust diagnostic template for the PAH ionized fraction. Remarkably, most of the other RNe fall within the limits set by NGC 7023. Finally, PAH spectroscopic templates are constructed and verified as principal components. Template spectra derived from NGC 7023 and NGC 2023 compare extremely well with each other, with those derived for NGC 7023 successfully reproducing the PAH emission observed from NGC 2023.

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High energy electron irradiation of interstellar carbonaceous dust analogs: Cosmic ray effects on the carriers of the 3.4 µm absorption band

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The effects of cosmic rays on the carriers of the interstellar 3.4 µm absorption band have been investigated in the laboratory. This band is attributed to stretching vibrations of CH_3 and CH_2 in carbonaceous dust. It is widely observed in the diffuse interstellar medium (ISM), but disappears in dense clouds. Destruction of CH_3 and CH_2 by cosmic rays could become relevant in dense clouds, shielded from the external ultraviolet field. For the simulations, samples of hydrogenated amorphous carbon (a-C:H) have been irradiated with 5 keV electrons. The decay of the band intensity vs electron fluence reflects a-C:H dehydrogenation, which is well described by a model assuming that H_2 molecules, formed by the recombination of H atoms liberated through CH bond breaking, diffuse out of the sample. The CH bond destruction rates derived from the present experiments are in good accordance with those from previous ion irradiation experiments of HAC. The experimental simplicity of electron bombardment has allowed the use of higher energy doses than in the ion experiments. The effects of cosmic rays on the aliphatic components of cosmic dust are found to be small. The estimated cosmic ray destruction times for the 3.4 µm band carriers lie in the 10^8 yr range and cannot account for the disappearance of this band in dense clouds, which have characteristic lifetimes of 3×10^7 yr. The results invite a more detailed investigation of the mechanisms of CH bond formation and breaking in the intermediate region between diffuse and dense clouds.

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http://dx.doi.org/10.3847/0004-637X/831/1/51

Fullerenes and fulleranes in circumstellar envelopes

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Three decades of search have recently led to convincing discoveries of cosmic fullerenes. The presence of C_{60} and C_{60}^+ in both circumstellar and interstellar environments suggests that these molecules and their derivatives can be efficiently formed in circumstellar envelopes and survive in harsh conditions. Detailed analysis of the infrared bands from fullerenes and their connections with the local properties can provide valuable information on the physical conditions and chemical processes that occurred in the late stages of stellar evolution. The identification of C_{60}^+ as the carrier of four diffuse interstellar bands (DIBs) suggests that fullerene-related

compounds are abundant in interstellar space and are essential for resolving the DIB mystery. Experiments have revealed a high hydrogenation rate when C_{60} is exposed to atomic hydrogen, motivating the attempt to search for cosmic fulleranes. In this paper, we present a short review of current knowledge of cosmic fullerenes and fulleranes and briefly discuss the implications on circumstellar chemistry.

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Journal of Physics: Conference Series, Volume 728, Issue 5, (2016)

http://iopscience.iop.org/article/10.1088/1742-6596/728/5/052004/meta

Visible absorptions of potential diffuse ISM hydrocarbons: C_9H_9 and C_9H_5 radicals

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The laboratory detection of previously unobserved resonance-stabilized C_9H_5 and C_9H_9 radicals in the supersonic expansion of a hydrocarbon discharge source is reported. The radicals are tentatively assigned as acetylenic-substituted cyclopentadienyl C_9H_5 and vinyl-substituted benzyl C_9H_9 species. They are found to feature visible absorption bands that coincide with a few very weak diffuse interstellar bands toward HD183143 and HD204827.

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https://arxiv.org/abs/1610.07318

Announcements

1st Faraday Joint Interest Group Conference 2017

11-13 April, 2017 at the University of Warwick, Coventry, UK

Showcasing UK Physical Chemistry

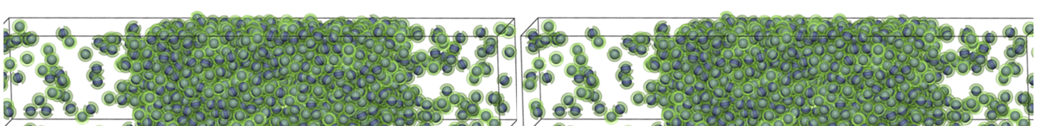
Organising Committee
Dr. Ann Dixon (Chair)
Dr. Carlos Avendaño
Prof. Wendy Brown
Dr. Sam Eden
Prof. Felix Fernandez-Alonso
Dr. Steven Lee
Prof. Martin McCoustra
Dr. Tanja van Mourik
Dr. Jan R. R. Verlet

Plenary and Parallel Sessions hosted by RSC Faraday Division Interest Groups
Astrophysical Chemistry Group
Biophysical Chemistry Group
British Carbon Group
Neutron Scattering Group
Photochemistry Group
Spectroscopy & Dynamics Group
Statistical Mechanics & Thermodynamics Group
Theoretical Chemistry Group

- Over **70** further contributed talks will be scheduled
- Poster prizes available for postgraduate and postdoctoral researchers
- Registration fee includes two nights ensuite accommodation, meals, and conference dinner

Confirmed Speakers
Professor Chris Dobson
Professor Ifor Samuel
Professor Peter Bruce
Dr. Józef Lewandowski
Prof. Alexander Tielens
Dr. Sandra Brünken
Dr. Anthony Meijer
Prof. Achillefs Kapanidis
Prof. Tuomas Knowles
Prof. Dr. Alec Wodtke
Dr. Maria Sanz
Dr. Susan Quinn
Prof. Ian Sims
Dr. Bas van de Meerakker
Prof. David Lennon
Prof .Jeffrey Penfold
Dr Simon Titmuss
Dr Matthew Blakeley
...and more tbc

Registration Deadline: March 28, 2017
Registration fee:£240 (RSC), £275 (Non-RSC), £80 (Student)



http://www2.warwick.ac.uk/fac/sci/chemistry/news/events/faraday2017

AstroPAH Newsletter

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