

# AstropAH

A Newsletter on Astronomical PAHs

Issue 20 | July 2015



# Editorial

**Dear Colleagues,**

Welcome to release 20 of AstroPAH with a stunning Spitzer view of the Horsehead Nebula on the cover. This month we have an In Focus on the interdisciplinary meeting “Energetic Processing of Large Interstellar Molecules” held in Leiden.

Before going to our abstracts section, we would like to announce that our fellow editor, Alessandra Candian, has been awarded a prestigious VENI grant from NWO (Netherlands Organisation for Scientific Research). Congratulations Alessandra!

In our Abstracts section, you will find a diversity of paper abstracts on the discovery of a new carbon allotrope: “penta-graphene”, dust processing, the Anomalous Microwave Emission, H<sub>2</sub> formation on PAHs, variations in the 3.3 μm feature, vinyl substituted PAHs, grand-PAHs, and last but not least the exciting [laboratory confirmation of C<sub>60</sub><sup>+</sup> as the carrier of two diffuse interstellar bands](#) published last week in Nature! Jan Cami, a leading expert on fullerenes in space, has kindly provided us with the following quote on this great event:

“Twenty-one years ago, in 1994, Bernard Foing and Pascale Ehrenfreund (my MSc advisor) searched for the electronic bands of C<sub>60</sub><sup>+</sup> in the interstellar medium – and found them, in the form of two diffuse interstellar bands (DIBs) at 9577 and 9632 Å ([Foing & Ehrenfreund 1994](#)). This was no easy feat since that part of the spectrum is heavily contaminated by telluric lines. The search was inspired by laboratory measurements ([Fulara et al. 1993](#)), but there was the catch: the experimental spectra were obtained with matrix isolation spectroscopy, a technique that results in wavelength shifts and broadening of the bands compared to gas-phase measurements. However, both newly found DIBs showed consistent shifts with respect to the matrix spectra, showed similar intensity variations and band widths and profiles. Thus, [Foing & Ehrenfreund \(1994\)](#) (and later also [Foing & Ehrenfreund 1997](#)) had a good case. A cold, gas-phase spectrum was all that was needed to confirm and prove this identification beyond any reasonable doubt. This has turned out to be a very challenging enterprise – taking more than twenty years to complete – but now confirmation has come in a spectacular way, with experiments from the group of John Maier in Switzerland as described in a Nature paper authored by Ewen Campbell ([Campbell et al. 2015](#)). Note that Pascale and Bernard wrote an associated “News and Views” perspective on these experiments ([Ehrenfreund & Foing 2015](#)).

These experiments not only confirm the presence of  $C_{60}^+$  in space, but they also represent the first identification of a few DIBs. I am certainly not the only one who is very excited by the prospects for finding more DIBs related to fullerenes. Indeed, based on the DIB strengths, [Foing & Ehrenfreund \(1994\)](#) estimate that 0.3 – 0.9% of the cosmic carbon could be in the form of  $C_{60}^+$ . Even if only a fraction of these end up in fullerene compounds (e.g. with hydrogen or metals – or why not, with PAHs), that would constitute a large enough column density to be responsible for several more DIBs ([Cami 2014](#)). These are very exciting times!”

Finally, we would like to draw your attention to the third announcement for ISPAC 2015, France, in our Meetings section.

Due to the holiday break in August, we will not have an issue next month. As always, you can send us your contributions anytime. For publication in September, see the deadlines below. Would you like to see your picture as Picture of the Month, your project featured in our In Focus, or distribute your latest paper or upcoming event amongst our community, we encourage you to contact us.

Enjoy the summer!

**The Editorial Team**

**Next issue: 22 September 2015.  
Submission deadline: 11 September 2015.**

# AstroPAH Newsletter

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## PAH Picture of the Month

Spitzer view of the region surrounding the Horsehead nebula: in blue the light emitted at 3.6  $\mu\text{m}$  and in cyan (blue-green) at 4.5  $\mu\text{m}$ , both of which come mainly from hot stars. Green represents the 8  $\mu\text{m}$  light (PAHs) and red represents 24  $\mu\text{m}$  light (dust). In the inset, the Horsehead nebula as seen in visible light by the Hubble Space Telescope.

**Credits:** NASA/JPL-Caltech

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*Design by Isabel Aleman*

## Energetic Processing of Large Interstellar Molecules

by Ronnie Hoekstra, Henrik Cederquist and Xander Tielens



*Figure 1 - Meeting participants, photo taken in the inner courtyard of the Snellius building.*

On May 11-13, 2015, the first interdisciplinary meeting on **Energetic Processing of Large Interstellar Molecules** took place in Leiden at the Snellius site of the Lorentz Center. The meeting aimed at bringing together experts in the field of molecular astrophysics and specialists in molecular interaction research. With this in mind, the meeting was co-organized and co-sponsored by the XLIC (XUV/X-ray light and fast ions for ultrafast chemistry COST Action CM1204) network and the NWO Dutch Astrochemistry Network (DAN), and the Dutch Top Research School NOVA. The Lorentz center hosted the meeting at its Snellius site where Aimée Reinards organized the practical details in an excellent way.

The expert meeting aimed at overviewing the state of the art in experimental and theoretical studies on energetic processing of large molecules by ions, electrons, and photons and its implications for the evolution of astrophysically relevant molecules. The fields of expertise of the participants therefore covered molecular physics, physical chemistry, and astronomy. It included molecular physicists involved in laboratory or quantum chemical studies on the interaction of energetic ions or photons with large molecules, and astronomers involved in studies of the origin and evolution of large molecules in space. The more specific objective of the workshop was to **identify and initiate joint experimental, theoretical, and observational studies with the aim of understanding energetic processing of large molecules of astrophysical relevance, including in particular polycyclic aromatic hydrocarbons and carbon chains and fullerenes.**

To facilitate the identification of joint challenges across scientific disciplinary borders, the program started off with talks that introduced the mutual subfields to the participants, highlighting the key questions, challenges, and opportunities. These introductory talks were given by Els Peeters, Nigel Mason, and Franck Lépine. Four half-day topical sessions of 3 or 4 invited talks provided an in-depth view into the four directions of:

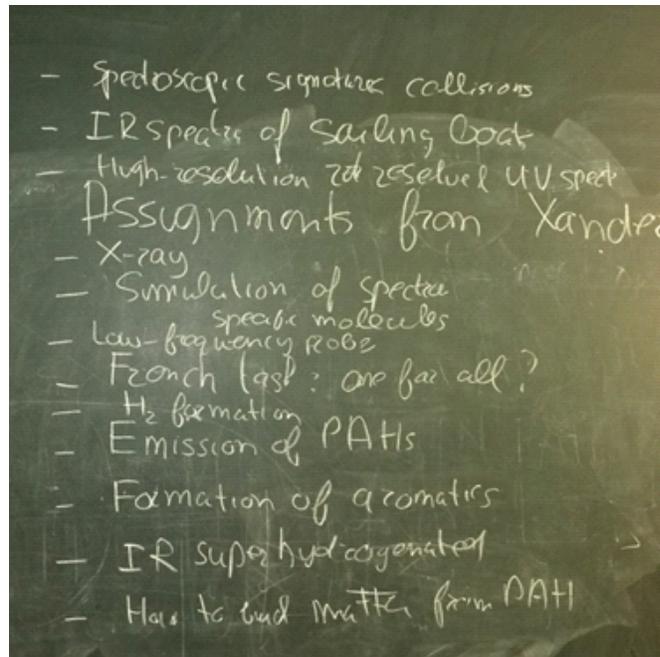
- **“Large molecules in space”** (Elisabetta Micelotta, Jan Cami and Marin Chabot),
- **“Molecular processes and structure”** (Liv Hornekær, Henning Zettergren, Stéphanie Cazaux and Yang Wang),
- **“Particle interactions”** (Paul Scheier, Thomas Schlathölter and Michael Gatchell), and
- **“Photonic interactions”** (Geert Reitsma, Christine Joblin and Jos Oomens).

**Figure 2** - List of topics from the workshop:

- Spectroscopic signature (of) collisions
- IR spectra of sailing boat
- High resolution rotationally resolved UV spectra

Assignments from Xander:

- X-ray
- Simulation of spectra for specific molecules
- Low frequency probe
- French task: one for all?
- H<sub>2</sub> formation
- Emission of PAHs
- Formation of aromatics
- IR (spectra of) superhydrogenated (PAHs)
- How to build matter from PAHs



Each of the topical sessions was concluded by a plenary discussion in which specific points were further clarified, and challenges for future research addressed. The discussion sessions were very lively. The very high, overall degree of participation was inspired by the excellent talks and the setting. The Lorentz center is fully geared to the creation of an inspiring, informal, academic environment and atmosphere for open discussions.

The ample time left in the schedule for informal splinter discussions led to a further scientific cross-fertilization. In the concluding session, many topics for concerted research efforts were discussed and generic, prototypical molecular systems identified, that should serve as linking pin systems in projects involving members of the two networks, represented by XLIC and the astronomy network. The original list of topics as it emerged on the blackboard is shown in Figure 2.

**It was decided to have a successor meeting on Energetic Processing of Large Molecules (EPoLM, April 11-13, 2016). EPoLM will be held in conjunction with the XLIC Stockholm meeting which runs from April 13-15. At that meeting we will find out which of the topics can be tick marked solved. See you next year in Stockholm!**

### The organizers:

Ronnie Hoekstra  
Henrik Cederquist  
Xander Tielens



**Ronnie Hoekstra** is Full Professor at the University of Groningen. He is head of the Quantum Interactions and Structural Dynamics Group at the Zernike Institute for Advanced Materials (Groningen) and the EUV Plasma Dynamics group at the Advanced Research Center for Nanolithography (Amsterdam). E-mail: [r.a.hoekstra@rug.nl](mailto:r.a.hoekstra@rug.nl).



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**Xander Tielens** is Professor of Physics and Chemistry of Interstellar Space at Leiden University. In 2009 he received an Advanced Grant from the European Research Council (ERC) and in 2012 a Spinoza Prize from the Netherlands Organisation for Scientific Research (NWO). He is member of the Royal Netherlands Academy of Arts and Sciences. E-mail: [tielens@strw.leidenuniv.nl](mailto:tielens@strw.leidenuniv.nl).

# Abstracts

## Penta-graphene: A new carbon allotrope

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A 2D metastable carbon allotrope, penta-graphene, composed entirely of carbon pentagons and resembling the Cairo pentagonal tiling, is proposed. State-of-the-art theoretical calculations confirm that the new carbon polymorph is not only dynamically and mechanically stable, but also can withstand temperatures as high as 1000 K. Due to its unique atomic configuration, penta-graphene has an unusual negative Poisson's ratio and ultrahigh ideal strength that can even outperform graphene. Furthermore, unlike graphene that needs to be functionalized for opening a band gap, penta-graphene possesses an intrinsic quasi-direct band gap as large as 3.25 eV, close to that of ZnO and GaN. Equally important, penta-graphene can be exfoliated from T12-carbon. When rolled up, it can form pentagon-based nanotubes which are semiconducting, regardless of their chirality. When stacked in different patterns, stable 3D twin structures of T12-carbon are generated with band gaps even larger than that of T12-carbon. The versatility of penta-graphene and its derivatives are expected to have broad applications in nanoelectronics and nanomechanics.

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PNAS, 2015, 112 (8), 2372-2377

<http://www.pnas.org/content/112/8/2372.abstract>

# Dust processing in the Carina nebula region

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Dust processing in the Carina nebula is investigated based on mid- to far-infrared spectroscopy with *Infrared Space Observatory (ISO)*. Mapping observations over a central  $40' \times 20'$  area of the nebula with PHT-S, SWS, and LWS onboard *ISO* not only reveal spectroscopically that the mid-infrared unidentified infrared (UIR) bands at 6.2, 7.7, 8.6, and 11.3  $\mu\text{m}$  are absent in the ionized region, but also indicate that the 11.3  $\mu\text{m}$  may behave differently from the other three UIR bands near the edge of the ionized region, suggesting a variation either in the size distribution or in the ionization fraction of the band carriers. The correlation of [NII] 122  $\mu\text{m}$  and [SII] 35  $\mu\text{m}$  line emissions observed with SWS and LWS are reinvestigated based on the recent atomic data as well as the latest cosmic abundance, suggesting that a large fraction ( $> 70\%$ ), if not all, of silicon returns to the gas phase in the Carina nebula, suggesting that silicates cannot survive in harsh conditions, such as massive star-forming regions. The present observations clearly show dust processing taking place in active regions in the Galaxy.

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Planetary and Space Science, in press (2015)

<http://www.sciencedirect.com/science/article/pii/S0032063315001014>

# Characterizing Extragalactic Anomalous Microwave Emission in NGC 6946 with CARMA

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Using 1 cm and 3 mm CARMA and 2 mm GISMO observations, we follow up the first extragalactic detection of anomalous microwave emission (AME) reported by Murphy et al. in an extranuclear region (Enuc. 4) of the nearby face-on spiral galaxy NGC 6946. We find the spectral shape and peak frequency of AME in this region to be consistent with models of spinning dust emission. However, the strength of the emission far exceeds the Galactic AME emissivity given the abundance of polycyclic aromatic hydrocarbons (PAHs) in that region. Using our galaxy-wide 1 cm map (21" resolution), we identify a total of eight 21"x21" regions in NGC 6946 that harbour AME at  $> 95\%$  significance at levels comparable to that observed in Enuc. 4. The remainder of the galaxy has 1 cm emission consistent with or below the observed Galactic AME

emissivity per PAH surface density. We probe relationships between the detected AME and dust surface density, PAH emission, and radiation field, though no environmental property emerges to delineate regions with strong versus weak or non-existent AME. On the basis of these data and other AME observations in the literature, we determine that the AME emissivity per unit dust mass is highly variable. We argue that the spinning dust hypothesis, which predicts the AME power to be approximately proportional to the PAH mass, is therefore incomplete.

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MNRAS 449, 809 (2015)

<http://adsabs.harvard.edu/abs/2015MNRAS.449..809H>

## **H<sub>2</sub> formation on PAHs in photodissociation regions: a high-temperature pathway to molecular hydrogen**

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Molecular hydrogen is the most abundant molecule in the Universe. It is thought that a large portion of H<sub>2</sub> forms by association of hydrogen atoms to polycyclic aromatic hydrocarbons (PAHs). We model the influence of PAHs on total H<sub>2</sub> formation rates in photodissociation regions (PDRs) and assess the effect of these formation rates on the total cloud structure. We set up a chemical kinetic model at steady state in a PDR environment and included radiative transfer to calculate the chemistry at different depths in the PDR. This model includes known dust grain chemistry for the formation of H<sub>2</sub> and a H<sub>2</sub> formation mechanism on PAHs. Since H<sub>2</sub> formation on PAHs is impeded by thermal barriers, this pathway is only efficient at higher temperatures ( $T > 200$  K). At these temperatures the conventional route of H<sub>2</sub> formation via H atoms physisorbed on dust grains is no longer feasible, so the PAH mechanism enlarges the region where H<sub>2</sub> formation is possible. We find that PAHs have a significant influence on the structure of PDRs. The extinction at which the transition from atomic to molecular hydrogen occurs strongly depends on the presence of PAHs, especially for PDRs with a strong external radiation field. A sharp spatial transition between fully dehydrogenated PAHs on the outside of the cloud and normally hydrogenated PAHs on the inside is found. As a proof of concept, we use coronene to show that H<sub>2</sub> forms very efficiently on PAHs, and that this process can reproduce the high H<sub>2</sub> formation rates derived in several PDRs.

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A&A 579, A72 (2015)

<http://www.aanda.org/articles/aa/abs/2015/07/aa23165-13/aa23165-13.html>

<http://arxiv.org/abs/1504.08276>

# Variations in the 3.3 $\mu\text{m}$ feature and Carbonaceous Dust in AKARI Data

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A wealth of near infrared spectroscopic data for a large number of galactic objects was recorded with AKARI during its active lifetime. The hydrocarbon emission features around 3.3 – 3.5  $\mu\text{m}$  are modelled here as a series of 6 Voigt profiles arising due to hydrogen atoms found in different molecular structures within the emitting spectroscopic carriers. This model is compared and contrasted with a model consisting of 3 Gaussian profiles and found to produce a superior fit to AKARI data. Analysis of the 6 Voigt model shows that the 3.3  $\mu\text{m}$  aromatic hydrocarbon band is well described by two components at 3.28  $\mu\text{m}$  and 3.30  $\mu\text{m}$ . We confirm that the 3.28  $\mu\text{m}$  band is due to emission from aromatic molecules, and find a good correlation between the 3.28  $\mu\text{m}$  and 3.41  $\mu\text{m}$  bands, assigned to bay-hydrogen sites and linking methylene groups respectively. Results are discussed in terms of molecular processing and dust formation.

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Planetary and Space Science, in press (2015)

<http://www.sciencedirect.com/science/article/pii/S0032063315001555>

# Vibrational spectroscopic study of vinyl substituted polycyclic aromatic hydrocarbons

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The mid infrared emission features observed in various astrophysical sources are attributed to polycyclic aromatic hydrocarbon (PAH) molecules. The models of emission spectra from a collection of PAHs show uncertainty in matching the 6.2  $\mu\text{m}$  feature. This indicates the need to consider a larger variety of PAHs and PAH derivatives. Chemical pathways towards formation of PAHs in the astrophysical environments involve vinyl substituted PAHs as intermediate products. Vibrational spectroscopic study of vinyl-PAHs is reported in the present work. The vinyl group is substituted at similar positions in eight different PAHs. The obtained optimized structures show that vinyl substitution at 2 position in acenes gives planar geometry, while all other vinyl-PAHs are non-planar. Infrared spectra is simulated for neutrals as well as for cations. The results are compared with the spectra of corresponding plain PAHs and analyzed for possible match with astrophysical observations. New features, due to vinyl group in the composite spectra, identified at 6.64, 6.92, 7.27, 8.77 and 10.35  $\mu\text{m}$  fall close to some sub features of the observed emission spectra. The paper provides data that may be used in the emission models particularly along proto planetary nebulae type cool objects.

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Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 151, 1, 2015

<http://www.sciencedirect.com/science/article/pii/S1386142515300093>

## PAH Emission at the Brightest Locations of PDRs: the Grand-PAH hypothesis

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The PAH emission observed in the Spitzer-IRS spectra of bright mid-IR locations of NGC7023, NGC2023 and NGC1333 were analyzed. These objects show large variations in PAH band ratios when studied through spectral mapping. Nevertheless, the mid-IR spectra at these bright spots show a remarkably similar PAH emission. We used the NASA Ames PAH IR Spectroscopic Database to fit the observations and analyze the derived PAH populations. Our results show that PAH emission in the 5–15  $\mu\text{m}$  range appears to be rather insensitive to variations of the radiation field. Similar PAH populations of neutral small-to-medium sized PAHs (~50%), with ionized species contributing in slightly less than 50%, provide very good fits. Analyzing the degeneracy of the results shows that subtle (but intrinsic) variations in the emission properties of individual PAHs lead to observable differences in the resulting spectra. On top of this, we found that variations of <30% in the PAH abundances would lead to noticeable spectral differences between the three PDRs. Therefore PAH populations must be remarkably similar at these different lines-of-sight. To account for this, we suggest the concept of grandPAHs as a unique mixture of the most stable PAHs emitting at these spots. Using NGC7023 as an example, the grandPAHs refer to the robust PAH population that results from the intense processing of PAHs at the border limit between the PDR and the molecular cloud where, due to the UV radiation that destroys the PAH population, the abundance of PAHs starts decreasing as we move towards the star.

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ApJ, 807, 99 (2015)

<http://iopscience.iop.org/0004-637X/807/1/99/>

# Laboratory confirmation of $C_{60}^+$ as the carrier of two diffuse interstellar bands

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The diffuse interstellar bands are absorption lines seen towards reddened stars<sup>1</sup>. None of the molecules responsible for these bands have been conclusively identified<sup>2</sup>. Two bands at 9,632 ångströms and 9,577 ångströms were reported in 1994, and were suggested to arise from  $C_{60}^+$  molecules (ref. 3), on the basis of the proximity of these wavelengths to the absorption bands of  $C_{60}^+$  measured in a neon matrix<sup>4</sup>. Confirmation of this assignment requires the gas-phase spectrum of  $C_{60}^+$ . Here we report laboratory spectroscopy of  $C_{60}^+$  in the gas phase, cooled to 5.8 kelvin. The absorption spectrum has maxima at  $9,632.7 \pm 0.1$  ångströms and  $9,577.5 \pm 0.1$  ångströms, and the full widths at half-maximum of these bands are  $2.2 \pm 0.2$  ångströms and  $2.5 \pm 0.2$  ångströms, respectively. We conclude that we have positively identified the diffuse interstellar bands at 9,632 ångströms and 9,577 ångströms as arising from  $C_{60}^+$  in the interstellar medium.

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# Meetings

## **Third Announcement**

### **ISPAC 2015**

### **International Symposium on Polycyclic Aromatic Compounds (PACs)**

**Bordeaux – France**  
**September 13-17, 2015**

<http://ispac2015.ism.u-bordeaux1.fr/?lang=en>

Dear colleagues,

This is the third announcement of the ISPAC 2015 symposium. The scientific topics cover physical, chemical, and biological properties of PACs, including a session devoted to astrophysical purposes: "PACs in interstellar media" (session chair: J. Mascetti, ISM, Univ. Bordeaux).

Observations have shown that PAH and PAC molecules are abundant and ubiquitous in the interstellar medium (ISM). Although much progress has been made over the last 25 years on the nature of PAHs and their role in the physics and chemistry of the ISM, still more remains to be discovered on their chemical reactivity, including the relationship between PAH molecules, hydrogenated amorphous carbon (HAC) and carbonaceous grains, the catalytic role of PAHs in the formation of molecular hydrogen, and the UV-photochemistry of PAHs.

The session is organized as a series of oral presentations (20-30 min) followed by short discussions (5-10 min). Invited speakers: C. Joblin (IRAP, Toulouse, France), C. Jäger (Univ. Jena, Germany), L. Hornekær (Aarhus Univ., Denmark), J. Cernicharo (INTA-CSIC, Spain), E. Dartois (IAS, Univ. Paris Sud, France), A. Simon (Univ. UPS Toulouse, France).

Registration is open till August 1st, and it is still possible to submit an abstract for poster presentation. Scientific programme, details and registration are available on the website.

We hope to welcome you in Bordeaux, the best 2015 European destination, in September !

**THE LOCAL ORGANIZING COMMITTEE:**

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