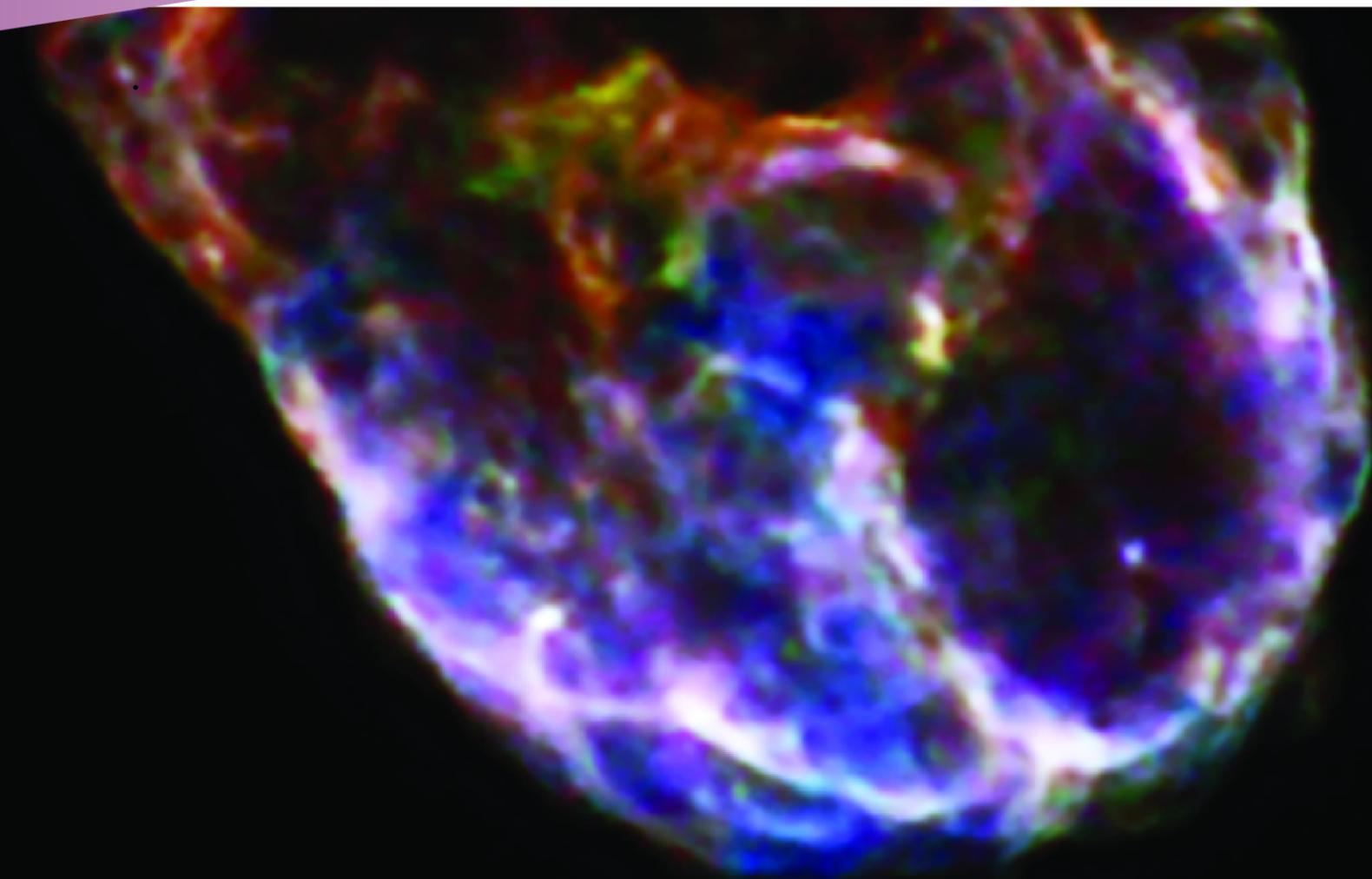


AstropAH

A Newsletter on Astronomical PAHs

Issue 17 | April 2015



Destroying PAHs

Editorial

Dear Colleagues,

Welcome to our 17th edition of AstroPAH. This issue's Picture of the Month features an X-ray image of the supernova remnant N132D in the Large Magellanic Cloud. This supernova remnant shows signs of PAH processing.

In Focus we have an interview with Dr. Melanie Schnell, who has just been awarded an ERC starting grant to work, amongst other topics, on rotational spectroscopy of PAH complexes.

In our abstracts section, you can find new studies on PANHs, PAH clusters, nano-diamonds, and dust as well as a look into unidentified emission features. Not included in AstroPAH, but now available online, are [the abstracts of the 69th International Symposium on Molecular Spectroscopy](#) (June 16-20, 2014 at The University of Illinois at Urbana-Champaign).

We would like to draw your attention to our meetings and announcements sections featuring two interesting meetings next September – the symposium to honour Lou Al-lamandolas contributions to the molecular Universe in Annapolis (USA) and the International Symposium on Polynuclear Aromatic Hydrocarbons in Bordeaux (France) – and the recent launched journal Molecular Astrophysics.

We thank you all for your contributions and please keep them coming. You can send us your contributions anytime. For publication in May, 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 (astropah@strw.leidenuniv.nl).

The Editorial Team

**Next issue: 19 May 2015.
Submission deadline: 8 May 2015.**

AstroPAH Newsletter

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PAH Picture of the Month

Chandra X-ray Observatory view of the supernova remnant (SNR) N132D, in the Large Magellanic Cloud. The colors in this image show emission due to low energy X-rays (red, 0.3-0.5 keV), intermediate energy X-rays (green, 0.5-0.75 keV) and high energy X-rays (blue, 0.75-7 keV). N132D is one of the very few SNRs showing clear evidence for large PAH molecules being destroyed by the blast wave shock (Tappe et al, 2012, ApJ, 754, 132).

Credits: NASA/CXC/NCSU/K. J. Borkowski et al.

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Design by Isabel Aleman

In Focus

Interview with Melanie Schnell

Tell us about yourself.

Melanie: "I am a physical chemist by training with a molecular physics and theoretical chemistry background as well. With my PhD research in the group of Jens-Uwe Grabow at the University of Hannover, I started to work in the field of high-resolution rotational spectroscopy. My main research focus was on investigating highly flexible molecules, but I soon also got in contact with my first PAH. . .

After my PhD I changed the field a bit to develop new methods to guide, decelerate and trap neutral, polar molecules in the gas phase using electric fields via their Stark effect – a very fascinating area of research.

Since 2011, I am back in molecular spectroscopy. I am currently a Max Planck research group leader at the Max Planck Institute for the Structure and Dynamics of Matter in Hamburg. In the group, we have a strong focus on investigating the structure, dynamics, and chirality of molecules and molecular complexes in the gas phase using broadband rotational spectroscopy employing the new chirp approach. Among others, we are interested in molecules of biological relevance. We also have a strong focus on molecular complexes, to learn about the interplay between the different molecular interaction forces.

As you all know, rotational spectroscopy is also ideally suited to study molecules of astrochemical interest – both in the laboratory and by using ground-based radioastronomy observatories, and we are just starting to establish this as a new research branch in our group."

When and why did you start studying rotational spectroscopy of PAHs?

Melanie: "My interest in PAHs dates back to my PhD research in the group of Jens-Uwe Grabow at the University of Hannover. During my PhD research, I developed an improved setup for precisely measuring the Stark effect of polar molecules and thus determining their dipole moments using cavity-based Fourier transform microwave spectroscopy. In 2003, Frank Lovas from the National Institute of Standards and Technology in Gaithersburg (USA) asked us if we could measure the Stark effect of corannulene, $C_{20}H_{10}$. In Gaithersburg, he already studied its ro-



tational spectrum. $C_{20}H_{10}$ can be understood to be the cap of fullerene C_{60} , saturated with hydrogen atoms, as shown in **Figure 1**. From a rotational spectroscopists point of view, it is an amazingly beautiful symmetric top with C_{5v} symmetry. I was fascinated by the fact that a molecule consisting purely from carbon and hydrogen can have a dipole moment of more than 2 D.”

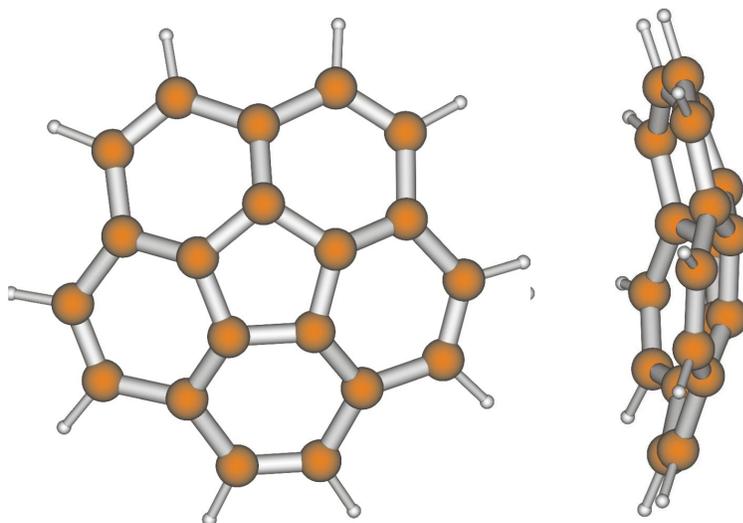


Figure 1 - Structure of corannulene. Its dipole moment of 2.07 D was measured in 2005 (Lovas et al. 2005, *J. Am. Chem. Soc.* 127, 4345-9). We are planning to extend these studies in the next years.

You recently acquired an ERC grant for your AstroRot project. What does AstroRot entail?

Melanie: "In the ERC Starting grant AstroRot we will combine broadband rotational spectroscopy studies in the laboratory with telescope observations, to explore the molecular complexity in interstellar space. We aim at discovering new molecule classes and key chemical processes. So far, mostly physical reasons were investigated for the observed variations in molecular abundances. We are interested in studying the influence of chemistry on the molecular composition of the Universe.

One focus will be placed on instrument development for our laboratory spectroscopy studies. Figure 2 shows a photo of our broadband rotational spectrometer that operates in the low frequency range from 2-8.5 GHz. We are just starting to extend its frequency ranges to have direct overlap with the new array telescopes (ALMA), i.e., starting in the 70 GHz range. We will exploit both the cold conditions of a molecular jet and the higher temperatures in a gas cell to mimic different interstellar conditions. Measurements in the gas cell will allow us to also study rotational emission of molecules in vibrationally excited states.

The key advantages of chirped-pulse Fourier transform microwave spectroscopy are accurate transition intensities, tremendously reduced measurement times, and unique mixture compatibility. We want to apply this to study PAHs and their complexes (see below).

Furthermore, I am also fascinated by the observation that specific isotopologues, such as deuterated ammonia ND_3 or NHD_2 , exhibit increased abundances in interstellar space com-

pared to what would be expected by their elemental natural abundances. Chemistry is discussed to be the reason for these higher abundances. We want to perform more studies in the laboratory to further explore this phenomenon.”

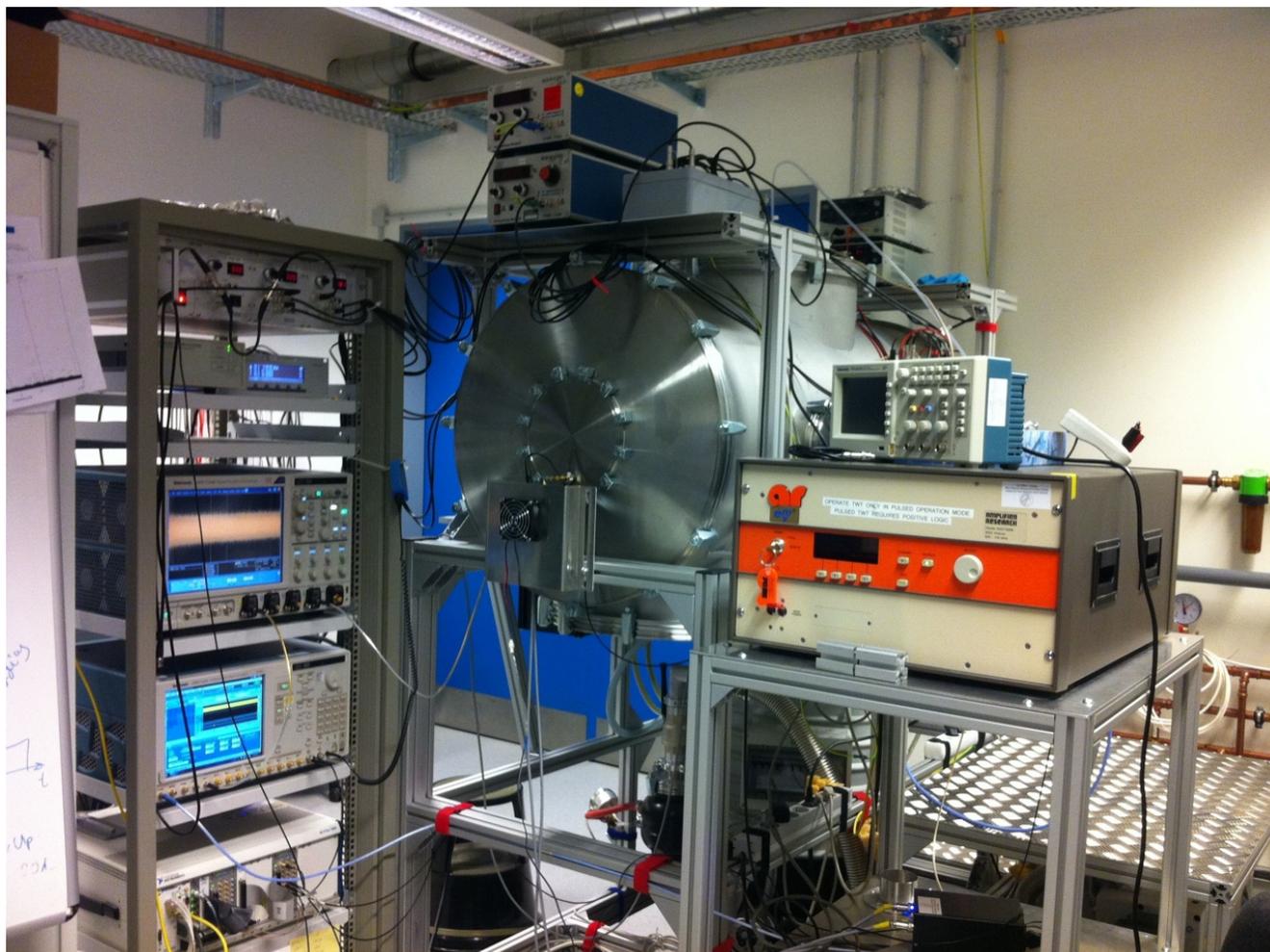


Figure 2 - Picture of our broadband rotational spectrometer covering the low frequency range from 2 to 8.5 GHz.

Which PAHs or related molecules will you be studying for that project?

Melanie: “We have a long-standing interest in symmetric PAHs such as corannulene, $C_{20}H_{10}$. In 2005, we were the first to report their rotational spectra and their unexpectedly large dipole moment of 2.07 D that arises from its curvature. As a consequence, all ten C-H bonds are roughly pointing into the same direction so that their individual polarizations add up.

We are interested in studying the rotational spectra of corannulene and its complexes with water and with itself. Furthermore, in the 2005 study, we did not succeed to study its ^{13}C isotopologues in natural abundance. With the broadband rotational spectroscopy approach we hope to be able to achieve this, which will allow us to precisely determine its molecular structure.

We are also interested in complexes of corannulene with other, smaller polyaromatic hydrocarbons. Since the molecular spectra can be expected to be very rich, broadband rotational spectroscopy will be the ideal technique to study these systems.”

How do you experience work-home balance?

Melanie: "Work-home or work-life balance in a scientific environment is an ambivalent topic for me. On the one hand, our working environment is highly flexible. Often, we can plan our daily schedule rather freely so that it can be combined with the time we need to take care of children, for example. On the other hand, however, conferences, beamtimes or observatory times let us travel a lot, which require complicated arrangements. Furthermore, when we as scientists work on qualifying ourselves for the next stage of academic position, it typically coincides with the time when we also plan to start a family, which can be very exhausting."

Do you have any advice for early-career researchers?

Melanie: "I think it is important to find a research area that fascinates one, to find research questions that drive one's curiosity. This will ensure that research remains curiosity-driven which, to my opinion, is a good way to ensure unexpected new findings and insights."

From a career-planning point of view, I think it would be optimal to change the area of research after the PhD to learn something new during the PostDoc period. These two research areas can then be naturally combined to form a new, unique research direction."

Abstracts

Photoluminescence of silicon-vacancy defects in nanodiamonds of different chondrites

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Photoluminescence spectra show that silicon impurity is present in lattice of some nanodiamond grains (ND) of various chondrites as a silicon-vacancy (SiV) defect. The relative intensity of the SiV band in the diamond-rich separates depends on chemical composition of meteorites and on size of ND grains. The strongest signal is found for the size separates enriched in small grains; thus confirming our earlier conclusion that the SiV defects preferentially reside in the smallest (≤ 2 nm) grains. The difference in relative intensities of the SiV luminescence in the diamond-rich separates of individual meteorites are due to variable conditions of thermal metamorphism of their parent bodies and/or uneven sampling of nanodiamonds populations. Annealing of separates in air eliminates surface sp^2 -carbon, consequently, the SiV luminescence is enhanced. Strong and well-defined luminescence and absorption of the SiV defect is a promising feature to locate cold (< 250 °C) nanodiamonds in space.

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Accepted for publication in Meteoritics and Planetary Science

<http://arxiv.org/abs/1502.08031>

Dust dynamics and evolution in expanding HII regions. I. Radiative drift of neutral and charged grains

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We consider dust drift under the influence of stellar radiation pressure during the pressure-driven expansion of an HII region using the chemo-dynamical model MARION. Dust size distribution is represented by four dust types: conventional polycyclic aromatic hydrocarbons (PAHs), very small grains (VSGs), big grains (BGs) and also intermediate-sized grains (ISGs), which are larger than VSGs and smaller than BGs. The dust is assumed to move at terminal velocity determined locally from the balance between the radiation pressure and gas drag. As Coulomb drag is an important contribution to the overall gas drag, we evaluate a grain charge evolution within the HII region for each dust type. BGs are effectively swept out of the HII region. The spatial distribution of ISGs within the HII region has a double peak structure, with a smaller inner peak and a higher outer peak. PAHs and VSGs are mostly coupled to the gas. The mean charge of PAHs is close to zero, so they can become neutral from time to time because of charge fluctuations. These periods of neutrality occur often enough to cause the removal of PAHs from the interior of the HII region. For VSGs, the effect of charge fluctuations is less pronounced but still significant. We conclude that accounting for charge dispersion is necessary to describe the dynamics of small grains.

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MNRAS 449, 440 (2015)

<http://mnras.oxfordjournals.org/content/449/1/440>

The electronic spectra of protonated nitrogen-substituted polycyclic aromatic hydrocarbon molecules

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Aims This study was designed to examine the viability of protonated nitrogen-substituted polycyclic aromatic hydrocarbons (H⁺PANHs) as candidates for the carriers of the diffuse interstellar bands (DIBs).

Methods We obtained the electronic spectra of two protonated PANH cations, protonated acridine and phenanthridine, using parent ion photo-fragment spectroscopy and generated theoretical electronic spectra using *ab initio* calculations.

Results We show that the spectra of the two species studied here do not correspond to known DIBs. However, based on the general properties derived from the spectra of these small protonated nitrogen-substituted PAHs, we propose that larger H⁺PANH cations represent good candidates for DIB carriers due to the expected positions of their electronic transitions in the

UV-visible and their narrow spectral bands.

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Accepted for publication in *Astronomy & Astrophysics*

<http://arxiv.org/abs/1503.03329>

A Tale of Three Mysterious Spectral Features in Carbon-Rich Evolved Stars: The 21 μm , 30 μm , and “Unidentified Infrared” Emission Features

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The mysterious “21 μm ” emission feature seen almost exclusively in the short-lived proto-planetary nebula (PPN) phase of stellar evolution remains unidentified since its discovery two decades ago. This feature is always accompanied by the equally mysterious, unidentified “30 μm ” feature and the so-called “unidentified infrared” (UIR) features at 3.3, 6.2, 7.7, 8.6, and 11.3 μm which are generally attributed to polycyclic aromatic hydrocarbon (PAH) molecules. The 30 μm feature is commonly observed in all stages of stellar evolution from the asymptotic giant branch (AGB) through PPN to the planetary nebula phase. We explore the interrelations among the mysterious 21 μm , 30 μm , and UIR features of the 21 μm sources. We derive the fluxes emitted in the observed UIR, 21 μm , and 30 μm features from published *ISO* or *Spitzer/IRS* spectra. We find that none of these spectral features correlate with each other. This argues against a common carrier (e.g., thiourea) for both the 21 μm feature and the 30 μm feature (otherwise these two features should correlate). This also does not support large PAH clusters as a possible carrier for the 21 μm feature.

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Astrophys. J. 802, 39 (2015)

<http://adsabs.harvard.edu/abs/2015ApJ...802...39M>

PAH Clusters as Sources of Interstellar Infrared Emission

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Polycyclic aromatic hydrocarbons (or PAHs) have been the subject of astrochemical research for several decades as principal sources of the interstellar aromatic infrared emission bands. PAH clusters could possibly contribute to these emission bands, but a lack of data on their

infrared properties has made this hypothesis difficult to evaluate. Here we investigate homogeneous neutral PAH clusters by measuring the mid-infrared absorption spectra of the five nonlinear PAH molecules phenanthrene, chrysene, pyrene, perylene, and benzo[*ghi*]perylene within solid argon ice at a fixed temperature of 5 K. We attribute observed spectral shifts in their principal absorption bands as a function of argon/PAH ratio to clustering of the PAH molecules within the argon matrix. These shifts are related to the cluster structures forming in the matrix and the topology of the monomer PAH molecule. We predict that interstellar PAH molecules that are relatively large (no fewer than 50 carbon atoms per molecule) and compact will have clusters that contribute to the asymmetrically red-shaded profile of the interstellar 11.2 μm emission band.

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The Astrophysical Journal, 801, 108 (2015)

<http://iopscience.iop.org/0004-637X/801/2/108/article>

Meetings

From interstellar ices to polycyclic aromatic hydrocarbons:

A symposium to honor Lou Allamandola's contributions to the molecular Universe

**Annapolis - Maryland - USA
September 13-17, 2015**

****Deadline for abstract submission: 26 June 2015****

This is the first announcement of the meeting "From interstellar ices to polycyclic aromatic hydrocarbons: A symposium to honor Lou Allamandola's contributions to the molecular Universe". Abstracts should be submitted by June 26 for consideration. Details on the meeting and registration will be available on the website in the near future:

<http://ices2pahs.strw.leidenuniv.nl/index.html>

Extensive advances in the field of Astrochemistry have been made thanks to simultaneous efforts in astronomical infrared spectroscopy and to dedicated laboratory simulations and theoretical studies aimed at reproducing observed spectra throughout the interstellar medium. The molecular complexity, both organic and mineral, found in inter/proto-stellar and solar system environments have been attributed to primarily grain-surface and bulk chemistry reactions.

This symposium will be comprised of contributions from participants working on dedicated laboratory experiments, theoretical calculations of basic processes and chemical reaction networks, as well as astronomical observations of complex molecules and, more generally solid state materials in space. This gathering is in honor of a major influence to this area of Astrochemistry, Dr. Louis Allamandola, one of the leading spokespersons of the interstellar polycyclic aromatic hydrocarbon (PAH) model.

The scientific topics of this meeting include:

- Ices - Spectroscopy, Energetic Processing
- Surface Chemistry
- PAHs in Ices

- Identification, Observation, and models of PAHs
- Formation of complex species in Ices - Astrobiology

The format of the meeting will consist of invited talks, contributed talks, and posters. A list of invited speakers will be available on the website soon.

The Symposium will be held at the Historic Inns of Annapolis located in Annapolis, MD USA (<http://www.historicinnsofannapolis.com/>).

We are looking forward to an exciting meeting and hope to welcome you in Annapolis this fall.

The Scientific Organizing Committee:

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Max Bernstein (NASA/HQ)
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International Symposium on Polynuclear Aromatic Hydrocarbons

'Cité Mondiale Convention Centre' in Bordeaux , France

September 13-17, 2015

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

ISPAC 2015 will focus on the research of Polycyclic Aromatic Compounds (PACs) on multiple fronts of analytical measurements, toxicology, organic synthesis, human exposure and health effects, and environmental presences, sources, fate and transport.

It is a forum that brings together researchers worldwide to communicate, learn and advance the field of PAC. In addition, we intend to have an exhibition involving chemical products, analytical instrumentations and services involving PACs.

We will welcome proposals for short courses, arranged sessions and vendors' seminars. Several best presentation awards will be distributed to young researchers. Finally the ISPAC 2015 Award will be given to a prominent research scientist in the field of PACs.

ORGANISERS: ISM / CNRS

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Announcements

NEW JOURNAL: Molecular Astrophysics

The journal is welcoming submissions!

<http://www.elsevier.com/locate/molap>

Molecular Astrophysics aims to provide a platform for scientists studying the chemical processes that form and deconstruct molecules, and control chemical abundances in the universe, particularly on Solar System objects such as planets, moons, and comets, in the atmospheres of exoplanets, as well as in regions of star and planet formation in the Interstellar Medium of galaxies.

This journal is subscription based with the option to publish Open Access.

First issue expected in fall 2015 and freely available online for the first year!

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