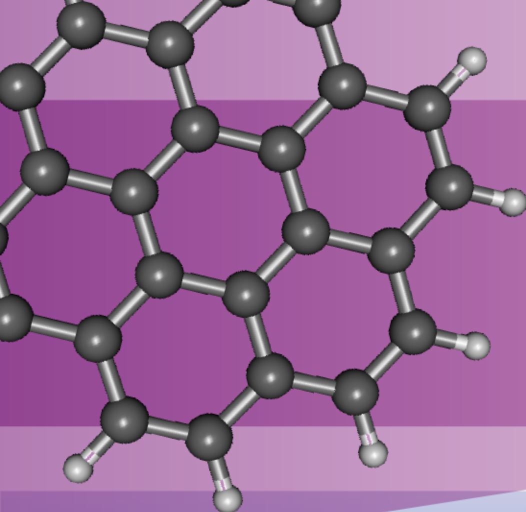
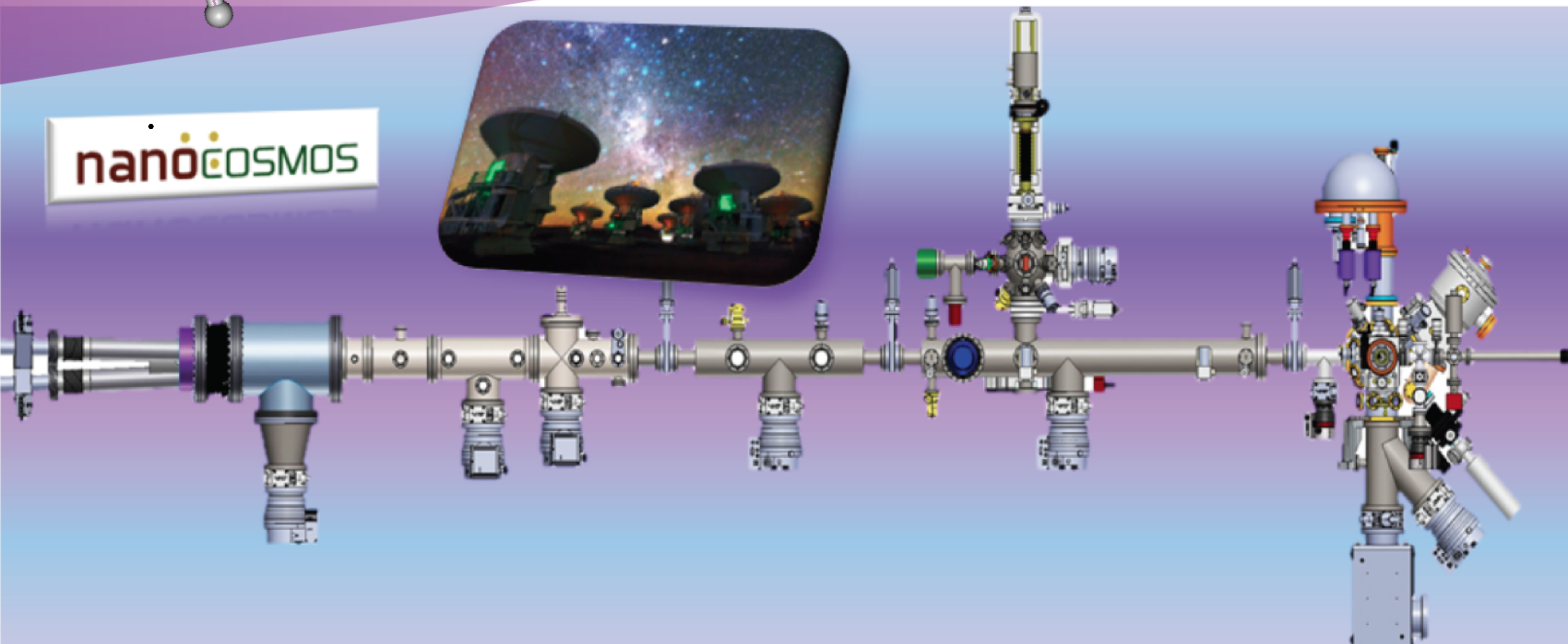
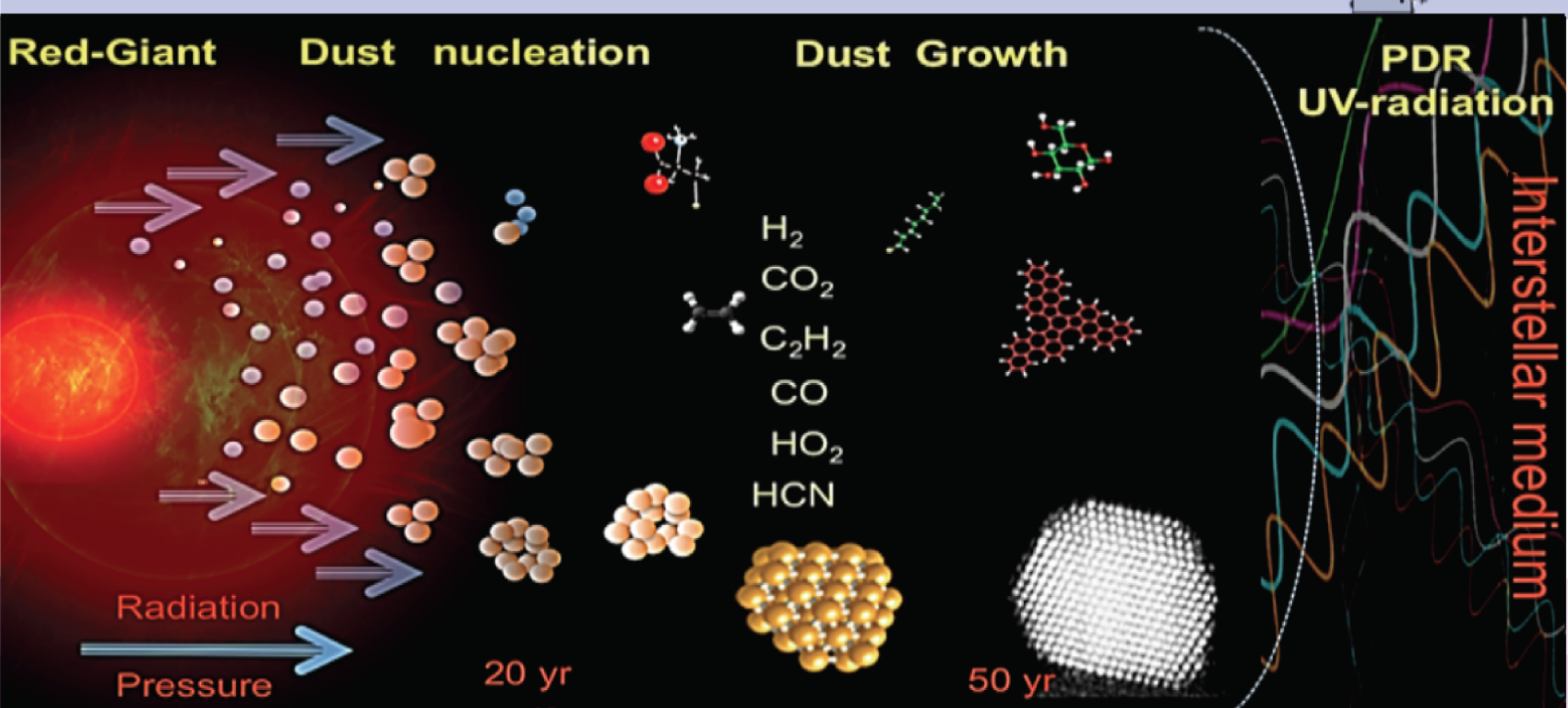


AstroPAH

A Newsletter on Astronomical PAHs

Issue 19 | June 2015





Editorial

Dear Colleagues,

Welcome to release 19 of AstroPAH!

In this issue, you will find an In Focus piece on the NANOCOSMOS project, a synergy among multiple disciplines to provide a cutting-edge view on cosmic dust formation. Our cover shows pictures that illustrate main features of the project.

In our abstracts section, you will find new studies on the photochemistry of PAHs and on their galactic and extragalactic emissions. Check also the second announcement for the symposium in honour of Lou Allamandola's contributions to the molecular universe for which the registration and abstract submission is now open.

We thank you all for your contributions. You can send us your contributions anytime. For publication in July, 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.

The Editorial Team

Next issue: 21 July 2015.
Submission deadline: 10 July 2015.

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PAH Picture of the Month

NANOCOSMOS - coupling observations and laboratory experiments.

Credits: NANOCOSMOS Team; ESO/B. Tafreshi/TWAN

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Design by Isabel Aleman

NANOCOSMOS:
an ERC-funded project to understand the formation and evolution of Cosmic Dust

José Cernicharo, Christine Joblin & José Ángel Martín-Gago

Dust grains play a fundamental role in the evolution of the Interstellar Medium and are intimately related to the life cycle of stars and to the formation of rocky planets in planetary disks around young stars. It is now accepted that dust grains are formed in the cool atmospheres of evolved stars (Asymptotic Giant Branch - AGB - stars, Wolf-Rayet stars, planetary nebulae, novae and supernovae ejecta). AGB stars are considered to account for 50-60% of interstellar dust in the Local Universe. However the physical and chemical processes leading to the formation and evolution of dust and its interaction with the surrounding gas are poorly understood. The **NANOCOSMOS** project (Gas and Dust from the Stars to the Laboratory: Exploring the NANOCOSMOS) will try to unveil these fundamental questions through a novel focus: unprecedented sub-arcsecond resolution observations of the envelopes of evolved stars combined with sophisticated laboratory simulations involving techniques in a highly-controlled ultra-high-vacuum environment.

The understanding of the processes that lead to the formation of dust grains impacts our knowledge of the physical and chemical properties of these grains and has therefore profound implications at all the astrophysical levels, from the formation of planetary systems to the study of the high-redshift Universe.

The European Research Council awarded NANOCOSMOS with a competitive Synergy grant in 2014 for a period of six years. The project is led by three principal investigators (J. Cernicharo, C. Joblin and J. A. Martín-Gago) with the support and expertise of the host institutions CSIC (Consejo Superior de Investigaciones Científicas) and CNRS (Centre National de la Recherche Scientifique). The whole team (cf. **Figure 1**) gathers almost 80 scientists and engineers from different top research areas such as Astrophysics, Surface Physics, Molecular Physics, Chemical Physics, Quantum Chemistry, Spectroscopy, Vacuum, Electrical and Mechanical Engineering.

One of the main goals of NANOCOSMOS will be to shed light onto the dust formation scenario in AGB stars. In these stars, dust chemistry is mainly governed by the C/O ratio. For C/O$<$1 (O-rich AGB stars), metal oxides together with silicates are formed. On the other hand for C/O$>$1 (C-rich AGBs), silicon carbide (SiC) and amorphous carbon grains are the predominant species due to the convective mixing processes that bring carbon from the interior to the

Figure 1 - *The NANOCOSMOS team members at the Kick-Off Meeting in the CSIC headquarters.*

stellar surface (the so-called third dredge-up in stellar nucleosynthesis). Typical dust grain sizes can vary from nanometer to several hundred nanometers at the end of the dust formation zone. Condensation temperatures range between 1,500 K and 2,500 K in the photosphere. This picture is shown in **Figure 2** for the well-studied proto-typical C-rich star IRC+10216.

NANOCOSMOS first approach to deal with this complex scenario consists of high-angular (sub-arcsecond) resolution observations with the Atacama Large Millimeter/submillimeter Array (ALMA) interferometer and the Very Large Telescope Interferometer (VLTI) to unveil the spatial distribution of each molecular species in the innermost shells of the photosphere of IRC+10216 and other prominent AGB stars. This will allow us to understand the role of these species in the formation of dust seeds and their ulterior growth. In particular the spatial distribution of matter as traced with CO and HCN will give us more clues on the opacities of the atmospheres of C-rich stars. This leads to a decrease of the effective temperature, thus favoring the formation of dust seeds. The spatial distribution of these molecules has been derived only for those arising in the external layers far from the photosphere of the star where photochemical processes induced by the interstellar radiation field modify the molecular content. In addition, High-electron-mobility transistor (HEMT) receivers will be developed in the 32-50 and 72-116 GHz range and used to observe a large number of AGB stars at different evolutionary stages using the 40-m millimeter wave telescope located at Yebes (Instituto Geográfico Nacional, IGN, Spain). These observations will constitute a legacy of NANOCOSMOS providing useful information to understand dust formation and evolution in evolved stars. These receivers will also be used to characterize the gas composition in the different experiments that will be performed in the project. A gas evolution chamber will be built to simulate the chemistry in regions irradiated by ultraviolet photons.

First spectral surveys of IRC+10216 carried out with ALMA (0.6 arcsecond angular resolution, Cycle 0 observations) have revealed hundreds of previously undetected narrow unidentified U-lines. These lines must be formed in a region very close to the photosphere of the star

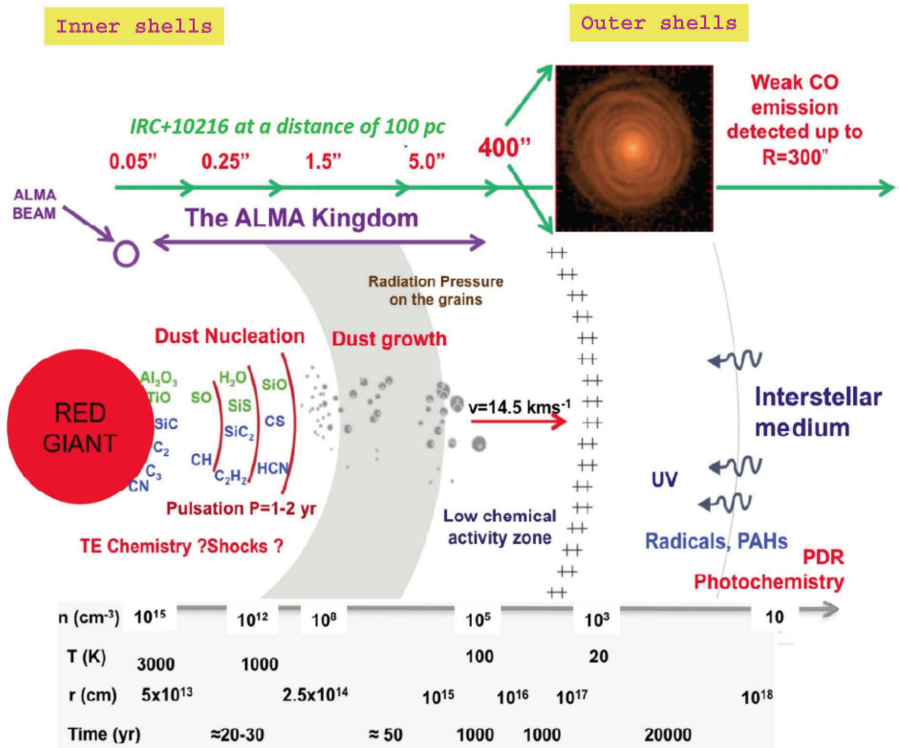

Figure 2 - *Conditions and mechanisms involved in dust grain formation and evolution in AGBs.*

(see **Figure 3**) thus playing an important role in the dust growth processes. These lines could arise from small silicon carbon clusters, whose building blocks are currently unknown. Identifying these U-lines should give us more insights into this question. Furthermore, NANOCOSMOS will provide a detailed and well-quantified view of the regions where dust is formed and the key processes at work. Laser Ablation Chirped-Pulse Fourier Transform Microwave Spectroscopy of SiC rods and other materials will be performed in order to assign the laboratory spectral identifications to the observed ones.

Another important goal to be addressed by the NANOCOSMOS project is the formation of Polycyclic Aromatic Hydrocarbons (PAHs) whose presence is revealed in regions that are irradiated by ultraviolet photons and is especially conspicuous in the protoplanetary and planetary nebula stages of evolved stars. Our current understanding of PAHs is limited by several factors including their large size for theoretical and experimental studies, the confusion-limiting observations in the mid-infrared range of the broad emission features at 6.2, 7.7, 8.6, 11.3 and 12.7 μm, e.g. there is no individual spectroscopic identification of one PAH, and the current lack of identifications in UV-visible spectroscopy. In order to better constrain the PAH population, NANOCOSMOS will explore several formation routes, e.g. the evolutionary scenario that favors the conversion of very small carbonaceous grains into PAHs and the UV radiation-driven polymerization processes proposed for their formation.

It will encompass 5 independent vacuum chambers:

- **MICS (Multiple Ion Cluster Source) chamber.** The MICS is a new optimized route for cluster growth of a standard technique based on a sputtering gas. It will allow the formation of nanoparticles of controlled elemental composition by atomic aggregation.
- **NEON chamber** that will separate neutral from ionized nanoparticles as well as a mass

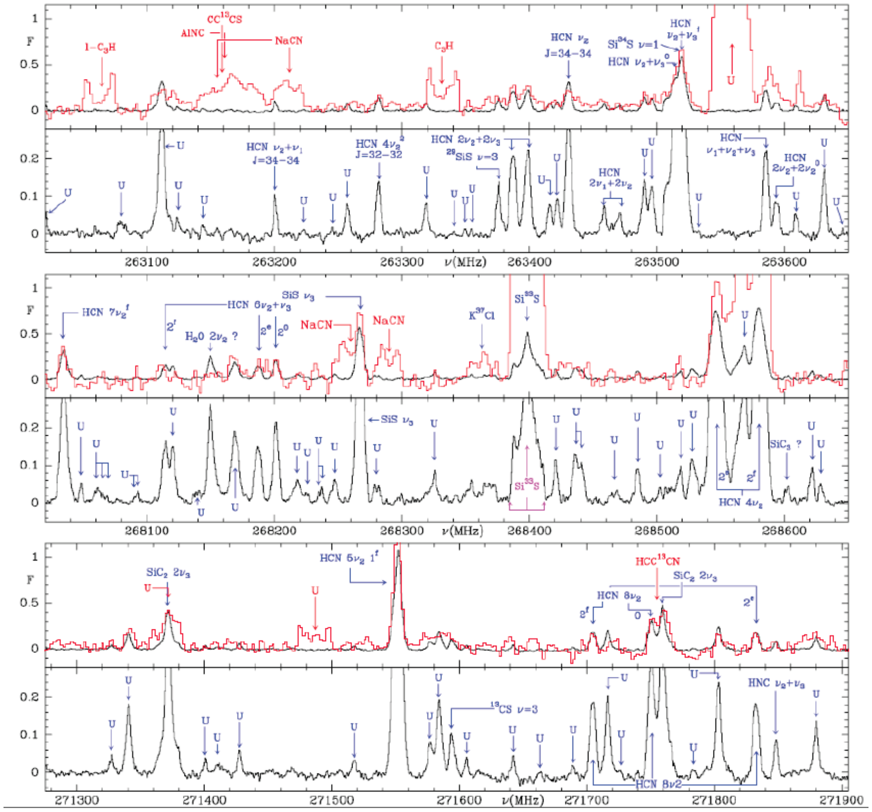

Figure 3 - *Narrow U-lines in the mini-frequency spectral survey of IRC+10216 (from Cernicharo et al., 2013, ApJ, 778, L25).*

selection. It also accelerates, simulating the radiation pressure, and anneals the formed clusters.

- **INTERACTION chamber.** Interaction and chemical reactions will be induced between the generated nanoparticles and molecules in the gas phase (H_2, CH_4, C_2H_2, etc.).
- **INFRA chamber.** In-flight analysis will be performed through UV, visible, near-mid and far-infrared spectroscopy as well as microwave spectroscopy with the new HEMT receivers that will provide the opportunity to study second/minute time-dependent changes in the gas composition using these extremely sensitive radio astronomical receivers.
- **ANA chamber.** This will allow us to collect the nanoparticles to perform X-ray photoelectron spectroscopy (XPS), thermal desorption spectroscopy (TDS), Auger electron spectroscopy (AES) and Ultraviolet photoelectron spectroscopy (UPS) in-situ. Also some in-situ processing can be performed here.

In summary, the Stardust machine will combine different techniques to achieve original studies on individual nanoparticles, their processing to produce complex molecules, the chemical evolution of their precursors, and their reactivity with abundant astronomical molecules. The simulation chambers will be equipped with state-of-the-art in situ and ex situ diagnostics.

The particles that will be collected in the Stardust machine in Madrid will be transferred to the NANOCOSMOS experimental setups developed in Toulouse, AROMA and PIRENEA 2, by means of a vacuum suitcase. The new setup Stardust Molecular Analyzer (AROMA) will perform mass spectrometry analysis of the molecular content (PAHs and other molecular species) of the nanoparticles that will be produced in the different simulation chambers

(Stardust machine and cold plasma reactors). We will be able to combine microprobe spatial resolution capabilities with access to the detailed molecular chemical structure by performing photo-dissociation studies. Another objective of NANOCOSMOS is to demonstrate the potential of this set-up for the characterization of extraterrestrial samples, such as meteoritic grains. The PIRENEA 2 setup consists of cryogenic ion traps and is designed to study the physical and chemical properties of the produced particles in cosmic conditions. These studies will include UV processing and reactivity in isolated conditions together with optical spectroscopy and will be compared to surface science experiments. This setup will also allow us to tackle fundamental questions related to PAHs and associated species (complexes, carbonaceous nanograins, etc.).

NANOCOSMOS is an ambitious project that will try to assess the properties of cosmic dust particles and their impact on the evolution of astronomical objects, from Cosmology to Planet Formation and the Origin of Life. The synergy in NANOCOSMOS between astrophysicists, engineers, molecular and plasma physicists, surface scientists, including both experimentalists and theoreticians is the key to provide a cutting-edge view of cosmic dust.

MORE INFORMATION:

http://www.icmm.csic.es/nanocosmos/

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Abstracts

Very Large Telescope observations of *Gomez's Hamburger:* Insights into a young protoplanet candidate

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Planets are thought to form in the gas and dust disks around young stars. In particular, it has been proposed that giant planets can form via gravitational instability of massive extended disks around intermediate mass stars. However, direct observations to constrain this mechanism lack. We have spatially resolved the 8.6 and 11.2 μm emission of a massive edge on protoplanetary disk around an A star, *Gomez's Hamburger* (GoHam), using VISIR at the Very Large Telescope. A compact region situated at a projected distance of 350 $\pm$ 50 AU South of the central star is found to have a reduced emission. This asymmetry is fully consistent with the presence of a cold density structure, or clump, identified in earlier CO observations, and we derive physical characteristics consistent with those observations: a mass of 0.8 – 11.4 Jupiter masses (for a dust to gas mass ratio of 0.01), a radius of the order of 10^2 astronomical units, a local density of the order of 10^7 cm^{-3}. Based on this evidence, we argue that this clump, which we call GoHam b, is a promising candidate for a young protoplanet formed by gravitational instability, that could be representative of the precursors of massive planets observed around A

stars, like HR 8799 or Beta-pictoris. Further studies at high angular resolution are needed to better constrain the physical properties of this object in order to confirm this proposal.

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Spatially Resolved *Spitzer-IRS* Spectral Maps of the Superwind in M82

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We have mapped the superwind/halo region of the nearby starburst galaxy M82 in the mid-infrared with *Spitzer-IRS*. The spectral regions covered include the H_2 S(1)-S(3), [NeII], [NeIII] emission lines and PAH features. We estimate the total warm H_2 mass and the kinetic energy of the outflowing warm molecular gas to be between $M_{warm} \sim 5-17\times10^6$ $M_\odot$ and $E_K \sim 6-20\times10^{53}$ erg. Using the ratios of the 6.2, 7.7 and 11.3 micron PAH features in the IRS spectra, we are able to estimate the average size and ionization state of the small grains in the superwind. There are large variations in the PAH flux ratios throughout the outflow. The 11.3/7.7 and the 6.2/7.7 PAH ratios both vary by more than a factor of five across the wind region. The Northern part of the wind has a significant population of PAH's with smaller 6.2/7.7 ratios than either the starburst disk or the Southern wind, indicating that on average, PAH emitters are larger and more ionized. The warm molecular gas to PAH flux ratios (H_2/PAH) are enhanced in the outflow by factors of 10 – 100 as compared to the starburst disk. This enhancement in the H_2/PAH ratio does not seem to follow the ionization of the atomic gas (as measured with the [NeIII]/[NeII] line flux ratio) in the outflow. This suggests that much of the warm H_2 in the outflow is excited by

shocks. The observed H_2 line intensities can be reproduced with low velocity shocks ($v < 40$ km s^{-1}) driven into moderately dense molecular gas ($10^2 < n_H < 10^4$ cm^{-3}) entrained in the outflow.

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Carbon/hydrogen clusters [$C_nH_x^+$] formation from laser irradiation of coronene

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This article presents the photo induced dehydrogenation of a cooled molecular jet of coronene, exposed to 266 nm laser radiation. Using unfocused laser radiation of 1064 nm, synchronously coupled with the ionization laser pulses, a system recently developed. Molecular beams were produced by laser desorption of coronene. Analysis of the photoproducts made by time-of flight mass spectrometer showed that a wide variety of ionic species were formed; more than 300 different species were observed. The results showed carbon clusters C_n^+ with n up to 24 as well as carbon/hydrogen clusters $C_nH_x^+$ with masses higher than 300 m/z. The effect on the laser irradiance on the formation of different ions, in the range from 109 W/cm^2 to 1010 W/cm^2, is discussed as it is reflected on the evolution from the big ions to the smaller ones.

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On the origin of the 11.3 micron unidentified infrared emission feature

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The 11.3 μm emission feature is a prominent member of the family of unidentified infrared emission (UIE) bands and is frequently attributed to out-of-plane bending modes of polycyclic aromatic hydrocarbon (PAH) molecules. We have performed quantum mechanical calculations of 60 neutral PAH molecules and found that it is difficult to reconcile the observed astronomi-

cal feature with any or a mix of these PAH molecules. We have further analyzed the fitting of spectra of several astronomical objects by the NASA PAH database program and found that reasonable fittings to the observed spectra are only possible by including significant contributions from oxygen and/or magnesium containing molecules in the mix. A mixed of pure PAH molecules, even including units of different sizes, geometry and charged states, is unable to fit the astronomical spectra. Preliminary theoretical results on the vibrational spectra of simple molecules with mixed aromatic/aliphatic structures show that these structures have consistent bundles of vibrational modes and could be viable carriers of the UIE bands.

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Laboratory Photo-chemistry of PAHs: Ionization versus Fragmentation

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Interstellar polycyclic aromatic hydrocarbons (PAHs) are expected to be strongly processed by vacuum ultraviolet photons. Here, we report experimental studies on the ionization and fragmentation of coronene ($C_{24}H_{12}$), ovalene ($C_{32}H_{14}$) and hexa-peri-hexabenzocoronene (HBC; $C_{42}H_{18}$) cations by exposure to synchrotron radiation in the range of 8 – 40 eV. The results show that for small PAH cations such as coronene, fragmentation (H-loss) is more important than ionization. However, as the size increases, ionization becomes more and more important and for the HBC cation, ionization dominates. These results are discussed and it is concluded that, for large PAHs, fragmentation only becomes important when the photon energy has reached the highest ionization potential accessible. This implies that PAHs are even more photo-stable than previously thought. The implications of this experimental study for the photo-chemical evolution of PAHs in the interstellar medium are briefly discussed.

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ApJ, 804, 1, L7 (2015)

http://iopscience.iop.org/2041-8205/804/1/L7/

Properties of Polycyclic Aromatic Hydrocarbons in the northwest photon dominated region of NGC 7023. III. Quantifying the traditional proxy for PAH charge and assessing its role

Christiaan Boersma[1], **Jesse Bregman**[1] **and Louis J. Allamandola**[1]

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Polycyclic aromatic hydrocarbon (PAH) emission in the Spitzer/IRS spectral map of the northwest photon dominated region (PDR) in NGC 7023 is analyzed. Here, results from fitting the 5.2-14.5 μm spectrum at each pixel using exclusively PAH spectra from the NASA Ames PAH IR Spectroscopic Database (www.astrochem.org/pahdb/) and observed PAH band strength ratios, determined after isolating the PAH bands, are combined. This enables the first quantitative and spectrally consistent calibration of PAH charge proxies. Calibration is straightforward because the 6.2/11.2 μm PAH band strength ratio varies linearly with the ionized fraction (PAH ionization parameter) as determined from the intrinsic properties of the individual PAHs comprising the database. This, in turn, can be related to the local radiation field, electron density, and temperature. From these relations diagnostic templates are developed to deduce the PAH ionization fraction and astronomical environment in other objects. The commonly used 7.7/11.2 μm PAH band strength ratio fails as a charge proxy over a significant fraction of the nebula. The 11.2/12.7 μm PAH band strength ratio, commonly used as a PAH erosion indicator, is revealed to be a better tracer for PAH charge across NGC 7023. Attempting to calibrate the 12.7/11.2 μm PAH band strength ratio against the PAH hydrogen adjacency ratio (duo+trio)/solo is, unexpectedly, anti-correlated. This work both validates and extends the results from Paper I and Paper II

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ApJ, 806, 121 (2015)

http://iopscience.iop.org/0004-637X/806/1/121/

Second Announcement

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

Abstract submission and registration are now open
Deadline for abstract submission: 26 June 2015

Dear colleagues,

This is the second 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:

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 composed 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 can be found on the conference website.

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:

Stefanie Milam (NASA/GSFC)
Alexander Tielens (Univ. Leiden)
Jason Dworkin (NASA/GSFC)
Doug Hudgins (NASA/HQ)
Jamie Elsila (NASA/GSFC)
Murthy Gudipati (NASA/JPL)
Max Bernstein (NASA/HQ)
Louis d'Hendecourt (Université Paris-Sud)

AstroPAH Newsletter

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