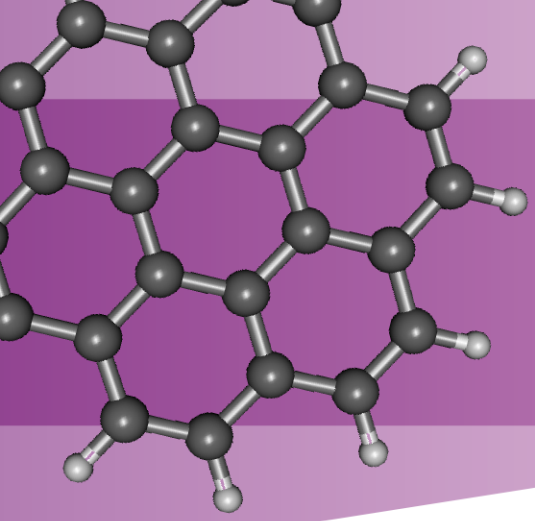
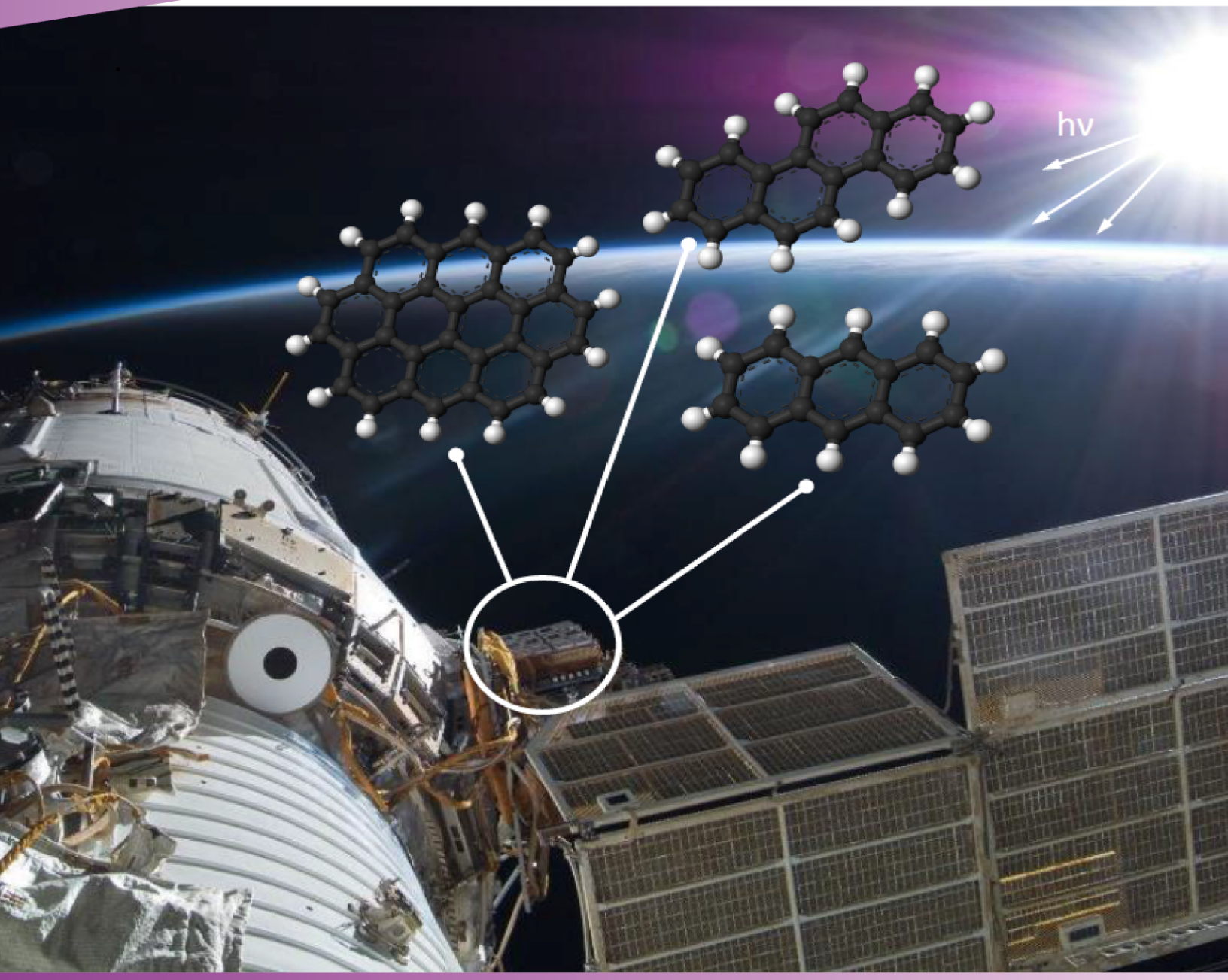


AstroPAH

A Newsletter on Astronomical PAHs

Issue 16 | March 2015



Editorial

Dear Colleagues,

Welcome to the 16th release of AstroPAH!

This month the Picture of the Month features art illustrating the ORGANIC Experiment on EXPOSE-R on board the International Space Station. The first results of this experiment have just been published (see Bryson et al. 2015 in the abstract section). Andreas Elsaesser (Leiden University) and Kathryn Bryson (NASA Ames) talk about this and other experiments in space exposure platforms in the *In Focus* section.

As usual, we have abstracts covering many interesting themes. Do not miss any!

We would like to take the occasion to congratulate Christine Joblin, who has been recently awarded with the prestigious Silver Medal from the French National Center for Scientific research (CNRS). Christine, whose inspiring interview for AstroPAH can be found in AstroPAH Issue 4 (http://astropah-news.strw.leidenuniv.nl/AstroPAH_0004.pdf), received this prize for the "originality, quality and importance of her work, recognized at both national and international level" (http://www.cnrs.fr/fr/recherche/prix/medaillesargent.htm).

We thank you all for your contributions and suggestions. Please, keep them coming! You can send us your contributions at any time. 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: 21 April 2015.
Submission deadline: 3 April 2015.

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PAH Picture of the Month

Cover art illustrating the ORGANIC experiment on EXPOSE-R on board of the International Space Station (ISS). The sample (including PAH molecules) experienced the exposure to solar, cosmic and particle irradiation for about 22 months, with the aim to test the predicted long-term stability of organic molecules.

Credits: Andreas Elsaesser and NASA.

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Design by Isabel Aleman

Current, Past and Future Space Exposure Platforms for Astrochemistry and Astrobiology

by Andreas Elsaesser & Kathryn Bryson

Electromagnetic and cosmic radiation is the main energy source and key driver of astrochemical processes in space. The stability, or instability, of various classes of organic molecules is of high interest to the astrochemistry but also to the astrobiology community. Its implications span from "What is the reservoir of organic molecules in the interstellar medium?" to "How did life evolve on Earth?" and "Which molecules are suitable as biomarkers for life detection missions to other planets?".

Carbon is found in space in all its allotropic forms: diamonds, graphite, and fullerenes (Cataldo et al. 2004; Cataldo & Pontier-Johnson 2002). More than 170 individual carbon-based molecules are detected in interstellar and circumstellar regions (http://www.astro.uni-koeln.de). Numerous organic compounds are observed or have been sampled from our solar system, including planetary surfaces/atmospheres, comets, meteorites, and interplanetary dust. The investigation of the life cycle of organic compounds is highly relevant for cosmochemistry, the origin of life, and the search for life on other planets. An in-depth understanding of the evolution and radiation processing of organic compounds in space requires laboratory studies and theoretical models to support the interpretation of astronomical data. Experiments in low Earth orbit (LEO) offer the unique opportunity to expose samples to the real space environment with a combination of UV and ionizing radiation, vacuum, and microgravity. Space-based experiments are conducted in part due to the difficulty of accurately simulating the entire space environment (such as UV radiation, galactic cosmic ray radiation, microgravity temperature etc.) in the laboratory. Two decades of successful experiments on the International Space Station (ISS) and free-flying satellites have provided new information about the evolution of organic and biological material in space and planetary environments (Guan et al. 2010; Horneck et al. 2010; Rabbow et al. 2012).

Amongst those was the BIOPAN series (BIOPAN-0 to BIOPAN-06), a multi-user facility for astrobiology and radiobiology. The BIOPAN facilities were installed on the outside of the Russian FOTON capsule and stayed typically 14-16 days in Earth orbit where samples could be exposed to the space and radiation environment (Burger 1995; Demets et al. 2005). On BIOPAN a variety of samples were studied ranging from microbiological samples to higher life forms

but also organic molecules such as amino acids and nucleobases (Guan et al. 2010). Part of BIOPAN-05 was the ORGANICS experiment, investigating the stability of polycyclic aromatic hydrocarbons (PAHs) under short space flight conditions (Ehrenfreund et al. 2007). ORGANICS was planned as a precursor experiment for long-term exposure experiments of PAHs in space. A new exposure facility mounted on the outside of the ISS made these long-term exposure experiments possible with the launch of first EXPOSE-E in 2007 (Rabbow et al. 2012) and then later EXPOSE-R in 2009 (Bryson et al. 2011). The ORGANIC experiment on EXPOSE-R (Fig. 1) was investigating the long-term stability of PAHs over an exposure period in LEO of about 22 months. The ORGANIC experiment spent 682 days outside the ISS, providing continuous exposure to the cosmic-, solar- and trapped-particle radiation background and $\sim$2900 h of unshadowed solar illumination with a calculated total (full-spectrum) irradiation dose.

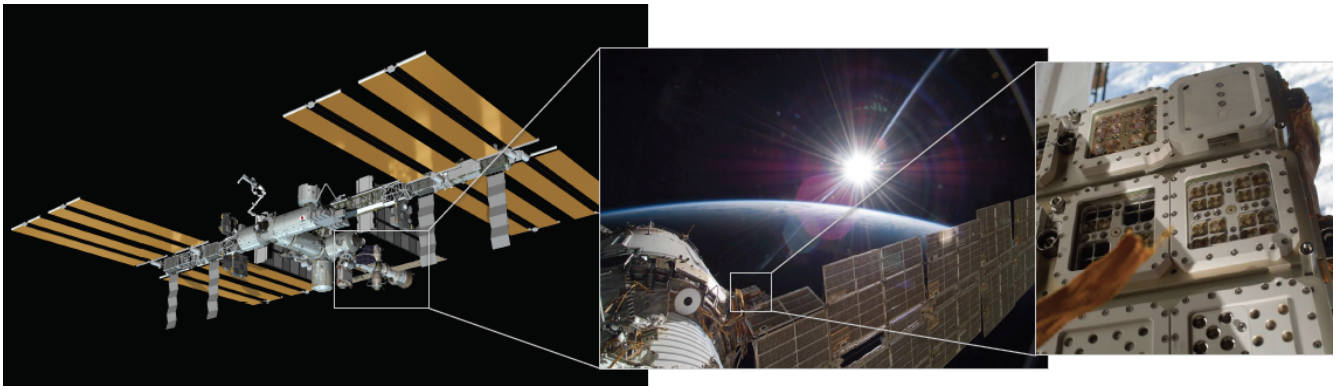

Figure 1 - *Expose-R facility on the ISS, mounted on the outside of the Russian Zvezda module (Image credit: NASA).*

Results from ORGANIC are highlighted in this issue of the PAH Newsletter (Bryson et al. 2015), confirming the stability of compact PAHs. The ORGANIC experiment on EXPOSE-R consists of 14 samples: 11 selected PAHs and the fullerenes C_{60}, C_{70} and a $C_{60}/C_{70}/C_{84}$ mixture. The samples were exposed to UV and particle radiation in the ISS environment (Fig. 1). A carrier with identical samples - not exposed to UV irradiation - was mounted below the carrier. These samples were designated "Dark" samples. In addition to the flight samples, mission ground reference sample carriers (referred to as Experiment Sequence Test (EST) samples) were exposed to vacuum, UV radiation and temperature fluctuation mimicking those on the ISS in a planetary simulation chamber at the Microgravity User Support Center (MUSC) at the German Aerospace Center (DLR). Finally, a complete set of Ground Control Samples was also stored under dark conditions at room temperature in a desiccator from the time of film deposition in August 2009. Limited spectral changes were observed in most cases pointing to the stability of PAHs and fullerenes under space exposure conditions. The results of these experiments confirm the known trend in the stability of PAH species according to molecular structure: compact PAHs are more stable than non-compact PAHs, which are themselves more stable than PAHs containing heteroatoms, the last category being the most prone to degradation in the space environment. The depletion rate was estimated to be of the order of 85 $\pm$ 5 % over the 17 equivalent weeks of continuous unshadowed solar exposure in the most extreme case of tetracene (smallest, non-compact PAH sample), shown on Fig. 2. The insignificant spectral changes (below 10%) measured for solid films of large or compact PAHs and fullerenes indicate a high stability under the range of space exposure conditions investigated on EXPOSE-R. New samples for the successor platform of EXPOSE-R, called EXPOSE-R2, were launched on July 24th 2014. The experiment was activated in November 2014 and will remain in LEO for 12-18 months. Besides microbial and higher organisms samples, EXPOSE-R2 is investigating thin

films of key pigments as well as mineral-associated amino acids for the experiments BIOMEX (de Vera et al. 2012) and P.S.S. (Photochemistry on the Space Station).

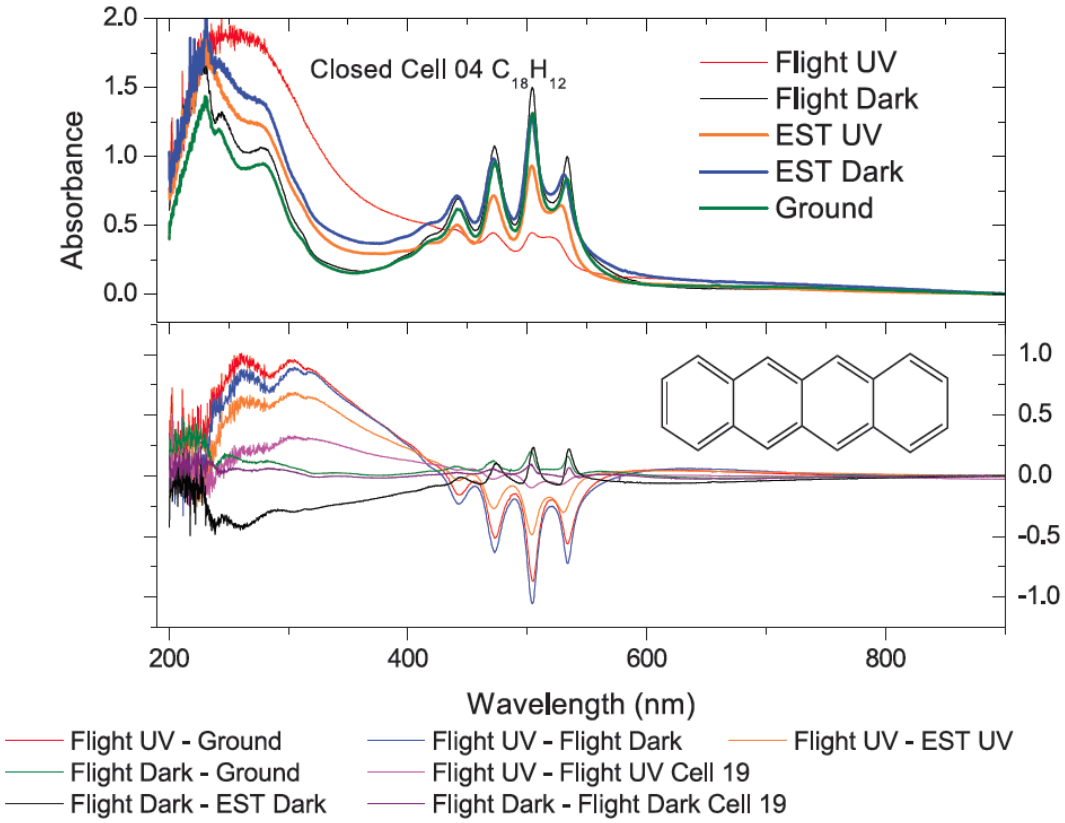

Figure 2 - *UV-Vis spectra of tetracene films deposited on a MgF2 disk (top panel) and calculated residual spectra (bottom panel). The samples exposed to space conditions (Flight UV) show strong changes in absorbance due to UV photolysis leading to absorbance spectral residuals of the order of 10 - 20% for bands in the 400 - 600 nm range (from Bryson et al. 2015).*

Typical astrochemistry samples for space exposure experiments such as BIOPAN and EXPOSE are prepared as transparent organic thin films on optical windows which are integrated into sample cells before being exposed to solar and cosmic radiation. To date, this represents the best analogue to assess the stability of a variety of types and sizes of carbon compounds in replicates. In particular, the stabilities of biomarkers such as amino acids and nucleobases, as well as aromatic hydrocarbons, have been the targets of these experiments (Ehrenfreund et al. 2007; Guan et al. 2010). Amino acids, the building blocks of proteins, are generally the most abundant single class of molecules in a bacterial cell followed by nucleobases (the building blocks of DNA and RNA). Both represent important target molecules in the search for life. PAHs are abundant and ubiquitous in galactic and extragalactic regions, protoplanetary disks, and solar system objects (Sephton 2002; Tielens 2008). Spectral measurements indicate that PAHs in space form a large variety of individual compounds, clusters, and PAH-related molecules (Tielens 2013). A class of aromatic molecules, the quinones, has been formed in numerous laboratory simulations of UV-photolyzed interstellar and planetary ices containing PAHs (Ashbourn et al. 2007; Bernstein et al. 1999). Due to their biological significance in electron transfer processes, the photostability of quinones is of great interest to the astrobiology community. Furthermore, the interaction of organic molecules with inorganic surfaces and their potential catalytic action is becoming increasingly studied in the context of life detection on other planets. The capability to study the effect of organics in contact with inorganic materials in space offers

new possibilities to test theories and models with regard to the origin of life and the search for life.

Most exposure platforms in the past allowed only pre- and postflight-analysis due to their passive nature. The recent progress in active in-situ monitoring of the degradation of organics in LEO using free-flying satellites represents a breakthrough (Mattioda et al. 2012; Nicholson et al. 2011). The O/OREOS mission (Fig. 3) was designed as a demonstration mission for in-situ spectroscopy but also delivered scientifically highly valuable data on the stability of quinones, porphyrins, amino acids and PAHs (Ehrenfreund et al. 2014; Bramall et al. 2012). Free-flying nano-satellites however lack the possibility for sophisticated and elaborate post-flight analysis on ground.

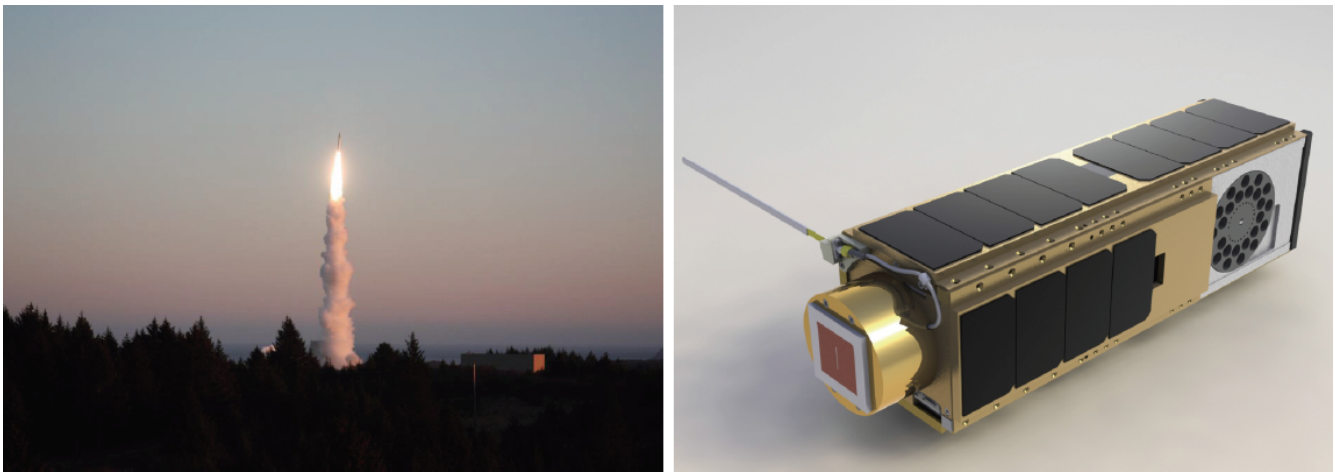

Figure 3 - *Launch of the O/OREOS from Kodiak Island, Alaska, US on November 19th 2010 (left) and (right) drawing of the O/OREOS nanosatellite with its two payloads, SESLO and SEVO, the latter equipped with a miniaturized UV-Vis spectrometer (Image Credit NASA).*

The in-situ concept is also planned for future exposure platforms on the ISS, for example in a new project called OREOcube (Elsaesser et al. 2014). OREOcube is carrying miniaturized UV-Vis spectrometers able to monitor organic-inorganic composite thin films while being exposed to solar and cosmic radiation. OREOcube samples however will be brought back to Earth similar to samples from previous passive exposure platform on the ISS in order to perform non-destructive as well as destructive in depth analyses to understand the effects of space exposure. OREOcube therefore combines the advantages of in-situ measurement capabilities with pre- and post-flight analysis.

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References:

Ashbourn, S.F.M. et al., 2007. Meteoritics & Planetary Science, 42, pp.2035-2041
Bernstein, M.P. et al., 1999. Science (New York, N.Y.), 283(February), pp.1135-1138
Bramall, N.E. et al., 2012. Planetary and Space Science, 60(1), pp.121-130
Bryson, K.L. et al., 2015. International Journal of Astrobiology, 14(01), pp.55-66
Bryson, K.L. et al., 2011. Advances in Space Research, 48(12), pp.1980-1996
Burger, F., 1995. Biopan - a multi-purpose exposure facility for space research. In pp. 313-318
Cataldo, F. et al., 2004. Origins of Life and Evolution of the Biosphere, 34, pp.13-24
Cataldo, F. & Pontier-Johnson, M.A., 2002. Fullerenes, Nanotubes and Carbon Nanostructures, 10, pp.1-14
Demets, R. et al., 2005. Advances in Space Research, 36, pp.311-316
Ehrenfreund, P. et al., 2014. Acta Astronautica, 93(2014), pp.501-508
Ehrenfreund, P. et al., 2007. Planetary and Space Science, 55(2007), pp.383-400
Elsaesser, A. et al., 2014. Langmuir: the ACS journal of surfaces and colloids, 30(44), pp.13217-27
Guan, Y.Y. et al., 2010. Planetary and Space Science, 58, pp.1327-1346
Horneck, G. et al., 2010. Microbiology and molecular biology reviews: MMBR, 74(650), pp.121-156
Rabbow, E. et al., 2012. Astrobiology, 12, pp.374-386
Sephton, M. a, 2002. Natural product reports, 19(0), pp.292-311
Tielens, A. G.G.M., 2008. Annual Review of Astronomy and Astrophysics, 46, pp.289-337
Tielens, A. G.G.M., 2013. Reviews of Modern Physics, 85(SEPTEMBER), pp.1021-1081
De Vera, J.-P. et al., 2012. Planetary and Space Science, 74(1), pp.103-110

Abstracts

First results of the ORGANIC experiment on EXPOSE-R on the ISS

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The ORGANIC experiment on EXPOSE-R spent 682 days outside the International Space Station, providing continuous exposure to the cosmic-, solar- and trapped-particle radiation background for fourteen samples: 11 polycyclic aromatic hydrocarbons and three fullerenes. The thin films of the ORGANIC experiment received, during space exposure, an irradiation dose of the order of 14 000 MJ m^{-2} over 2900 h of unshadowed solar illumination. Extensive analyses were performed on the returned samples and the results compared to ground control measurements. Analytical studies of the returned samples included spectral measurements from the vacuum ultraviolet to the infrared range and time-of-flight secondary ion mass spectrometry. Limited spectral changes were observed in most cases pointing to the stability of PAHs and fullerenes under space exposure conditions. Furthermore, the results of these experiments confirm the known trend in the stability of PAH species according to molecular structure: compact PAHs are more stable than non-compact PAHs, which are themselves more stable than PAHs containing heteroatoms, the last category being the most prone to degradation in the space environment. We estimate a depletion rate of the order of 85$\pm$5% over the 17 equivalent weeks of continuous unshadowed solar exposure in the most extreme case tetracene (smallest, non-compact PAH sample). The insignificant spectral changes (below 10%) measured for solid films of large or compact PAHs and fullerenes indicate a high stability under the range of space exposure conditions investigated on EXPOSE-R.

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http://goo.gl/IxVoGz

Accurate spectroscopy of polycyclic aromatic compounds: from the rotational spectrum of fluoren-9-one in the millimeter wave region to its infrared spectrum.

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The rotational spectrum of fluoren-9-one, a small oxygenated polycyclic aromatic hydrocarbon, has been recorded and assigned in the 52-74.4 GHz region. The determined small negative value of the inertia defect (-0.3 u Å^2) has been explained in terms of vibrational-rotational coupling constants calculated at the B3LYP/cc-pVTZ level of theory. Vibrational anharmonic analysis together with second-order vibrational perturbation theory approximation was applied both to fluorenone and its reduced form, fluorene, to predict the mid- and near-infrared spectra. The data presented here give precise indication on the fluorenone ground state structure, allow for an accurate spectral characterization in the millimeter wave and infrared regions, and hopefully will facilitate extensive radio astronomical searches with large radio telescopes.

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http://scitation.aip.org/content/aip/journal/jcp/142/2/10.1063/1.4905134

A Crossed Molecular Beam and Ab Initio Study on the Formation of 5- and 6-Methyl-1,4- dihydronaphthalene ($C_{11}H_{12}$) via the reaction of Meta-tolyl (C_7H_7) with 1,3-Butadiene (C_4H_6)

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The crossed molecular beam reactions of the meta-tolyl radical with 1,3-butadiene and D6-1,3- butadiene were conducted at collision energies of 48.5 kJ mol^{-1} and 51.7 kJ mol^{-1}. The reaction dynamics propose a complex-forming reaction mechanism via addition of the meta-tolyl radical with its radical center either to the C1 or C2 carbon atom of the 1,3-butadiene reactant

forming two distinct intermediates, which are connected via migration of the meta-tolyl group. Considering addition to C1 proceeds by formation of a van-der-Waals complex below the energy of the separated reactants, we propose that in cold molecular clouds holding temperatures as low as 10 K, the reaction of the meta-tolyl radical with 1,3-butadiene is de-facto barrier less. At elevated temperatures such as in combustion processes, the reaction can also proceed via addition to C2 by overcoming the entrance barrier to addition (11 kJ mol^{-1}). Eventually, the resonantly stabilized free radical intermediate $C_{11}H_{13}$ undergoes isomerization to a cis form, followed by rearrangement through two distinct ring closures at the para- and ortho-position of tolyl radical to yield cyclic intermediates. These intermediates then emit a hydrogen atom forming 6- and 5-methyl-1,4-dihydronaphthalene via tight exit transition states. The steady state branching ratio, 70.0% and 29.2%, at the collision energy of 51.7 kJ mol^{-1}, of 6- and 5-methyl-1,4-dihydronaphthalene, respectively, is determined mainly by the rates of reverse ring opening of cyclic intermediates. The formation of the thermodynamically less stable 1-meta-tolyl-trans-1,3-butadiene was found to be a less important pathway (0.8%). The reaction of the meta-tolyl radical with 1,3-butadiene leads without entrance barrier to two methyl substituted PAH derivatives holding 1,4-dihydronapthalene cores: 5- and 6-methyl-1,4-dihydronaphthalene thus providing a barrierless route to odd-numbered PAH derivatives under single collision conditions.

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Phys. Chem. Chem. Phys. (2015), in press
http://pubs.rsc.org/en/content/articlelanding/2015/cp/c5cp00311c#!divAbstract

Mixed aliphatic and aromatic composition of evaporating very small grains in NGC 7023 revealed by the 3.4/3.3 μm ratio

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Context. A chemical scenario was proposed for photon-dominated regions (PDRs) according to which UV photons from nearby stars lead to the evaporation of very small grains (VSGs) and the production of gas-phase polycyclic aromatic hydrocarbons (PAHs).

Aims. Our goal is to achieve better insight into the composition and evolution of evaporating very small grains (eVSGs) and PAHs through analyzing the infrared (IR) aliphatic and aromatic emission bands.

Methods. We combined spectro-imagery in the near- and mid-IR to study the spatial evolution of the emission bands in the prototypical PDR NGC 7023. We used near-IR spectra obtained with the IRC instrument onboard AKARI to trace the evolution of the 3.3 μm and 3.4 μm bands, which are associated with aromatic and aliphatic C−H bonds on PAHs. The spec-

tral fitting involved an additional broad feature centered at 3.45 μm that is often referred to as the plateau. Mid-IR observations obtained with the IRS instrument onboard the *Spitzer* Space Telescope were used to distinguish the signatures of eVSGs and neutral and cationic PAHs. We correlated the spatial evolution of all these bands with the intensity of the UV field given in units of the Habing field G_0 to explore how their carriers are processed.

Results The intensity of the 3.45 μm plateau shows an excellent correlation with that of the 3.3 μm aromatic band (correlation coefficient R = 0.95) and a relatively poor correlation with the aliphatic 3.4 μm band (R=0.77). This indicates that the 3.45 μm feature is dominated by the emission from aromatic bonds. We show that the ratio of the 3.4 μm and 3.3 μm band intensity ($I_{3.4}/I_{3.3}$) decreases by a factor of 4 at the PDR interface from the more UV-shielded layers ($G_0 \sim 150, I_{3.4}/I_{3.3} = 0.13$) to the more exposed layers ($G_0 > 1 \times 10^4\,, I_{3.4}/I_{3.3} = 0.03$). The intensity of the 3.3 μm band relative to the total neutral PAH intensity shows an overall increase with G_0, associated with an increase of both the hardness of the UV field and the H abundance. In contrast, the intensity of the 3.4 μm band relative to the total neutral PAH intensity decreases with G_0, showing that their carriers are actively destroyed by UV irradiation and are not efficiently regenerated. The transition region between the aliphatic and aromatic material is found to correspond spatially with the transition zone between neutral PAHs and eVSGs.

Conclusions. We conclude that the photo-processing of eVSGs leads to the production of PAHs with attached aliphatic sidegroups that are revealed by the 3.4 μm emission band. Our analysis provides evidence for the presence of very small grains of mixed aromatic and aliphatic composition in PDRs.

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An embedded active nucleus in the OH megamaser galaxy IRAS16399-0937

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We present a multiwavelength study of the OH Megamaser galaxy (OHMG) IRAS16399-0937, based on new HST/ACS F814W and Hα+[N II] images and archive data from HST, 2MASS, Spitzer, Herschel and the VLA. This system has a double nucleus, whose northern (IRAS16399N) and southern (IRAS16399S) components have a projected separation of $\sim$6" (3.4 kpc) and have previously been identified based on optical spectra as a Low Ionization Nuclear Emission Line Region (LINER) and starburst nucleus, respectively. The nuclei are embedded in a tidally distorted common envelope, in which star formation is mostly heavily obscured. The infrared spectrum is dominated by strong polycyclic aromatic hydrocarbon (PAH), but deep silicate and molecular absorption features are also present, and are strongest in the IRAS16399N nucleus. The 0.435-500 μm SED was fitted with a model including stellar, ISM and AGN torus components using our new MCMC code, CLUMPYDREAM. The results indicate that the IRAS16399N contains an AGN ($L_{bol} \sim 10^{44}$ ergs/s) deeply embedded in a quasi-spherical distribution of optically-thick clumps with a covering fraction ≈ 1. We suggest that these clumps are the source of the OHM emission in IRAS16399-0937. The high torus covering fraction precludes AGN-photoionization as the origin of the LINER spectrum, however, the spectrum is consistent with shocks ($v \sim 100 - 200$ km s^{-1}). We infer that the $\sim 10^8$ M$_\odot$ black-hole in IRAS16399N is accreting at a small fraction (~ 1%) of its Eddington rate. The low accretion-rate and modest nuclear SFRs suggest that while the gas-rich major merger forming the IRAS 16399-0937 system has triggered widespread star formation, the massive gas inflows expected from merger simulations have not yet fully developed.

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PAH radiative cooling and fragmentation kinematics studied within an electrostatic ring

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Radiative cooling of polycyclic aromatic hydrocarbon (PAH) cations has been studied using a compact electrostatic ion storage ring, the Mini-Ring, in a time range up to 8 ms. The time evolution of the internal energy distribution of the ensemble of the stored ions was probed using laser induced photo-dissociation at different storage times. For anthracene cation, the observed fast radiative cooling is attributed to fluorescence from thermally excited electronic states populated via inverse internal conversion [1]. In this paper we report on the measurement of the population decay of anthracene cations with a given internal energy. This population decay, directly related to the time shift of the internal energy distribution, is attributed to the radiative cooling mechanism and could be compared with the calculated fluorescence emission rate due to the electronic transition.

By detecting the emitted neutral fragments with a position sensitive detector, information on the fragmentation channels and their qualitative branching ratios were obtained for various PAHs. An odd-even effect was observed for the successive dehydrogenation of pyrene cation $C_{16}H^+_{10-n}$ (n=0-4). This effect is interpreted as an alternation in the dissociation energies and is in agreement with recent calculations [2].

[1] S. Martin, J. Bernard, R. Brédy, B. Concina, C. Joblin, M. Ji, C. Ortéga and L. Chen, Phys. Rev. Lett. 110, 063003 (2013)

[2] B. West, F. Useli-Bacchitta, H. Sabbah, V. Blanchet, A. Bodi, P. M. Mayer and C. Joblin, J. Phys. Chem. A 118, 7824 (2014)

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Small molecules from the decomposition of interstellar carbons

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We have studied the molecular products of the photo-induced decomposition of hydrogenated amorphous carbon (HAC) and solid hexane, C_6H_{14}, using mass spectroscopy. Mass spectra of HAC are dominated by simple hydrocarbon molecules having fewer than four carbon atoms. Notable products include C_3H_2, phenyl, C_6H_5, benzene, C_6H_6, and a variety of partially dehydrogenated alkane molecules with the composition C_nH_{2n-1}. Hexane, chosen as a representative solid alkane, has a more complex mass spectrum which includes C_n and a number of hydrocarbon molecules with up to 10 carbon atoms. As alkyl radicals, C_nH_{2n-1}, are commonly found in the decomposition of alkanes, we have used high precision density functional theory to simulate the infrared spectrum of 1-, 2-, and 3-hexyl radicals as well as that of the 3-hexyl ion, C_6H_{13+}. The latter could be detectable in interstellar/circumstellar sources via a strong feature at 3.66 μm. The appearance of C_3H_2 as a decomposition product of photodissociated HAC may be related to the ubiquitous presence of c-C_3H_2 in the interstellar medium. The production of such molecules in the interstellar medium through a “top-down” chemistry deriving from the decomposition of HAC is discussed.

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A theoretical study on the vibrational spectra of Polycyclic Aromatic Hydrocarbon molecules with aliphtaic sidegroups

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The role of aliphatic side groups on the formation of astronomical unidentified infrared emission (UIE) features is investigated by applying the density functional theory (DFT) to a series of molecules with mixed aliphatic-aromatic structures. The effects of introducing various aliphatic groups to a fixed polycyclic aromatic hydrocarbon (PAH) core (ovalene) are studied. Simulated spectra for each molecule are produced by applying a Drude profile at T=500 K while the molecule is kept at its electronic ground state. The vibrational normal modes are classified using a semi-quantitative method. This allows us to separate the aromatic and aliphatic vibrations and therefore provide clues to what types of vibrations are responsible for the emissions bands at different wavelengths. We find that many of the UIE bands are not pure aromatic vibrational bands but may represent coupled vibrational modes. The effects of aliphatic groups on the formation of the 8 μm plateau are quantitatively determined. The vibrational motions of methyl ($-CH_3$) and methylene ($-CH_2-$) groups can cause the merging of the vibrational bands of the parent PAH and the forming of broad features. These results suggest that aliphatic structures can play an important role in the UIE phenomenon.

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Top-down formation of fullerenes in the interstellar medium

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Fullerenes have been recently detected in various circumstellar and interstellar environments, raising the question of their formation pathway. It has been proposed that they can form by the photo-chemical processing of large polycyclic aromatic hydrocarbons (PAHs). Following our previous work on the evolution of PAHs in the NGC 7023 reflection nebula, we evaluate, using photochemical modeling, the possibility that the PAH $C_{66}H_{20}$ (i.e. circumovalene) can lead to the formation of C_{60} upon irradiation by ultraviolet photons. The chemical pathway involves full dehydrogenation, folding into a floppy closed cage and shrinking of the cage by loss of C_2

units until it reaches the symmetric C_{60} molecule. At 10" from the illuminating star and with realistic molecular parameters, the model predicts that 100% of $C_{66}H_{20}$ is converted into C_{60} in $\sim 10^5$ years, a timescale comparable to the age of the nebula. Shrinking appears to be the kinetically limiting step of the whole process. Hence, PAHs larger than $C_{66}H_{20}$ are unlikely to contribute significantly to the formation of C_{60}, while PAHs containing between 60 and 66 C atoms should contribute to the formation of C_{60} with shorter timescales, and PAHs containing less than 60 C atoms will be destroyed. Assuming a classical size distribution for the PAH precursors, our model predicts absolute abundances of C_{60} are up to several 10^{-4} of the elemental carbon, i.e. less than a percent of the typical interstellar PAH abundance, which is consistent with observational studies. According to our model, once formed, C_{60} can survive much longer than other fullerenes because of the remarkable stability of the C_{60} molecule at high internal energies.Hence, a natural consequence is that C_{60} is more abundant than other fullerenes in highly irradiated environments.

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