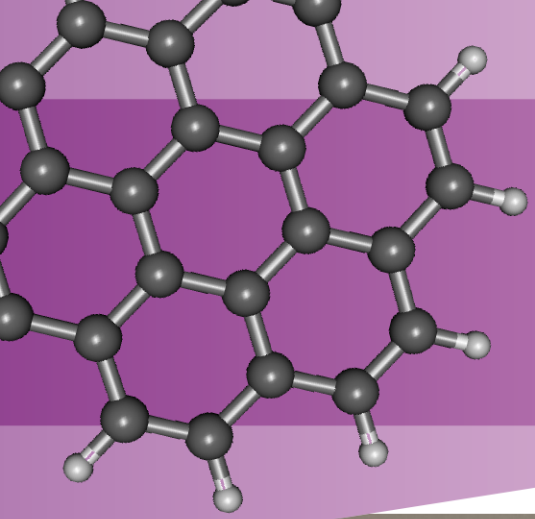

# AstroPAH

A Newsletter on Astronomical PAHs

Issue 43 | November 2017

# JWST SELFIE

# Editorial

**Dear Colleagues,**

Welcome to the 43rd issue of AstroPAH featuring a selfie of the James Webb Space Telescope (JWST). Last week, we received the fantastic news that the Early Release Science proposal linked to PAH research has been awarded. We would like to congratulate the team led by Olivier Berné, Els Peeters and Emilie Habart for this well-deserved achievement.

This month's *In Focus*, written by Olivier Pirali and Jean-Blaise Brubach, presents the Far-Infrared AILES Beamline of Synchrotron SOLEIL, its auxiliary setups and some of the PAH research performed there.

Don't forget to check out the Abstract section. We have interesting reads on the photochemistry of coronene in ices, dissociative ionisation of adamantane, water clustering on PAH surfaces, and the spatial extent of PAHs in the disk of a Herbig star.

If you would like to suggest a person, facility or research project to put in the spotlight, please send us an email! We welcome all suggestions you may have for our In Focus and Picture of the Month sections. Did you receive an award or other great news? Let us know too. We can also promote meetings and vacancies for you, and please keep us up to date on your papers. As always you can send your contributions anytime. For publication in December, you can find the deadlines below.

We thank you all for your contributions so far!

**The Editorial Team**

**Next issue: 21 December 2017.**
**Submission deadline: 8 December 2017.**

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## PAH Picture of the Month

Optical engineer Larkin Carey took a selfie, reflecting onto James Webb Space Telescope's secondary mirror, as part of a test to verify the telescope's optics. More information here

**Credits:** Bell Aerospace.

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

# The Far-Infrared AILES Beamline of Synchrotron SOLEIL

**by Olivier Pirali and Jean-Blaise Brubach**

SOLEIL, an acronym in French for Optimized Light Source of Intermediate Energy for the LURE [1] laboratory, is a research center located on the Plateau de Saclay in Saint Aubin, France. It is an electron accelerator producing synchrotron radiation emitted by relativistic electrons of 2.75 GeV nominal energy. The SOLEIL electron storage ring has a circumference of 354 m. The synchrotron radiation is generated by bending the trajectory of the electrons using a magnetic field (Lorentz force), hence producing an extremely narrow high brilliance light beam tangentially to the electrons' trajectory. Today, 29 operational beamlines extract this radiation covering a wide range of the electromagnetic spectrum from the THz frequencies (few $\mu$eV) to hard X-rays (100 keV). The synchrotron radiation is pulsed (the repetition rate is 352 MHz in the most frequent operation mode of the machine) and can be polarized. SOLEIL covers fundamental research needs in physics, chemistry, material sciences, life sciences, Earth sciences, and atmospheric sciences [1]. It both hosts its own research activities and is a user facility for the international scientific community.

For several beamlines, part of their research activities center around astrophysics applications. In particular the AILES (Advanced Infrared Line Exploited for Spectroscopy), DESIRS (Dichroïsme Et Spectroscopie par Interaction avec le Rayonnement Synchrotron) and SMIS (Spectroscopy and Microscopy in Infrared using Synchrotron) beamlines have relatively strong involvements in the study of PAHs and interstellar dust analogs. DESIRS is an undulator-based beamline covering the VUV range (5-40 eV) with a unique combination of ultra high resolution spectral purity, flux and fully variable polarization. The SMIS spectromicroscopy beamline aims to deliver high brilliance infrared radiation in the 2.5-100 microns spectral range. The beamline is dedicated to microscopic analysis of a large variety of samples. In this article, we will focus on the far-infrared AILES beamline and the instrumentation which has been developed, in part, to study PAHs and related compounds.

[1] Laboratoire d'Utilisation du Rayonnement Electromagnétique

# The Far-Infrared AILES beamline

The AILES beamline was developed for absorption spectroscopy, and it is applied to the study of gas phase as well as condensed phase systems. It covers the electromagnetic spectrum region ranging from the mid- to far-infrared (IR) or THz range (4000 to 5 $cm^{-1}$).

In addition to the increase in flux and brilliance made possible by the Synchrotron Radiation, the beamline has been designed for a high level of mechanical stability to minimize the noise level. The synchrotron emission is extracted by a custom mirror and is redirected through a series of 8 mirrors before being refocused at the entrance of two Michelson-type Fourier-transform infrared (FTIR) interferometers. These two spectroscopic workstations are, in general, dedicated to rovibrational studies of molecular systems (AILES A, with the highest resolution at 0.001 $cm^{-1}$ or about 0.1 $\mu$eV) as well as to studies of optical properties of condensed matter (AILES B with a resolution of 0.007 $cm^{-1}$) [2]. The two experimental workstations are complemented by various sampling devices, enabling different studies of matter in gaseous, liquid and solid phases.

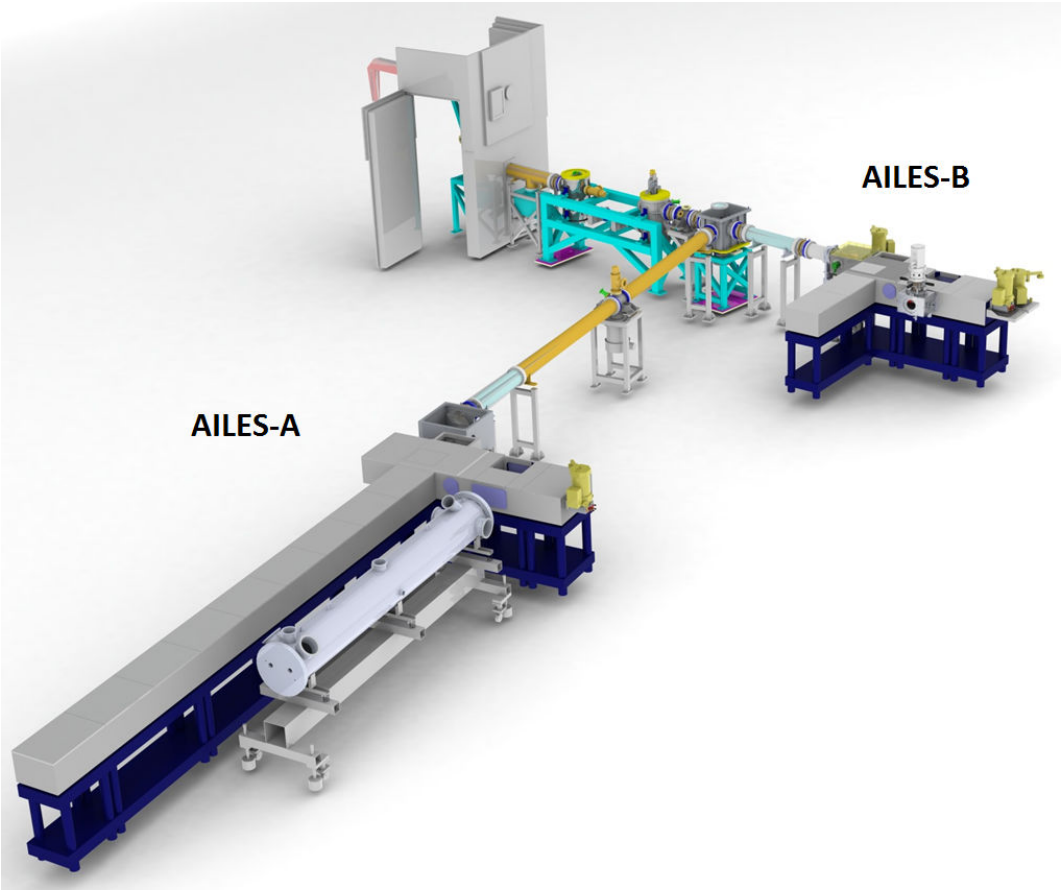


Figure 1: Schematic representation of the AILES beamline endstations. The two FTIR spectrometers allow the spectral characterization of various families of samples in a wide spectral range covering the THz, far-IR and IR spectral ranges.

# Rotationally Resolved far-IR spectroscopy of PAHs

On the AILES-A branch of the beamline, several experimental setups have been developed to record high resolution gas phase absorption spectra of not only neutral, weakly reactive species but also, radical species, ionic species (see e.g. ref [3]), and molecular complexes (see e.g. ref[4]). Starting a few years ago, we used both a room-temperature long pathlength cell and a supersonic jet expansion setup to record rotationally resolved spectra of the smallest members of the PAH family. Because of their sizes (even the smallest PAHs are considered among the largest species for which the rotational structure of vibrational bands can be resolved), very little was known on the rotational structure of the IR/far-IR bands of PAHs, and the IR band contours were always estimated using rotational constants calculated by DFT methods. Our project on the AILES beamline was to measure and analyze the rotational structures of several IR and far-IR bands of two-rings PAHs and their derivatives. In total, about 30 bands were fully analyzed and both ground state and excited states rotational constants were compared to anharmonic DFT calculations performed in collaboration with Manuel Goubet (PhLAM laboratory in Lille, France). Fig. 2 shows an example of such rotationally resolved spectra. The study of this relatively intense band of isoquinoline is a part of a recent article containing the full analysis of the most intense far-IR c-type bands of N-containing 2-rings PAHs derivatives [5].

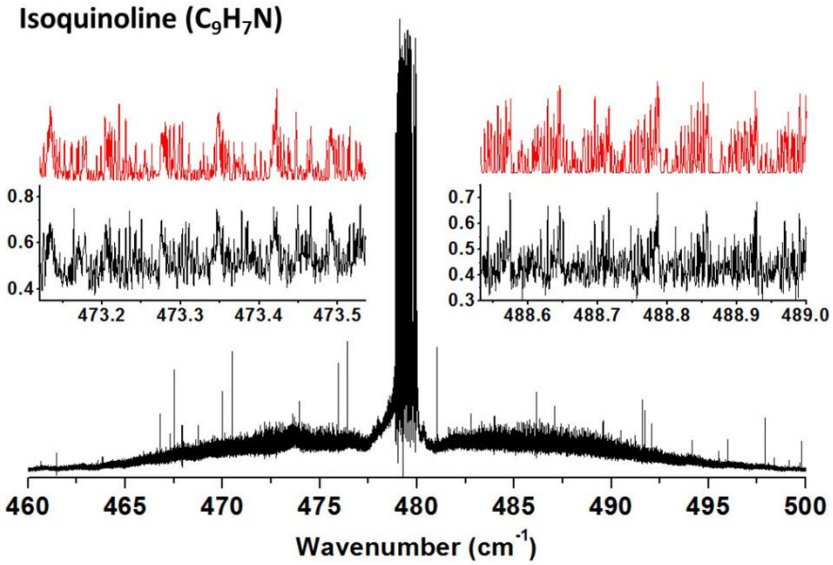


Figure 2: Rotationnally resolved spectrum of the so-called drumhead mode of isoquinoline centered around 480 $cm^{-1}$. In the insets the black traces are zoom-ins of the experimental spectrum, and the red traces are the simulation obtained from the set of derived rotational constants.

Recently, the spectral range available on the AILES beamline has been extended to millimeter and sub-millimeter ranges (70 GHz–950 GHz) thanks to a frequency multiplication chain. It allows us to study the pure rotation spectra of PAHs that have a permanent dipole moment in their ground state as well as finer effects such as rotation-vibration perturbations within the vibrationnally excited states of these molecules [6].

# Experimental setups of the AILES-B branch

The AILES-B branch of the beamline is devoted to condensed matter studies. In condensed matter, exploring the phase diagram as functions of thermodynamic parameters is a efficient way to modify properties of samples in order to understand the microscopic mechanism behind these properties. This ability to study the spectroscopic characteristics of materials as functions of pressure, temperature and/or time is a major issue for synchrotron-radiation-based research. The synchrotron IR light, several times more brilliant than conventional IR sources, is ideal to be coupled with setups requiring high photon flux. Several ensembles designed to investigate condensed matter in complex environments are available on the AILES beamline, and some of them are adapted to the studies of PAHs. For example, a low temperature cryostat setup (4 K–350 K) is used to study interstellar dust analogues, and a high pressure setup allows for the study of the evolution of various samples as a function of pressure and/or temperature.

Since 2007, the AILES beamline has been equipped with the cryostat allowing for spectroscopic measurements as of function of temperature (4 K–350 K) of various samples (solid, liquid or powder) in transmission or in reflexion (normal or grazing angle). In particular, the coupling of this cryostat to the synchrotron beam of the AILES beamline allows the study of the optical properties of analogues of interstellar silicate grains at low temperature in the FIR/submm range [7]. The far-infrared to millimeter wavelength (FIR-mm) range in astronomical observations is dominated by the thermal emission from large (10–100 nm) and cold (10–20 K) dust grains, which are in thermal equilibrium with the interstellar radiation field. However, the physics of the FIR-mm emission from such cold matter is not well understood as shown by the observed temperature dependance of the spectral index of the dust emissivity $\beta$, a similar behavior is also observed in characterization experiments of the spectral properties of dust analogues. Several studies have been performed on various dust analogues with Fe or Mg-rich amorphous silicate in the aims to provide spectroscopic data of realistic cosmic dust analogues to astronomers for the interpretation of observations.

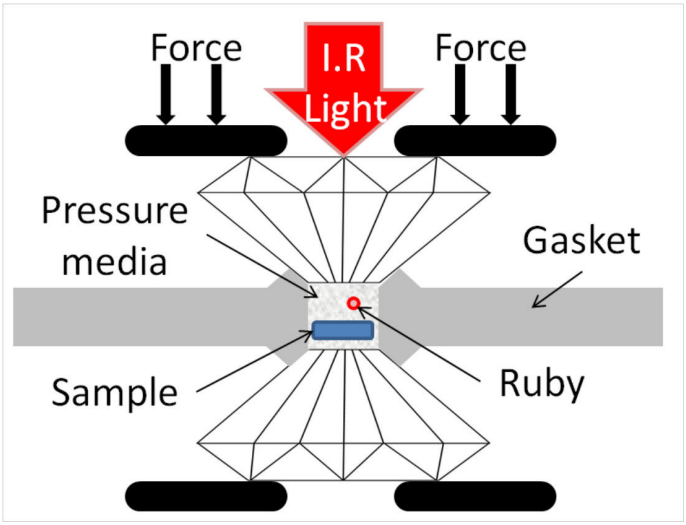


Figure 3: Schematic view of a DAC. The sample is inserted in the gasket hole between diamonds.

Recently, the AILES beamline has been equipped with a setup setup which allows for the rapid and reproducible measurement of the far IR spectra of samples under high pressure. In this configuration, the high photon flux synchrotron IR light is coupled with a high pressure setup based on Diamond Anvil Cells (see Figure 3). Diamonds are transparent in the IR and THz ranges and are therefore well suited for DAC based transmission or reflectivity experiments. The DAC can be used as the sample cell in such ensembles as our high pressure, low temperature (HPLT) setup [8]. The design and development of the HPLT was achieved with the following requirements(Figure 4): (i) The pressure applied to the sample can reach at least 20 GPa. The size of the sample typically ranges between 30 to 300 $\mu$m in diameter and 10 to 80 $\mu$m in thickness cf. Figure 4. (ii) The setup is compatible with a wide spectral range (all IR region down to 20 cm$^{-1}$). (iii) The temperature of the sample can reach 20 K. This implies that the vacuum inside the chamber is sufficient ($10^{-7}$ mbar at low temperature) to prevent the condensation of a large amount of residual water molecules on the cell, hence degrading the quality of the measurements. (iv) The setup allows for in situ change and reading of the pressure within the cell. (v) The optical setup allows for measurement of IR transmission or reflectivity.

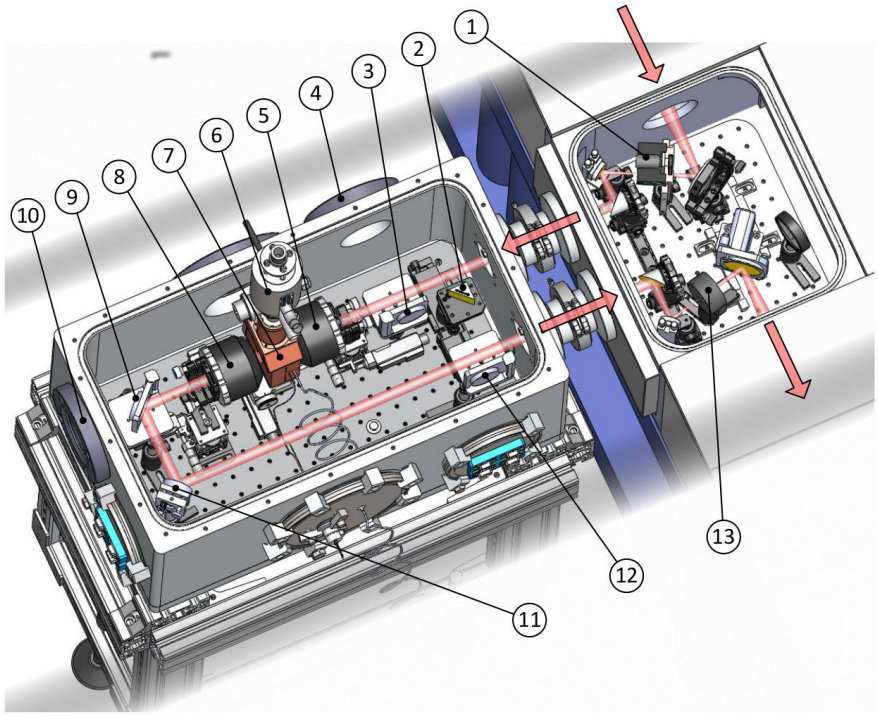


Figure 4: Component layout of the HPLT setup inserted in the vacuum chamber and spectrometer: (1) Polarizer, (2) knife-edge right angle mirror, (3, 9, 12) movable flat mirrors, (4, 10) viewports, (5, 8) cassegrain reflective objectives, (6) cryostat, (7) diamond anvil cell, (11) fixed flat mirror, (13) aperture.

The HPLT device now available at the AILES beamline allows studies by IR spectroscopy of PAHs in a wide range of thermodynamic conditions. Among them the superconducting mechanism in PAHs is still a matter of theoretical and experimental debate as shown for the studies of solid picene ($C_{22}H_{14}$) under pressure up to 8 GPa [9].

In summary, the AILES beamline of synchrotron SOLEIL provides several experimental setups suitable to the IR/far-IR spectroscopic study of PAHs and dust analogs in the gas phase and condensed phase. Potential users interested by the experimental opportunities of the beamline are invited to contact O. Pirali and J.-B. Brubach for details. Proposals for beamtime allocation are submitted by users twice a year (the deadlines are September 15th and February 15th) on the following website: http://sunset.synchrotron-soleil.fr/sun/


## Acknowledgments

The authors would like to thank the AILES beamline staff, and P. Roy the beamline manager. O. P. would like to thank M. A. Martin-Drumel and S. Gruet for their large implications in the development of the different experimental stations of the AILES-A branch.

**Olivier Pirali** (CNRS Researcher, Institut des Sciences Moléculaires d'Orsay, Université Paris-Saclay, France) obtained his PhD in 2004 on Fourier Transform spectroscopy in the far-IR (Université Paris-Sud). In 2005, he joined the Dennis Tokaryk group (Physics Department, University of New Brunswick, Canada) to study the electronic spectra of high spin multiplicity states of $N_2$ and $C_3$. He then did a post-doctoral fellowship in the Jos Oomens group (Nieuwegein, the Netherlands) where he studied the IR spectra of large C-bearing cations (PAHs and diamandoids) at the FELIX free electron laser facility. Olivier joined the French Research Science Center (CNRS) in 2006 to develop an activity on high resolution gas phase spectroscopy in the far-IR using the synchrotron continuum extracted by the AILES beamline of the SOLEIL facility. There, he studies the high resolution rotational and ro-vibrational spectra of large carbonated molecules (2-ring PAHs, their derivatives, diamondoids) as well as light open-shell molecules (radicals and ions).

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**Jean-Blaise Brubach** (Beamline Scientist, Synchrotron SOLEIL, Saint-Aubin) obtained his PhD on the dynamics of water molecules in bulk and in confining systems in 2002 (Université Paris-Sud). He joined SOLEIL in 2005. After his PhD, he obtained a postdoctoral position at the University of Pharmacology of Chatenay Malabry (Val de Marne, France) for the society Gattefossé S.A. where he studied lipid excipient for drug targeting for drug delivery. He has participated in the installation and development of the AILES beamline devoted to IR spectroscopy, particularly in the THz range. His main responsibility at the AILES beamline of SOLEIL is related to soft matter and bio-chemistry research.

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# Abstracts

## Photochemistry of Coronene in Cosmic Water Ice Analogs at Different Concentrations

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This work presents the photochemistry of ultraviolet (UV) irradiated coronene in water ices at 15 K, studied using mid-infrared Fourier transform (FTIR) spectroscopy for $C_{24}H_{12}$:$H_2O$ at concentrations of (1:50), (1:150), (1:200), (1:300), and (1:400). Previous UV irradiation studies of anthracene:$H_2O$, pyrene:$H_2O$, and benzo[ghi]perylene:$H_2O$ ices at 15 K have shown that aromatic alcohols and ketones, as well as $CO_2$ and $H_2CO$, are formed at very low temperatures. Likewise, here, in addition to the coronene cation, hydroxy-, keto-, and protonated coronene (coronene-$H^+$) are formed. The rate constants for the decay of neutral coronene and for the formation of the photoproducts have been derived. It is shown that PAHs and their UV-induced PAH:$H_2O$ photoproducts have mid-infrared spectroscopic signatures in the 5–8 µm region that can contribute to the interstellar ice components described by Boogert et al. (2008) as C1–C5. Our results suggest that oxygenated and hydrogenated PAHs could be in UV-irradiated regions of the ISM where water-rich ices are important.

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The Astrophysical Journal, 848, 112 (2017)

https://doi.org/10.3847/1538-4357/aa8c71

# The Spatial Extent of Polycyclic Aromatic Hydrocarbons Emission in the Herbig Star HD 179218

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We investigate, in the mid-infrared, the spatial properties of the Polycyclic Aromatic Hydrocarbons (PAHs) emission in the disk of HD 179218, an intermediate-mass Herbig star at ∼300 pc. We obtained mid-infrared images in the PAH-1, PAH-2 and Si-6 filters centered at 8.6, 11.3, and 12.5 µm, and N-band low-resolution spectra using CanariCam on the 10-m Gran Telescopio Canarias (GTC). We compared the point spread function (PSF) profiles measured in the PAH filters to the profile derived in the Si-6 filter, where the thermal continuum emission dominates. We performed radiative transfer modeling of the spectral energy distribution (SED) and produced synthetic images in the three filters to investigate different spatial scenarios. Our data show that the disk emission is spatially resolved in the PAH-1 and PAH-2 filters, while unresolved in the Si-6 filter. Thanks to very good observing conditions, an average full width at half maximum (FHWM) of 0.232″, 0.280″ and 0.293″ is measured in the three filters, respectively. Gaussian disk fitting and quadratic subtraction of the science and calibrator PSFs suggests a lower-limit characteristic angular diameter of the emission of ∼100 mas, or ∼40 au. The photometric and spectroscopic results are compatible with previous findings. Our radiative transfer (RT) modeling of the continuum suggests that the resolved emission should result from PAH molecules on the disk atmosphere being UV-excited by the central star. Simple geometrical models of the PAH component compared to the underlying continuum point to a PAH emission uniformly extended out to the physical limits of the disk model. Furthermore, our RT best model of the continuum requires a negative exponent of the surface density power-law, in contrast with earlier modeling pointing to a positive exponent. We have spatially resolved for the first time to our knowledge the PAHs emission in the disk of HD 179218 and set constraints on its spatial extent. Based on spatial and spectroscopic considerations as well as on qualitative comparison with IRS 48 and HD 97048, we favor a scenario in which PAHs extend out to large radii across the flared disk surface and are at the same time predominantly in an ionized charge state due to the strong UV radiation field of the 180 $L_{\odot}$ central star.

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A&A in press (2017)

http://arxiv.org/abs/1711.05202

# Dissociative Ionisation of Adamantane: A Combined Theoretical and Experimental Study

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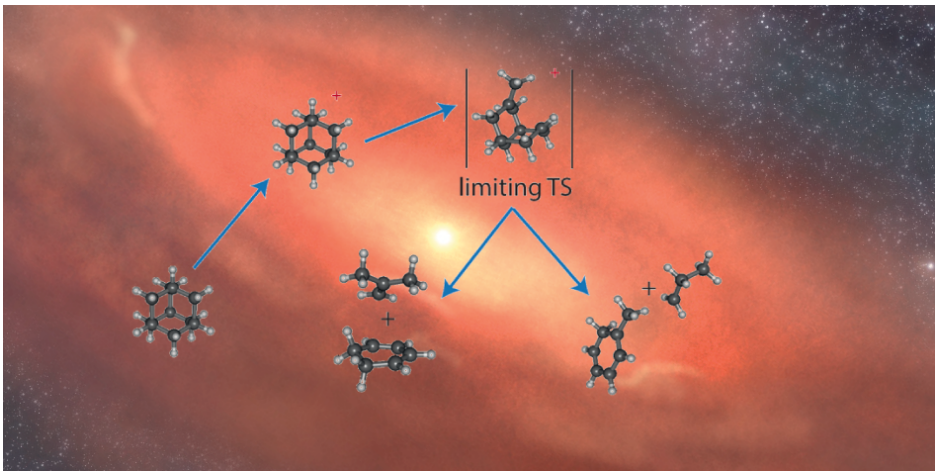


Figure 5: Adamantane, the smallest nanodiamond molecule, dissociates mostly through $C_4H_8$ and $C_3H_7$ loss, yielding small hydrocarbons as product. (Background ESO).

Diamond nanoparticles, or nanodiamonds, are intriguing carbon-based materials which, maybe surprisingly, are the most abundant constituent of presolar grains. While the spectroscopic properties of even quite large diamondoids have already been explored, little is known about their unimolecular fragmentation processes. In this paper we characterise the dissociative ionisation of adamantane ($C_{10}H_{16}$) - the smallest member of the diamondoid family - utilising imaging Photoelectron Photoion Coincidence (iPEPICO) spectroscopy and Density Functional Theory (DFT) calculations. We have found adamantane to dissociatively photoionise via several parallel channels of which H, $C_3H_7$ and $C_4H_8$ losses are the most important ones. Calculations confirm the existence of a rate-limiting transition state for the multiple C-loss channels, which is located at 10.55 eV with respect to neutral adamantane. In addition, we found dissociation channels leading to small cationic hydrocarbons, which may be relevant in the interstellar medium.

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Accepted for publication in Physical Chemistry Chemical Physics

http://dx.doi.org/10.1039/C7CP05957D

# Capturing the Elusive Water Trimer from the Stepwise Growth of Water on the Surface of the Polycyclic Aromatic Hydrocarbon Acenaphthene

**Amanda L. Steber[1,2,3,4], Cristóbal Pérez[1,2,3,4], Berhane Temelso[5], George C. Shields[5], Anouk Rijs[6], Brooks H. Pate[7], Zbigniew Kisiel[7], and Melanie Schnell[1,2,3,4]**

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Polycyclic aromatic hydrocarbons (PAHs) are key players in reaction chemistry. While it is postulated that they serve as a basis for ice grains, there has been no direct detection of PAHs in astronomical environments. We aim to investigate the hydration of PAHs to set a foundation for the future exploration of potential ice formation pathways. We report results from chirped pulse Fourier transform microwave spectroscopy and quantum-chemical calculations for the PAH acenaphthene and acenaphthene complexed with up to four water molecules. The acenaphthene-$(H_2O)_3$ complex is of particular interest as the elusive cyclic water trimer was observed. It appears in a slightly distorted configuration when compared with the pure water trimer. This is explained by hydrogen-bond net cooperativity effects. Binding energies for the complexes are presented. Our results provide insight into the onset of complex aggregation that could be occurring in extraterrestrial environments as part of ice grain formation.

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J. Phys. Chem. Lett. 8, 5744 (2017)

http://pubs.acs.org/doi/pdf/10.1021/acs.jpclett.7b02695

# Announcements

## Post-doc Position in Laboratory Astrophysics/Astrochemistry

### Advertised by: Gianfranco Vidali, Professor of Physics, Syracuse University, Syracuse, NY (USA)

**Deadline for Application: until filled**

The Physics Department at Syracuse University is soliciting applications for a post-doc position in the laboratory astrophysics/astrochemistry under the supervision of Prof. Gianfranco Vidali. A highly motivated and accomplished recent PhD graduate is sought to work on NSF-funded, ongoing experiments of molecule formation on analogs of dust grains in simulated space conditions. The position is for one year. A PhD in Physics or closely related fields is required. The candidate should have working experience in laboratory astrophysics/astrochemistry and/or surface science. Experience in working with ultra-vacuum technology, atomic/molecular beam techniques, and computer simulations is highly prized.
For full consideration please complete an online faculty application (https://www.sujobopps.com/postings/72239) and attach the following documents:

- CV/Resume
- Cover Letter
- A list of publications (attach to ”Other Document”)
- A list of professional references
- Research Statement (attach to ”Writing Sample”) describing research accomplishments and how the candidate would contribute to the research pursued in Prof. Vidali’s laboratory. Research statement not to exceed 3 pages.

To learn more about this position and to apply, go to: https://www.sujobopps.com/postings/72239. To learn more about research done in Prof. Vidali’s group, including recent research accomplishments, please go to http://astro.syr.edu or contact Prof. Gianfranco Vidali.

E-mail contact: gvidali@syr.edu
Webpage: http://astro.syr.edu

**AstroPAH Newsletter**

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