

AstroPAH

A Newsletter on Astronomical PAHs

Issue 23 | November 2015

A vibrant, multi-colored nebula or galaxy image. The center is a bright, white-yellow source of light, possibly a star or a young stellar object, from which several bright, white rays of light extend outwards. The surrounding gas and dust are composed of various colors, including shades of blue, green, red, and yellow, creating a dynamic and ethereal appearance against a dark, star-filled background.

Egg Nebula

Editorial

Dear Colleagues,

Welcome to the 23rd edition of AstroPAH!

Our Picture of the Month is the Egg Nebula, a beautiful pre-planetary nebula where small hydrocarbons have been detected.

Grab your cup of coffee and enjoy the In Focus about the FELIX Laboratory, three interesting papers on the fragmentation of PAH isomers, the chemisorption and diffusion of hydrogen on PAH flakes and the observation of C_{60}^+ and C_{60}^{2+} in the laboratory and in space, and news about future meetings and open positions.

We thank you all for your contributions and please keep them coming. You can send us your contributions anytime. For publication in December, 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 visit our webpage or contact us (links in the next page).

Best regards,

The Editorial Team

Next issue: 15 December 2015.

Submission deadline: 4 December 2015.

AstroPAH Newsletter

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PAH Picture of the Month

The Egg Nebula (CL 618) is a young planetary nebula, the dust and gas ejecta of an old low/intermediate mass star. Small hydrocarbons – C₆H₆, C₄H₂, C₄H₆ – were detected in this object (Cernicharo et al., 2001, ApJ, 546, L123). These molecules are probably associated with a toroid of gas and dust (dark lane in the image) that blocks the direct view of the central star. Dust particles in the nebula process and scatter the light from the star, creating the concentric rings structures and the beams of light seen in the image.

Credits: (Credit: ESA/Hubble, NASA)

CONTACT

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Newsletter Design: Isabel Aleman

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

Astrochemistry and PAH IR spectroscopy at the FELIX Laboratory

by Jordy Bouwman, Jos Oomens, and Britta Redlich

Already early on in the development of the PAH hypothesis, it was realized that ionized PAHs likely possess long lifetimes under the low-density conditions of the ISM and that their contribution to the observed emission bands may be substantial, especially in strongly irradiated regions of the ISM. Perhaps even more interesting, the IR spectra of radical cation PAHs were found to deviate substantially from those of their neutral counterparts, particularly in terms of relative intensities of the bands in the various ranges of the IR. The laboratory study of the IR spectra of ionized PAHs has therefore been of profound interest since the early days of the hypothesis.

Tandem mass spectrometry (MS) is an ideal tool to generate, store, manipulate and isolate gaseous ionic PAH species. Not only can one generate the radical cation of a (commercially available) neutral PAH molecule, the tandem mass spectrometer can be used as a “gas-phase test tube” in which one can let the ionic PAH undergo reactions and mass-select product ions of interest. Tandem MS thus allows one to study ionized PAHs in various forms, including protonated, dehydrogenated, deprotonated (anionic) and fragmented PAHs. Such experiments are typically not possible for neutral (condensed-phase) species as the mass spectrometer provides careful selection of the species of interest from a possible zoo of species present.

The density of ionized PAHs in any (storage) mass spectrometer is extremely low as a consequence of Coulombic repulsion between the ions; expressed in terms of pressure, typical ion trap mass spectrometers store ions at pressures well below 10^{-12} mbar. This is clearly many orders of magnitude too low for absorption spectroscopy methods, even using long path lengths such as in cavity-enhanced absorption methods. A particularly interesting alternative when working in a mass spectrometer is photo-dissociation spectroscopy: the degree of dissociation induced by a monochromatic source is recorded as a function of the wavelength of the radiation and used to determine the wavelength-dependent absorption strength of the ion. A plot of the dissociation yield versus wavelength is then used as a surrogate for the absorption spectrum (**see textbox 1**). The technique obviously relies on the availability of a laser tunable across the IR wavelength range of interest, which should also possess a sufficiently high output power to be able to induce dissociation by the absorption of multiple IR photons. The Free Electron Laser for Infrared eXperiments (FELIX) at our institute has proven to be an excellent light source for such experiments.^[1] **Textbox 2** gives an overview of the layout of the FELIX Laboratory and some key characteristics of the free electron lasers.

Infrared and THz Action spectroscopy

Infrared absorption spectroscopy is a standard tool for the investigation of molecules and matter. However, it is not straightforwardly applicable to species at very low densities in the gas phase, such as molecules in molecular beam expansions, ionic species, weakly-bound complexes and clusters. Several versions of the so-called action spectroscopy method have been developed to circumvent this problem. These techniques have in common that they measure the effects in the sample induced upon irradiation by the light instead detecting directly the absorption, *i.e.* the change in intensity of the transmitted light beam.

Mechanism of Action spectroscopy

Species under study are irradiated with the output of an infrared or THz (free electron) laser. When the laser frequency is in resonance with an allowed IR transition in the sample, photon absorption occurs, leading to an action, *e.g.* dissociation or ionization, which is detected mass spectrometrically. Monitoring the photodissociation yield as a function of the IR frequency provides the IR spectrum of the species. As the dissociation thresholds for covalently-bound species are higher than the IR photon energies, multiple photons need to be absorbed sequentially and call for a powerful light source. Wide frequency coverage is required to provide spectra that can be analysed to determine the structure of the species. This assignment generally requires the comparison with computed IR spectra for a given structure.

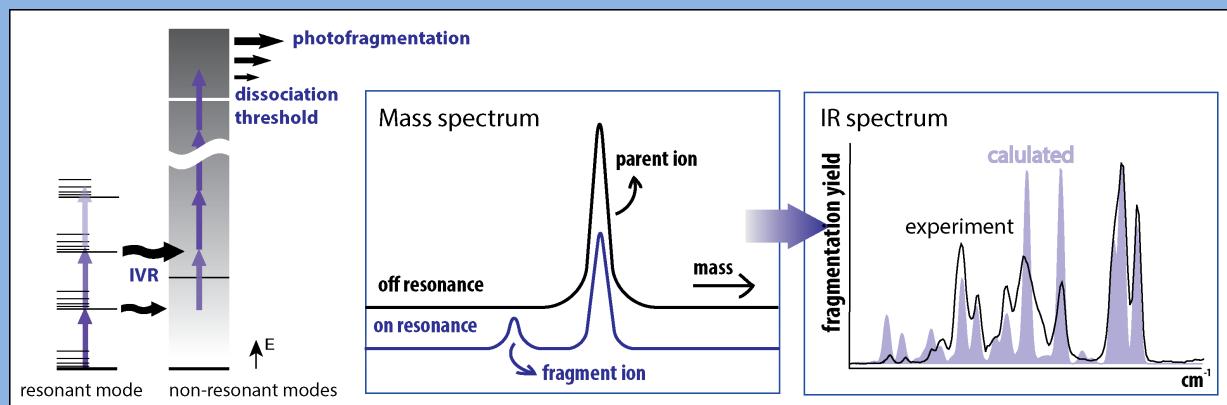
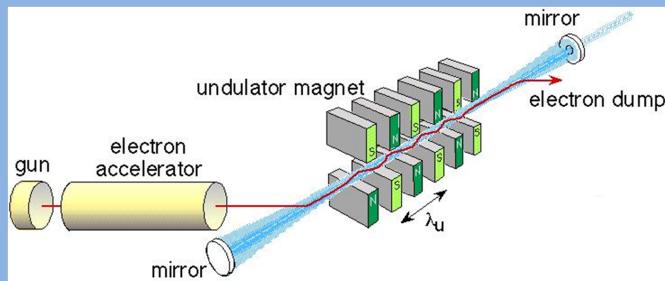


Figure 1: Left - *The mechanism of IR multiple photon excitation.* Infrared light is resonantly absorbed, the energy is redistributed and the sample is ready to absorb another photon. This process repeats until e.g. the dissociation threshold is reached, and photofragmentation occurs. Middle - *Mass spectrometric detection.* When the laser is tuned to resonance, a decrease in intensity of the parent ion peak and the appearance of the fragment ion peak are observed. Right – *Recording of the infrared spectrum.* By monitoring the fragmentation yield as a function of the IR wavelength, an IR spectrum can be constructed. Structural information can be inferred from comparison of this experimental spectrum with calculated IR spectra for candidate structures.

Experimental IR spectra for an extensive series of ionized PAHs and related molecules have been reported, starting with the radical cation versions of regular PAHs and PANHs.^[2,3] More exotic species, with no obvious neutral analogue have more recently come into focus. An interesting example is ionic H-deficient PAHs $[\text{PAH-H}]^+$. IR spectroscopy showed that despite the even-electron nature of these species, they possess radical (*i.e.* triplet) ground states^[4]. Based on quantum-chemical computations alone, deciding whether these ions have singlet or triplet ground electronic states is difficult. From an astro-chemical viewpoint, spectra for such species are typically not in PAH spectral databases, but are significantly different from the species in their singlet electronic state.

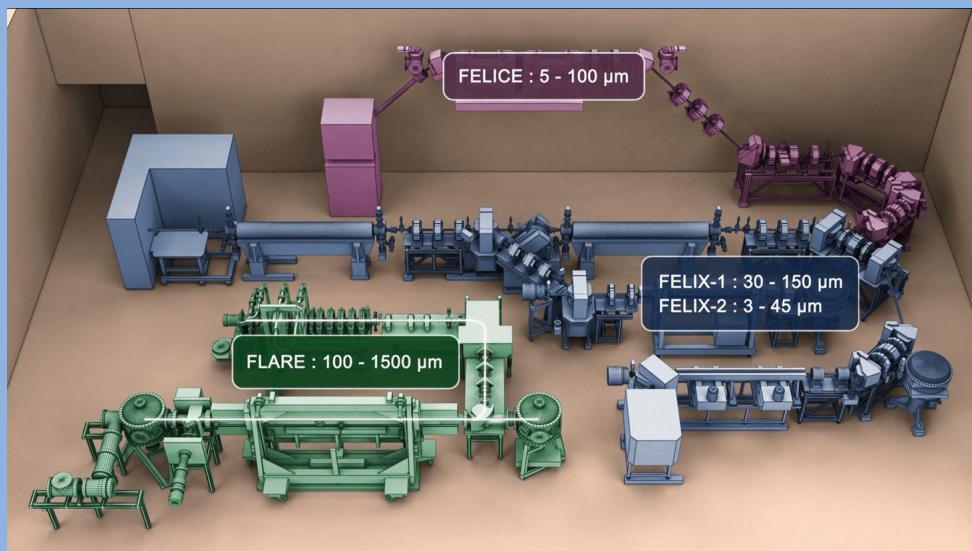
Free Electron Lasers

Free Electron Lasers (FELs) are versatile devices that can operate in the entire range of the electromagnetic spectrum and nowadays FELs exist around the world from the THz to the X-Ray regime. They are based on the radiation emitted by electrons as they move on a curved trajectory with a velocity close to the speed of light. For amplification of the spontaneously emitted light either very long undulators or a resonator cavity are required; the latter version is shown in the principle layout scheme.



FELIX Laboratory – Infrared and THz free electron lasers

The FELIX Laboratory operates two independent free electron lasers that together comprise 4 beam lines – FLARE, FEL-1, FEL-2 and FELICE providing pulsed, continuously tunable, high intensity infrared and THz radiation to 14 dedicated experimental stations.



The primary applications are found in areas benefitting either from the high brightness or the high fluence the FEL laser sources offer. Studies on saturation-relaxation phenomena e.g. applying techniques as pump-probe or photon-echo measurements make use of the high peak powers to investigate a variety of samples ranging from solid state to biological systems. Over the last decade, it has been demonstrated that the FELIX output has some unique features that make it highly suitable for IR-spectroscopy of (bio)molecules, complexes and clusters in the gas phase using various techniques summarized under 'action spectroscopy'. These require high fluence and a wide and continuous tuning range and provide structural information that is difficult if not impossible to obtain otherwise.

FELICE - The FELICE (Free Electron Laser for Intra-Cavity Experiments) beam line is the only FEL beam line in the world dedicated to intra-cavity experiments enabling optical studies on molecules, complexes and cluster throughout the infrared spectral region with unprecedented photon flux enabling new opportunities for e.g. very strongly bound systems such as PAHs.

The FELIX is an international user facility providing access and support to external user; for more Information: www.ru.nl/felix or felix@science.ru.nl.

Negatively charged PAHs (formally a deprotonated PAH) have also been investigated at the FELIX Laboratory and an example is shown in Figure 2^[5]. Anionic PAHs have been hypothesized to be abundantly present in dense regions of high metallicity, and have even been suggested to become the main carriers of negative charge in such regions. Forming the deprotonated PAHs in the mass spectrometer is a multi-step process that makes use of the ion-manipulation possibilities of a tandem mass spectrometer. PAHs are not very acidic and do not easily give up a proton. Therefore, the experiment utilized PAH carboxylic acid molecules, such as naphthoic acid (naphthalene with a -COOH functional group), as precursor. Electrospray ionization generates an abundant naphthoate anion, which under mild activation undergoes dissociation to yield a neutral CO₂ molecule and the naphthyl anion (C₁₀H₇⁻). This product can then be mass-isolated and its IR spectrum can be recorded by photo-dissociation (or detachment) spectroscopy using FELIX.

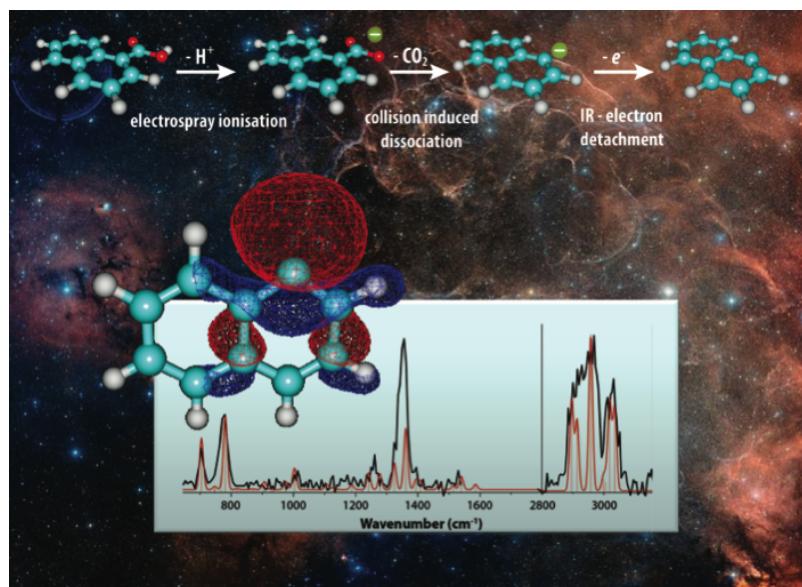


Figure 2 - Infrared spectrum of the naphthyl anion C₁₀H₇⁻. The anion is formed in an ion storage tandem mass spectrometer using naphthoic acid as a precursor. Interestingly, the negative charge is strongly localized, as suggested from the computed HOMO orbital.

Novel directions of tandem MS at the FELIX laboratory applied to interstellar PAH chemistry include the structural characterization of products formed in UV dissociative ionization of PAHs. Fragmentation by acetylene (C₂H₂) loss is one of the most common breakdown channels of PAHs. For the smallest PAH naphthalene (C₁₀H₈), this results in the formation of a C₈H₆⁺ fragment ion. The molecular structure of this product is certainly not a priori clear; multiple isomers are conceivable including phenylacetylene, benzocyclobutadiene, pentalene as well as various a-cyclic isomers. The IRMPD spectrum recorded for the mass-isolated C₈H₆⁺ fragment is shown in Figure 3 and compared with theoretically predicted spectra for the various isomers. Clearly, pentalene⁺ is the only product under our experimental conditions. These data provide the first unambiguous experimental evidence that naphthalene isomerizes to azulene – the (5-7) membered ring isomer of naphthalene – prior to dissociation. This process is found to occur in larger PAHs as well. This 6-to-5 membered ring isomerization may constitute the isomerization pathways that link PAHs to fullerenes under interstellar energetic processing conditions.

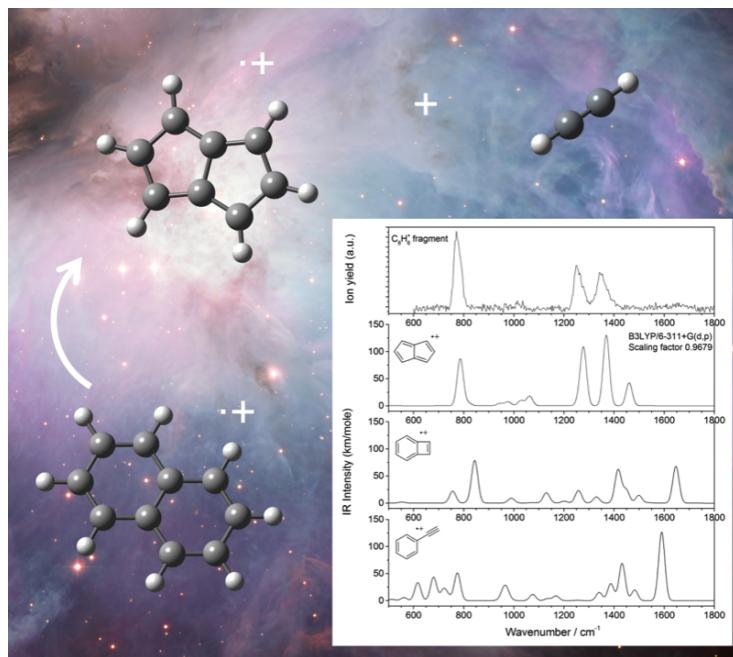


Figure 3 - The C_2H_2 -loss product that is formed in the 193 nm two-photon dissociative ionization of naphthalene is identified as pentalene $^+$ by means of infrared multiphoton dissociation.

Action spectroscopy studies at the FELIX Laboratory thus contribute to a better understanding of the IR spectra of PAHs in various forms. They provide accurate experimental verification of computed spectra constituting various PAH spectral databases, which are used directly in the interpretation of interstellar emission spectra.

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Abstracts

Isomer effects in fragmentation of Polycyclic Aromatic Hydrocarbons

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We have observed significant differences in the fragmentation patterns of isomeric Polycyclic Aromatic Hydrocarbon (PAH) cations following collisions with helium atoms at center-of-mass energies around 100 eV. This is in contrast to the situation at other collision energies or in photo-absorption experiments where isomeric effects are very weak and where the lowest-energy dissociation channels (H- and C₂H₂-loss) dominate in statistical fragmentation processes. In the 100 eV range, non-statistical fragmentation also competes and is uniquely linked to losses of single carbon atoms (CH_x-losses). We find that such CH_x-losses are correlated with the ionic ground state energy within a given group of isomers. We present results for three C₁₆H₁₀⁺, four C₁₈H₁₂⁺ and five C₂₀H₁₂⁺ isomers colliding with He.

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Int. J. Mass Spectrom. 2015, in press

<http://dx.doi.org/10.1016/j.ijms.2015.09.005>

Hydrogen atom chemisorption and diffusion on neutral and charged polycyclic aromatic hydrocarbon (PAH) flakes in the interstellar media

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Hydrogen atoms diffusion on a hydrocarbon flake is studied using PM6 and DFT programs using as models neutral and positive charged coronene. Chemisorption and potential energy surfaces and diffusion paths were calculated. Results show that diffusion occurs through C-C bonds. Edge effects are very important because the most stable adsorptions occur on hydrogenated border sites, so the diffusion is biased toward edge sites. Charged coronene has stronger adsorption energies than neutral systems. A large difference between barriers in neutral and charged systems was not observed in most of the cases. A discussion of modeling diffusion processes is presented.

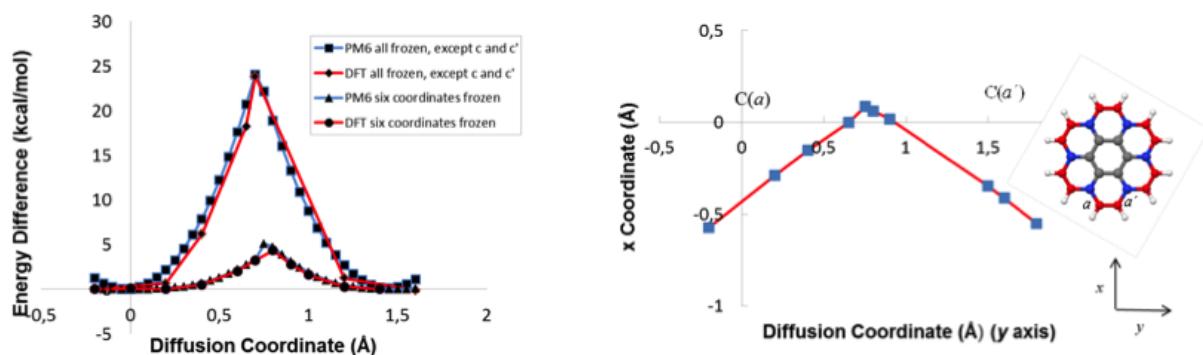


Figure 1: (a) Effect of distortion on diffusion barrier for $c \rightarrow c'$ migration of neutral system with PM6 and DFT. Two cases were considered: (i) optimization of only c and c' atoms (ii) all coordinates optimized, except 6 fixed coordinated to avoid coronene surface movement during H diffusion. (b) Diffusion pathway for H atom showing the x coordinate variation from a to a' sites located at the y axis.

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Chemical Physics Letters, 640, 11 (2015)

<http://www.sciencedirect.com/science/article/pii/S0009261415007484>

On observing C_{60}^+ and C_{60}^{2+} in laboratory and space

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Recently, we have measured the IR absorptions of C_{60}^+ , C_{60}^- , and C_{60}^{2+} in neon matrixes. Many, previously unknown absorptions were established. Here we compare our laboratory IR absorption spectra for C_{60}^+ and C_{60}^{2+} to the IR emission spectra of several astronomical objects that show C_{60} emission. We find that IR bands of C_{60}^+ are possibly present in the objects Tc1, SMP SMC 16, NGC 7023, NGC 2244 and SMP LMC 02. Infrared emission features possibly due to C_{60}^{2+} were identified in NGC 7023. To help with future observations of fullerene-related DIBs, we also revisited the oscillator strengths of the NIR absorptions of C_{60}^+ , and report significantly revised values. Additionally, we report the UV oscillator strengths of C_{60}^+ .

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<http://dx.doi.org/10.1051/0004-6361/201527234>

meetings

SECOND ANNOUNCEMENT International Symposium and Workshop on Astrochemistry - ISWA

Campinas, SP - Brazil
3 - 8 July 2016

Dear Colleagues,

This is the second announcement of the “INTERNATIONAL SYMPOSIUM AND WORKSHOP ON ASTROCHEMISTRY - ISWA”: Understanding the extraterrestrial molecular complexity through experiments, observations and models.

The main goal of this event is to bring together experimentalists, observers and theoreticians interested to contribute to the progress of the knowledge in astrochemistry. During the symposium, we will have two workshops: one focused on experimental astrochemistry and another focused on astronomical observations. The activities in the workshops will address proposal writing to the Brazilian Synchrotron Light Laboratory (LNLS) and data reduction for the Atacama Large Millimeter Array (ALMA) and the Large Latin American Millimeter Array (LLAMA) radio observatories. During this meeting we will also have the opportunity to follow a real astrochemical experiment at one of the beam lines of the LNLS. The experiment will simulate the interaction between UV and soft X-rays with astrophysical ice analogs.

The scientific topics of this meeting are:

- Astrophysical ices - Spectroscopy, Molecular processes, Energetic Processing (UV, X-rays, UV/VIS, Electrons, Ions)
- Formation of complex species in ices - Astrobiology
- Surface Chemistry, Thermal programmed desorption
- Gas phase experiments on astrochemistry
- Detection of molecules in astrophysical environments (radio, infrared)
- Astrochemical models, abundances, chemical evolution.

The format of the meeting will consist of lectures given by main speakers, oral presentations and posters. A list of invited speakers will be available on the website soon.

The Symposium will be held at the Historic Farm-Hotel **Solar das Andorinhas**, located in Campinas, SP, Brazil. The participants of the meeting will have a thematic conference dinner with a typical Brazilian winter party called “Festa Julina”, which includes also a bonfire, and typical drinks and foods.

Registration is open. The deadline for abstract submission is March 15th, 2016.

Details on the meeting and registration is available on our website:

<http://www1.univap.br/gaa/iswa>

Additional information can be obtained via email to:

iswa2016@gmail.com

We are looking forward to an exciting meeting and hope to welcome you in Brazil next year in the beginning of July.

The Scientific Organizing Committee:

Sergio Pilling (UNIVAP/Brazil), Chair
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The Local Organizing Committee:

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Announcements

CSH Fellowships in the Science of Habitability

Advertised by Prof. Kevin Heng

Application deadline: December 31, 2015

The Center for Space and Habitability (CSH) at the University of Bern, Switzerland, invites applications for multiple CSH Fellows. CSH Fellows are expected to be independent postdoctoral researchers, who will propose their own research programs based on addressing the following questions. We are particularly interested in applicants with interdisciplinary expertise in astrobiology, biology, chemistry and geology.

- What are the theoretical, historical and functional definitions of life? How may we search for it in the broader Universe?
- Is habitability a well-defined concept? How is it influenced by the atmosphere, surface, interior, geological and biological cycles, stellar environment and system architecture of a planet, moon or exoplanet? May we design falsifiable diagnostics to quantify the habitability of a planet, moon or exoplanet via measurements or data?
- What knowledge may we glean from space- and ground-based telescopes (for exoplanets) and space missions (for the Solar System)? Using an interdisciplinary approach, may we design novel techniques for interpreting data from existing facilities or novel facilities for the future?
- What are the broader, philosophical and non-scientific implications for the discovery of habitats and life in the Universe?

Each prospective candidate is expected to name two hosts/supervisors from the CSH and the University of Bern. The research proposal should explain why interacting with the selected hosts/supervisors would benefit the prospective CSH Fellow. The proposed research need not be closely aligned with the expertise of the hosts/supervisors, but it is expected to be broadly related and address the above questions decisively. Existing expertise, at the professor level,

include: planetary science and space instrumentation (Kathrin Altwegg, Ingo Leya, Nicolas Thomas, Peter Wurz), planet formation (Yann Alibert, Willy Benz, Christoph Mordasini), exo-planetary atmospheres (Kevin Heng), atmospheric/climate science (Niklaus Kaempfer, Christoph Raible, Thomas Stocker), geology (Klaus Mezger), chemistry (Olivier Muehlemann) and philosophy (Claus Beisbart).

Each CSH Fellowship is held for 2+1 years at the University of Bern and comes with a travel budget. The annual salary increases with experience and is competitive with the local standard of living. CSH Fellows are expected to contribute to the intellectual life of the CSH (co-host talks and visitors, lead discussions, organize coffees and lunches, etc). Applicants should submit a cover letter (with the names of 3 referees), a 2-page CV (including a list of publications) and a research proposal (up to 5 pages) as part of a **SINGLE PDF FILE**. The 3 letters of recommendation should be sent directly to Kevin Heng by the referees themselves.

For further information please check the following links:

[CSH Website](#), [Job Register](#)

Contact: Prof. Kevin Heng

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Center for Space and Habitability
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Research Associate in Theoretical Molecular Physics

Advertised by Dr. Sergey Yurchenko

Application deadline: 30 November 2015.

Duties and Responsibilities The project aims to provide data on molecular absorption processes of hydrocarbons important for modelling atmospheres of extrasolar planets and cool stars. The data will be calculated using high level ab-initio procedures based on the state-of-the-art electronic structure and variational nuclear motion methods. The results will form a part of the ExoMol database. A flavour of the project can be obtained from its web pages [ExoMol](#). We are looking for candidates with a solid research training in the quantum mechanics of medium size molecules and an interest in applications to astrophysical problems. The candidate will be responsible for performing high accuracy electronic structure and variational nuclear motion calculations on molecules such as propene and butane and generate associated transition probabilities; performing programming development as may be required for these calculations. The position is open from the **1st of April 2016**. This project is funded by STFC for 2 years in the first instance.

Key Requirements The successful applicant will have a PhD in Physics, Chemistry or a closely related discipline and expertise in relevant subject area with a background in theoretical molec-

ular physics and/or quantum chemistry. Experience in high accuracy electronic structure calculations, nuclear motion variational method of theoretical spectroscopy and program development skills would be an advantage. Knowledge of suitable computer programming techniques FORTRAN and Linux is essential. Candidates should also have excellent written and verbal communication skills, ability to analyse and write up data, ability to present complex information effectively to a range of audiences. We expect the candidate to be committed to high quality research and to be able to work collaboratively and as part of a team.

Further Details can be found at the link
[Research Associate in Theoretical Molecular Physics](#)

Contact: Dr Sergey Yurchenko

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PhD positions at Leiden Observatory

Leiden University, The Netherlands
<http://www.strw.leidenuniv.nl>

The Leiden Observatory invites applications for **several PhD position** as part of a general call. Positions are available in all the research areas in which the Observatory is active, such as stars and planetary systems, interstellar matter, star formation, astrochemistry, high energy astrophysics, galaxies, large scale structure, cosmology, instrumentation, computational astrophysics, laboratory astrophysics and astrochemistry, history of science, and science outreach. Examples of PhD projects currently available can be found here:

http://www.strw.leidenuniv.nl/phd/example_phds.php

In particular, the Leiden Observatory is very active on studies of **PAHs in space** (observational, theoretical, and experimental). PhD students from Leiden succeed exceptionally well on the international job market. Many of the faculty members, PhD students, and undergraduates have an international background. English is the common language. Application forms and instructions are available at:

<http://www.strw.leidenuniv.nl/phd/>

Applicants are requested to upload a curriculum vitae, a list of all university courses taken and transcripts of grades obtained, brief statements of research interests and experience, and the contact information for at least two referees. The successful candidates must have a MSc degree (or equivalent) by the starting date. The starting dates are negotiable.

Complete applications received by **December 1, 2015** will receive full consideration.

For more details see: <http://www.strw.leidenuniv.nl/jobs/index.php?node=6>

AstroPAH Newsletter

<http://astropah-news.strw.leidenuniv.nl>
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Next issue: 15 Dec. 2015
Submission deadline: 4 Dec. 2015