AstroPAH

A Newsletter on Astronomical PAHs

Issue 18 | May 2015

SOFIA by night

Editorial

Dear Colleagues,

Welcome to our 18th edition of AstroPAH. In this issue, we dedicate the *In Focus* and our Picture of the Month to the airborne observatory SOFIA. The call for proposals for this observatory has just been released and, as you can read in the *In Focus*, it provides a great opportunity to observe PAHs in space.

The abstracts section features papers on PAH growth, internally excited PAH species, PAH complexes, and the emergence of a carbon star. As requested by the organizers, we are publishing a new and corrected announcement for the International Symposium on Polycyclic Aromatic Compounds (ISPAC 2015) to be held in Bordeaux, France, next September.

A new IAU Commission on Laboratory Astrophysics (C.B5) has just been approved by the IAU Executive Committee. Check the full announcement on page 16.

Our team at AstroPAH is very happy to congratulate our colleague, Annemieke Petrignani, who was awarded a NWO/VIDI Grant to work on laboratory astrochemistry. Congratulations, Annemieke!

We thank you all for your contributions and please keep them coming. You can send us your contributions anytime. For publication in June, 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: 16 June 2015.
Submission deadline: 5 June 2015.

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PAH Picture of the Month

The SOFIA flying observatory taxis to the Christchurch terminal (NZ) after a nighttime flight to study celestial objects visible only from the Southern Hemisphere.

Credits: NASA / Carla Thomas

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Design by Isabel Aleman

SOFIA and its potential for PAH detection

by Ella Sciamma-O'Brien and the SOFIA team

Figure 1 - *The SOFIA observatory in flight.*

The **Stratospheric Observatory For Infrared Astronomy (SOFIA)** is a joint project between NASA and the German Aerospace Center Deutsches Zentrum für Luft und-Raumfahrt (DLR). SOFIA is an airborne observatory consisting of a specially modified Boeing 747SP aircraft with a 2.7 m telescope (with an effective aperture of 2.5 m) mounted in an open cavity in the aft section of the aircraft. This observatory can fly at altitudes as high as 13.7 km (45,000 ft), i.e. above 99.8% of the precipitable water vapor, which blocks much of the mid and far-infrared radiation from reaching ground-based telescopes. SOFIA has the potential to be a key element for chemical and dynamical studies of warm material in the universe, as well as for observations of deeply embedded sources and transient events. It is designed for at least two decades of operations and has joined the Spitzer Space Telescope (Werner et al., 2004 and Gehrz et al., 2007), Herschel Space Observatory (Pilbratt, 2003), and James Webb Space Telescope (JWST, Gardner et al., 2006) as one of the premier facilities for panchromatic observations in thermal IR and submillimeter astronomy.

The SOFIA telescope is designed to observe at elevations between +20 and +60 degrees, and at wavelengths between 0.3 and 1600 μm. In practice, the wavelength coverage of the observatory is dependent upon the current instrument suite. Currently, seven first generation science instruments have been developed for SOFIA. They include an occultation photometer (HIPO), near- (FLITECAM), mid- (FORCAST), and far-infrared (HAWC+) cameras, infrared spectrometers (EXES, FIFI-LS), and heterodyne receivers (GREAT). The facility science instruments (FORCAST, FLITECAM, HAWC+) and principal investigator science instruments (EXES, FIFI-LS, GREAT) are available to all General Investigators. HIPO is a special purpose PI-class science instrument and requires prior consultation with the instrument team, and approval before it can be proposed for. Except for the combination of HIPO and FLITECAM, which can be flown together, only one science instrument can be flown at a time. SOFIA began initial science flights in December 2010. Table 1 gives a brief overview of the observatory's current instrument suite. Below we describe in more details the two most useful instruments for PAH work: FORCAST and EXES.

Table 1 *- SOFIA Instruments.*

SOFIA instrument	Description	Built by PI	λ range (μm) spec. res. (λ/Δλ)	Field of View Array size
FORCAST	Fain Object infraRed CAMera for the SOFIA Telescope - Facility instrument Mid IR camera and grism spectrometer	Cornell T. Herter	5 – 40 R – 200	3.2' x 3.2' 256 x 256 Si:As, Si:Sb
GREAT	German Receiver for Astronomy at Terahertz Frequencies - PI instrument Heterodyne spectrometer	MPIIR, KOSMA DLR-WS R. Güsten	60 – 200 $R = 10^6 – 10^8$	Diffraction Limited Single pixel heterodyne
FIFI-LS	Field Imaging Far-IR Line Spectrometer PI instrument w/ facility-like capabilities Imaging grating spectrometer	DSI, Stuttgart A. Krabbe	42 – 210 R = 1000 – 3750	30' x 30' (Blue) 60' x 60' (Red) 2 – 16 x 5 x 5 Ge:Ga
HIPO	High-speed Imaging Photometer for Occultation – Special PI instrument	Lowel Obs. E. Dunham	0.3 – 1.1	5.6' x 5.6' 1024 x 1024 CCD
FLITECAM	First Light Infrared Test Experiment CAMera Facilty instrument New IR test camera and grism spectrometer	UCLA I. McLean	1 – 5 R ~ 2000	8.2' x 8.2' 1024 x 1024 InSb
HAWC+	High Resolution Airborne Wideband Camera Facility instrument Far IR bolometer camera	JPL C. D. Dowell	50 – 240	Diffraction Limited 12 x 32 Bolometer
EXES	Echelon-Cross-Echelle Spectrograph PI instrument Echelon spectrometer	UT/UC Davis NASA Ames M. Richter	4.5 – 28 $R=10^5, 10^4, 3000$	5' to 90' slit 1024 x 1024 Si:As

FORCAST

FORCAST is a facility class, mid/far-infrared camera and spectrograph. The instrument has two cameras that operate from ∼5-25 μm and 25-40 μm, with several filters available in both cameras. The cameras can be used individually over the whole wavelength range, or together for simultaneous imaging of the same field of view. Spectroscopy is also possible using a suite of six grisms.

FORCAST is of great value to the SOFIA community for imaging protostellar environments, young star clusters, molecular clouds, and galaxies. Multicolor information allows determination of dust properties (temperatures, optical depths, masses, composition), location of ionizing sources, and the morphology of star forming regions.

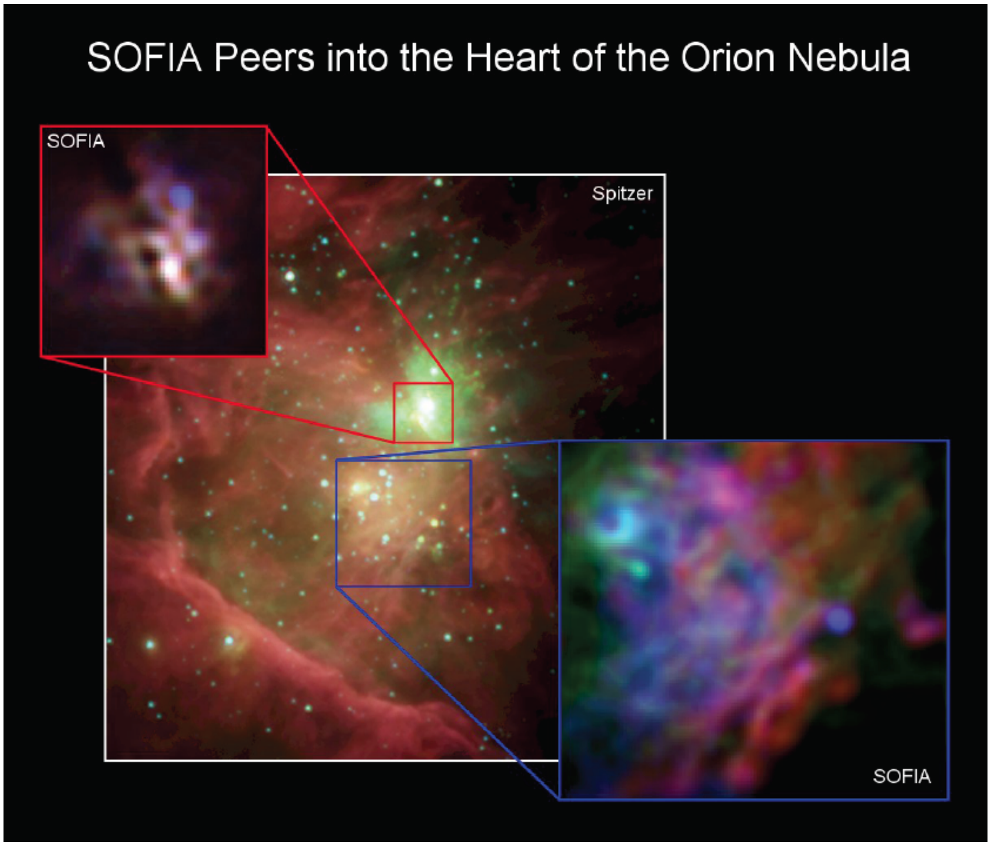

Figure 2 - *SOFIA/FORCAST 3-color mid-infrared images (blue box: 20, 31 and 37 μm, red box: 8, 20 and 37 μm) of the M42 star-forming region in Orion shown as inset on Spitzer image. These images show a complex distribution of interstellar dust and protostars in the Orion nebula. The SOFIA images were made at combinations of wavelengths and angular resolutions unavailable to any other ground- or space-based observatory. (Credits: J. De Buizer/FORCAST team; Spitzer image: NASA/Caltech-JPL).*

EXES

The Echelon-cross-Echelle Spectrograph (EXES) is a Principal Investigator-class, high- resolution mid-infrared spectrograph. EXES operates in the 4.5-28.3 μm wavelength region, at high (R$\sim$50,000-100,000), medium (R$\sim$5000-20,000) and low (R$\sim$1000-3000) spectral resolution. The instrument uses a 1024$\times$1024 Si:As detector array. High resolution is provided by an echelon a coarsely-ruled, steeply-blazed aluminum reflection grating along with an echelle grating to cross-disperse the spectrum. The echelon can be bypassed so that the echelle acts as the sole dispersive element. This results in single order spectra at medium- or low-resolution depending on the incident angle.

The low-resolution mode is ideally suited to settle some long-standing questions about astronomical PAHs specifically related to the strong 6.2μm PAH band and the weaker features between 5 and 6 μm. The 6.2 μm band originates from the PAH's skeletal C-C stretching vibrations while the weak bands between 5 and 6 μm are due to overtone, combination, and difference bands involving peripheral C-H stretching and bending vibrations. These bands are particularly important in view of the recent experimental and computational interest in the role of anharmonicity on the spectrum. The 6.2μm band is known to shift and has never been adequately resolved. To date, the only species known that can match the shift are PANHs, PAHs containing N within the hexagonal skeletal network. Apart from being a potentially significant reservoir of cosmic N, PANHs are also astrobiologically interesting. Regarding the weak 5-6 μm bands, because of the anharmonic effects, these bands also contain information about edge structures that is not revealed by the bands in the 3 or 10-15 μm regions. Taken together, these data reflect the PAH population's response to local conditions and these, in turn, shed light on the astrophysics in the emission regions.

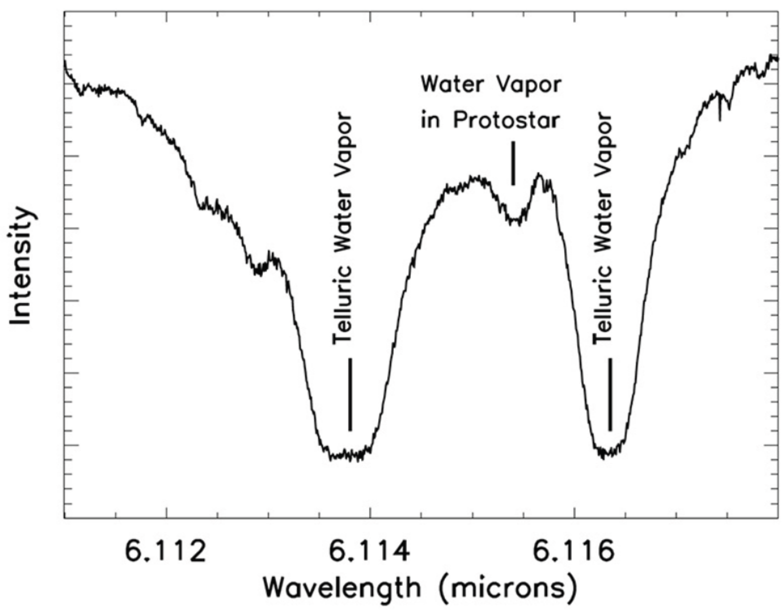

Figure 3 - *An EXES spectrum of high-mass protostar AFGL 2591 that shows a detection of H_2O vapor from the inner envelope or molecular ouflow. (Credit: N. Indriolo/EXES Team)*

EXES on SOFIA is able to observe molecular transitions that are blocked by the Earth's atmosphere for ground-based instruments. In particular, high spectral resolution enables the study of molecular hydrogen, water vapor, and methane from sources such as molecular clouds, protoplanetary disks, interstellar shocks, circumstellar shells, and planetary atmospheres.

SOFIA CALL FOR PROPOSALS CYCLE 4:

The Call for Proposals for the next SOFIA Cycle (Cycle 4) has just been released. The deadline for proposal submission is 9:00pm, Pacific Daylight Time, July 10, 2015.

MORE INFORMATION:

Information for Researchers - http://www.sofia.usra.edu/Science/
Cycle 4 Information - http://www.sofia.usra.edu/Science/proposals/cycle4/index.html

Abstracts

Molecular Growth Inside of Polycyclic Aromatic Hydrocarbon Clusters Induced by Ion Collisions

Rudy Delaunay[1,2], Michael Gatchell[3], Patrick Rousseau[1,2], Alicja Domaracka[1], Sylvain Maclot[1,2], Yang Wang[4,5], Mark H. Stockett[3], Tao Chen[3], Lamri Adoui[1,2], Manuel Alcamí[4,5], Fernando Martín[4,5,6], Henning Zettergren[3], Henrik Cederquist[3], and Bernd A. Huber[1]

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The present work combines experimental and theoretical studies of the collision between keV ion projectiles and clusters of pyrene, one of the simplest polycyclic aromatic hydrocarbons (PAHs). Intracluster growth processes induced by ion collisions lead to the formation of a wide range of new molecules with masses larger than that of the pyrene molecule. The efficiency of these processes is found to strongly depend on the mass and velocity of the incoming projectile. Classical molecular dynamics simulations of the entire collision process – from the ion impact (nuclear scattering) to the formation of new molecular species – reproduce the essential features of the measured molecular growth process and also yield estimates of the related absolute cross sections. More elaborate density functional tight binding calculations yield the same growth products as the classical simulations. The present results could be relevant to understand the physical chemistry of the PAH-rich upper atmosphere of Saturn's moon Titan.

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Witnessing the Emergence of a Carbon Star

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During the late stages of their evolution, Sun-like stars bring the products of nuclear burning to the surface. Most of the carbon in the Universe is believed to originate from stars with masses up to a few solar masses. Although there is a chemical dichotomy between oxygen-rich and carbon-rich evolved stars, the dredge-up itself has never been directly observed. In the last three decades, however, a few stars have been shown to display both carbon- and oxygen-rich material in their circumstellar envelopes. Two models have been proposed to explain this dual chemistry: one postulates that a recent dredge-up of carbon produced by nucleosynthesis inside the star during the Asymptotic Giant Branch changed the surface chemistry of the star. The other model postulates that oxygen-rich material exists in stable keplerian rotation around the central star. The two models make contradictory, testable, predictions on the location of the oxygen-rich material, either located further from the star than the carbon-rich gas, or very close to the star in a stable disk. Using the Faint Object InfraRed CAmera (FORCAST) instrument on board the Stratospheric Observatory for Infrared Astronomy (SOFIA) Telescope, we obtained images of the carbon-rich planetary nebula (PN) BD +30° 3639 which trace both carbon-rich polycyclic aromatic hydrocarbons (PAHs) and oxygen-rich silicate dust. With the superior spectral coverage of SOFIA, and using a 3D photoionisation and dust radiative transfer model we prove that the O-rich material is distributed in a shell in the outer parts of the nebula, while the C-rich material is located in the inner parts of the nebula. These observations combined with the model, suggest a recent change in stellar surface composition for the double chemistry in this object. This is evidence for dredge-up occurring $\sim$10^3 yr ago.

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MNRASL (2015) in press

http://arxiv.org/abs/1504.03349

Formation of H_2 from internally heated Polycyclic Aromatic Hydrocarbons: Excitation energy dependence

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We have investigated the effectiveness of molecular hydrogen (H_2) formation from Polycyclic Aromatic Hydrocarbons (PAHs) which are internally heated by collisions with keV ions. The present and earlier experimental results are analyzed in view of molecular structure calculations and a simple collision model. We estimate that H_2 formation becomes important for internal PAH temperatures exceeding about 2200 K, regardless of the PAH size and the excitation agent. This suggests that keV ions may effectively induce such reactions, while they are unlikely due to e.g. absorption of single photons with energies below the Lyman limit. The present analysis also suggests that H_2 emission is correlated with multi-fragmentation processes, which means that the $[PAH\text{-}2H]^+$ peak intensities in the mass spectra may not be used for estimating H_2-formation rates.

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http://dx.doi.org/10.1063/1.4917021

Electronically Excited States of PANH Anions

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The singly deprotonated anion derivatives of nitrogenated polycyclic aromatic hydrocarbons (PANHs) are investigated for their electronically excited state properties. These include single deprotonation of the two unique arrangements of quinoline producing fourteen different isomers. This same procedure is also undertaken for single deprotonation of the three nitrogenation isomers of acridine and the three of pyrenidine. It is shown quantum chemically that the quinoline-class of PANH anion derivatives can only produce a candidate dipole-bound excited state each, a state defined as the interaction of an extra electron with the dipole moment of the corresponding neutral. However, the acridine- and pyrenidine-classes possess valence

excited states as well as the possible dipole-bound excited states where the latter is only possible if the dipole moment is sufficiently large to retain the extra electron; the valence excitation is independent of the radical dipolar strength. As a result, the theoretical vertically computed electronic spectra of deprotonated PANH anion derivatives is fairly rich in the 1.5 eV to 2.5 eV range significantly opening the possibilities for these molecules to be applied to longer wavelength studies of visible and near-IR spectroscopy. Lastly, the study of these systems is also enhanced by the inclusion of informed orbital arrangements in a simply constructed basis set that is shown to be complete and efficient.

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http://pubs.rsc.org/en/content/articlelanding/2015/cp/c5cp01354b#!divAbstract

Rotation-vibration interactions in the spectra of polycyclic aromatic hydrocarbons: Quinoline as a test-case species

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Polycyclic aromatic hydrocarbons (PAHs) are highly relevant for astrophysics as possible, though controversial, carriers of the unidentified infrared emission bands that are observed in a number of different astronomical objects. In support of radio-astronomical observations, high resolution laboratory spectroscopy has already provided the rotational spectra in the vibrational ground state of several molecules of this type, although the rotational study of their dense infrared (IR) bands has only recently become possible using a limited number of experimental set-ups. To date, all of the rotationally resolved data have concerned unperturbed spectra. We presently report the results of a high resolution study of the three lowest vibrational states of quinoline C_9H_7N, an N-bearing naphthalene derivative. While the pure rotational ground state spectrum of quinoline is unperturbed, severe complications appear in the spectra of the ν45 and ν44 vibrational modes (located at about 168 cm^{-1} and 178 cm^{-1}, respectively). In order to study these effects in detail, we employed three different and complementary experimental techniques: Fourier-transform microwave spectroscopy, millimeter-wave spectroscopy, and Fourier-transform far-infrared spectroscopy with a synchrotron radiation source. Due to the high density of states in the IR spectra of molecules as large as PAHs, perturbations in the rotational spectra of excited states should be ubiquitous. Our study identifies for the first time this effect

and provides some insights into an appropriate treatment of such perturbations.

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http://dx.doi.org/10.1063/1.4913750

Electronic Spectroscopy of $[FePAH]^+$ Complexes in the Region of the Diffuse Interstellar Bands: Multireference Wave Function Studies on $[FeC_6H_6]^+$

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The low-energy states and electronic spectrum in the near-infraredvisible region of $[FeC_6H_6]^+$ are studied by theoretical approaches. An exhaustive exploration of the potential energy surface of $[FeC_6H_6]^+$ is performed using the density functional theory method. The ground state is found to be a $^4A_1$ state. The structures of the lowest energy states ($^4A_2$ and $^4A_1$) are used to perform multireference wave function calculations by means of the multistate complete active space with perturbation at the second order method. Contrary to the density functional theory results ($^4A_1$ ground state), multireference perturbative calculations show that the $^4A_2$ state is the ground state. The vertical electronic spectrum is computed and compared with the astronomical diffuse interstellar bands, a set of near-infrared-visible bands detected on the extinction curve in our and other galaxies. Many transitions are found in this domain, corresponding to d $\rightarrow$ d, d $\rightarrow$ 4s, or d $\rightarrow \pi^*$ excitations, but few are allowed and, if they are, their oscillation strengths are small. Even though some band positions could match some of the observed bands, the relative intensities do not fit, making the contribution of the $[Fe\text{-}C_6H_6]^+$ complexes to the diffuse interstellar bands questionable. This work, however, lays the foundation for the studies of polycyclic aromatic hydrocarbons (PAHs) complexed to Fe cations that are more likely to possess d $\rightarrow \pi^*$ and $\pi^* \rightarrow \pi^*$ transitions in the diffuse interstellar bands domain. PAH ligands indeed possess a larger number of π and π^* orbitals, respectively, higher and lower in energy than those of C_6H_6, which are expected to lead to lower energy d $\rightarrow \pi^*$ and d $\pi \rightarrow \pi^*$ transitions in $[FePAH]^+$ than in $[Fe\ C_6H_6]^+$ complexes.

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J. Chem. Phys. A, Article ASAP
http://pubs.acs.org/doi/abs/10.1021/acs.jpca.5b00438

Meetings

International Symposium on Polycyclic Aromatic Compounds

“Cité Mondiale Convention Centre” in Bordeaux, France

13 - 17 September 2015

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

It is with great pleasure that we invite you to attend the 2015 International Symposium on Polycyclic Aromatic Compounds conference, ISPAC 2015, to be held in Bordeaux, France.

ISPAC 2015 will focus on the research of Polycyclic Aromatic Compounds (PACs) on multiple fronts of analytical methods, synthesis of large PACs, physico-chemical properties, toxicology and environment. The scientific topics include an arranged session ”PACs in interstellar media”, with a keynote lecture by Dr Christine Joblin, IRAP, Toulouse, France.

The meeting will consist of invited talks, contributed talks and posters.

Registration is open (early-bird registration till June, 1st) and the abstract submission deadline is May, 15th. We hope to see you in Bordeaux, the Best European Destination in 2015!

ORGANISERS: Dr P. Garrigues (ISM) and Prof. J. Cachot (EPOC), University of Bordeaux

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International Symposium and Workshop on Astrochemistry - ISWA

Understanding the extraterrestrial molecular complexity through experiments, observations and models

Campinas, SP - Brazil
July 3-8, 2016

Dear colleagues,

This is the first 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 in experimental astrochemistry and other 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 programed 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” (http://www.hotelfazendasolardasandorinhas.com/indexingles.asp) 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” with 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 mailto: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
Edgar Mendoza (IAG-USP/Brazil), Co-Chair
Bertrand Lefloch (IPAG/France)
Cecilia Ceccarelli (IPAG/France)
Ewine van Dishoeck (Leiden Univ./NL)
Guillermo Muoz Caro (CAB-INTA/Spain)
Harold Linnartz (Leiden Univ./NL)
Heloisa Boechat-Roberty (OV-UFRJ, Brazil)
Jacques Lepine (IAG-USP/Brazil)
Kinsuk Acharyya (Virginia Univ./USA)
Michel Nuevo (NASA Ames/USA)
Nigel Mason (OU/UK)
Peter Woitke (St. Andrews Univ./UK)
Phillipe Boduch (GANIL-CIMAP/France)
Sun Kwok (HK Univ./China)
Yi-Jehng Kuan (Nat. Taiwan Normal Univ./Taiwan)

The Local Organizing Committee:

Sergio Pilling, Chair
Edgar Mendoza, Co-Chair
Isabel Aleman
Will Robson M. Rocha
Douglas Galante
Diana R. G. Gama

Announcements

New IAU Commission: Laboratory Astrophysics

Dear Colleagues and IAU Members,

a new IAU Commission on Laboratory Astrophysics (C.B5) has just been approved by the IAU Executive Committee. The Laboratory Astrophysics Commission will be launched at the end of the IAU XIXX General Assembly in Honolulu, this Summer.

We would like to ask for your support and encourage you to sign up for this new commission. Please note that you may sign-up for up to a maximum of 3 commissions. This step is **very** important for the success of the new commission.

IAU members should have received instructions for the signing-up process with a unique voting code. Please vote and encourage your colleagues to support Laboratory Astrophysics at the IAU.

Thank you for your support!

Proposers Laboratory Astrophysics Commission:

Farid Salama (NASA ARC)
Helen Fraser (The Open University)
Paul Barklem (Uppsala University)
Thomas Henning (Max Planck Institute)
Gianfranco Vidali (Syracuse University)

AstroPAH Newsletter

http://astropah-news.strw.leidenuniv.nl
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Next issue: 16 June 2015
Submission deadline: 5 June 2015