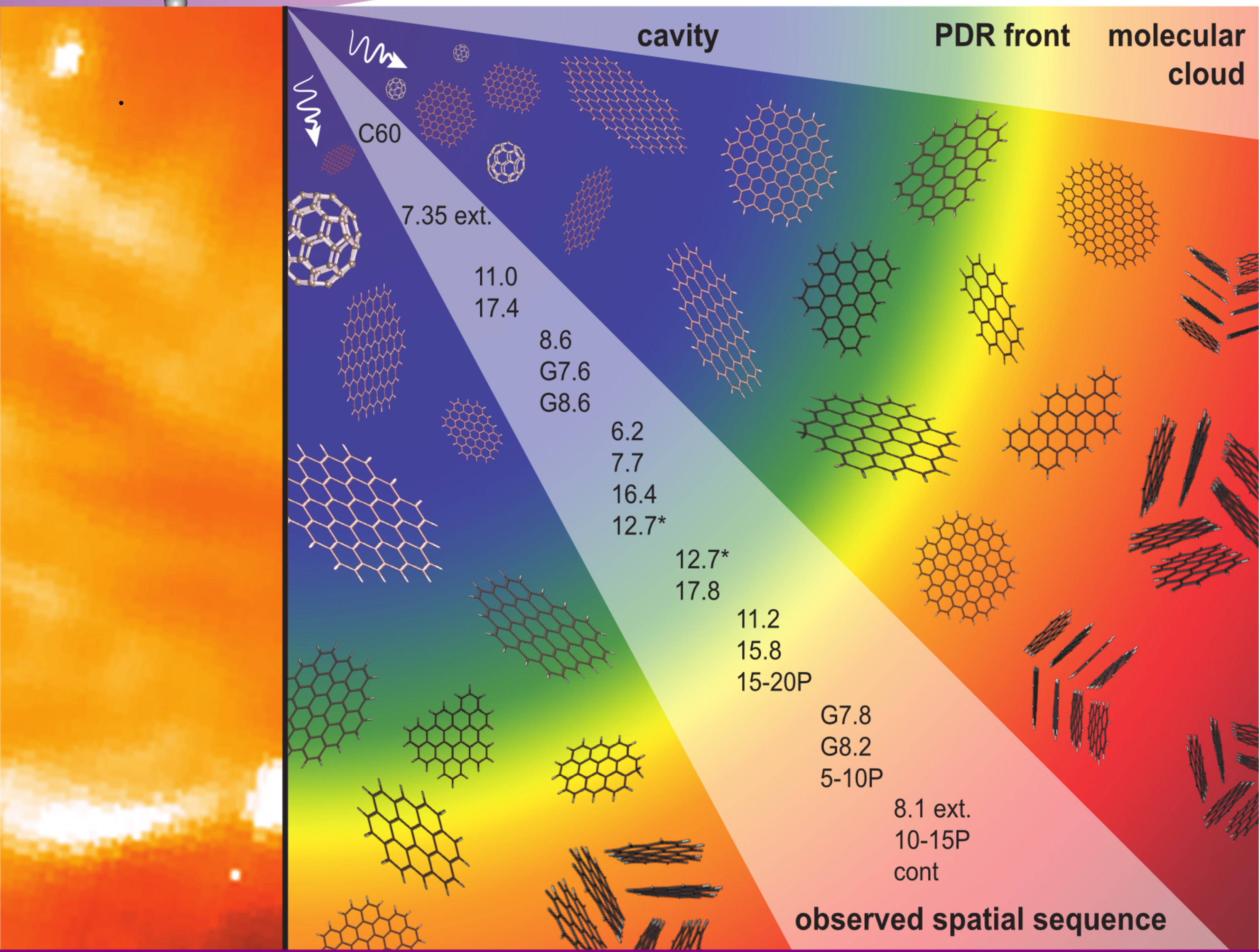
AstroPAH

A Newsletter on Astronomical PAHs

Issue 29 | June 2016



PAH Population in NGC 2023

Editorial

Dear Colleagues,

Welcome to the June issue of AstroPAH.

We would like to start this editorial with a congratulation to Christine Joblin, research director of Astrophysics and Planetology at CNRS, for the prestigious award she received at the start of this month. On June 6 2016, Christine Joblin was knighted *Chevalier* of the French *"Ordre national de la Légion d'honneur"* for her 23-year contribution to astrochemistry (link). Christine gave us a great interview in February 2014 (AstroPAH #4).

As for this month's AstroPAH, our Picture of the Month presents a state-of-the-art illustration of our understanding of the photochemical evolution of the interstellar PAH population in reflection nebulae, based on a picture of Heather Andrews and collaborators (2016) and modified by Els Peeters (2016). To learn about the science that is featured in this cartoon, we invite you to read our *In Focus* interview with Els Peeters, where she talks about her latest paper and her personal experiences as a scientist.

Papers highlighted in our Abstracts section cover the use of Raman Spectroscopy for identification and discrimination of PAHs and a vibrational study of deuterium containing PAH species. We also would like to direct your attention to our Meetings section presenting a conference of the COST action "Origins and Evolution of Life on Earth and in the Universe" and a conference on JWST.

We welcome contributions to AstroPAH. Visit our webpage or contact us for more information. For publication in June, see the deadlines below. We thank you all for your contributions so far.

Join us on Facebook.

The Editorial Team

Next issue: 19 July 2016.
Submission deadline: 8 July 2016.

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Contents

PAH Picture of the Month

The photochemical evolution of the interstellar PAH population in reflection nebulae (modified from Andrews et al. 2015, ApJ, 807, 99, Fig. 15). This figure exemplified the changes in the PAH population as they are more and more exposed to the strong radiation field of the central star in the evaporative flows associated with the Photodissociation Region (PDR) in NGC 2023. With increasing distance from the star, the figure shows the transition from the cavity closer to the star (left-hand side) to the PDR front and finally to the molecular cloud (right-hand side).

Credits: E. Peeters, adapted from Fig. 15 of Andrews et al. (2015, ApJ, 807, 99)

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

In Focus

An Interview with Els Peeters

Dr. Els Peeters is Associate Professor in the department of Physics and Astronomy at the University of Western Ontario, London, Canada and research scientist at the SETI Institute, Mountain View, California, USA. Her research focuses on the physics and chemistry of interstellar molecules and dust with a prime emphasis on polycyclic aromatic hydrocarbons (PAHs). She is an observational astronomer and has worked extensively with infrared observations from space-based telescopes, such as the Infrared Space Observatory (ISO), NASA's Spitzer Space Telescope and the Herschel Infrared Space Observatory, the Stratospheric Observatory for Infrared Astronomy (SOFIA) and ground-based telescopes (e.g. VLT, Gemini). She collaborates with (astro-)chemists to interpret the astronomical PAH characteristics.

When and why did you start studying PAHs?

During the summer following my 18th birthday, I was contemplating what I would study at the university. Many options were available (most related to science) but the final decision was made (and conveyed to my parents on a postcard) when I was sitting on an airplane for the first time and was fascinated by the fact that a plane could stay in the air so I enrolled in the 'Licentiaat in Physics' program at the Catholic University of Leuven (KUL) in Belgium. During one of my first calculus classes I met my future partner, Jan Cami. He and some other study friends (notably Bart Vandenbussche and Gwendolyn Meeus), were all active amateur astronomers, and introduced me to astronomy. As I wanted to do something exotic for my 4th year research project, I listed Astronomy and Nuclear physics as my first and second choice and yes, I was one of the lucky students that got into Astronomy. My research project was to study the central object of the Red Rectangle under the supervision of Christoffel Waelkens and Hans van Winckel. I truly enjoyed my 'stay' at the Instituut voor Sterrenkunde but unfortunately, no Ph.D. positions in Astronomy were available that year at the Institute. However, Christoffel

Waelkens gave me the opportunity to enroll in the European M.Sc. program in Astronomy. As I never looked for opportunities outside of Belgium or even outside of the KUL, this was a big change. During the first 6 months of this program, we followed courses at the University of Porto, Portugal. The second part of this program involved a research project at one of the participating European universities. At that time, my future plan was to become a teacher at a college and, in Belgium, this required a Ph.D. degree. So I had also applied for Ph.D. positions in Physics at the KUL and started my Ph.D. research in experimental low-temperature semiconductor physics halfway through my M.Sc. program. Since I wanted to finish what I started, I arranged that I could do the M.Sc. exams in Belgium while Prof. Waelkens kindly facilitated for me to do a research project again at the KUL, this time under the supervision of Conny Aerts on the topic of line-profile variations of slowly pulsating B stars. While my social life during these six months was almost nonexistent (during the day I worked on my Ph.D. research in Physics while in the evenings and weekends, I worked on my M.Sc. research in Astronomy), it was totally worth it. Fast forward one year. In the meantime, Jan had started a Ph.D. program in Astronomy in the Netherlands and learnt about two open Ph.D. positions in Astronomy, both to work with ISO-SWS observations. As I was not very happy with my Ph.D. research in Physics and valued my experience in Astronomy, I decided to apply to both positions. Sacha Hony took up the position with Rens Waters and, after two years of research in low temperature physics, I moved on to start a Ph.D. project with Xander Tielens and Pjotr Roelfsema at the University of Groningen and SRON . . . on PAHs. So . . . that's when and why I started studying PAHs: a somewhat random walk with chance opportunities along the way. I truly enjoyed my Ph.D. years in Astronomy (and the years following) and have never regretted the switch back to Astronomy.

Tell us about your latest paper.

Reference:
"The PAH emission characteristics of the reflection nebula NGC2023"
Peeters E., Bauschlicher C.W. Jr., Allamandola L.J., Tielens A.G.G.M., Ricca A., Wolfire M.G. 2016, ApJ, submitted

We very carefully looked into the spatial behaviour of the PAH emission in the reflection nebula NGC 2023: the amount of treasures buried in spectral maps of extended objects is truly amazing. We found that the PAH emission bands exhibit a variety of different spatial morphologies: i.e. their (peak) emission occurs at different distances from the illuminating source revealing a 'spatial sequence' within the PAH emission (see the Picture of the Month and its caption)). It is interesting to see (and confirm) that the PAH features behave independently from the underlying plateau emission. Moreover, the morphology of all the major PAH bands varies with wavelength indicating that multiple components contribute to a single feature. This is particular true for the 7 to 9 μm PAH emission as its spatial distribution continuously varies between two extremes which are bound between ∼7.35 and ∼8.1 μm.

Despite having distinct spatial morphologies, some PAH bands still show very strong correlations with each other, especially the traditional charge proxy bands at 6.2, 7.7 and 8.6 μm. We further explored this behaviour by decomposing the 7 to 9 μm PAH emission into 4 Gaussian components (G7.6, G7.8, G8.2 and G8.6; see Fig. 1). The G7.6 and G8.6 components exhibit the same spatial distribution and are the strongest correlated of all PAH components. In contrast, the G7.8 and G8.2 components have spatial distributions similar to that of the dust continuum emission and not the PAH feature emission, and are not as tightly correlated. Thus, at least two PAH subpopulations with different spatial distributions contribute to the 7 to 9 μm PAH emission.

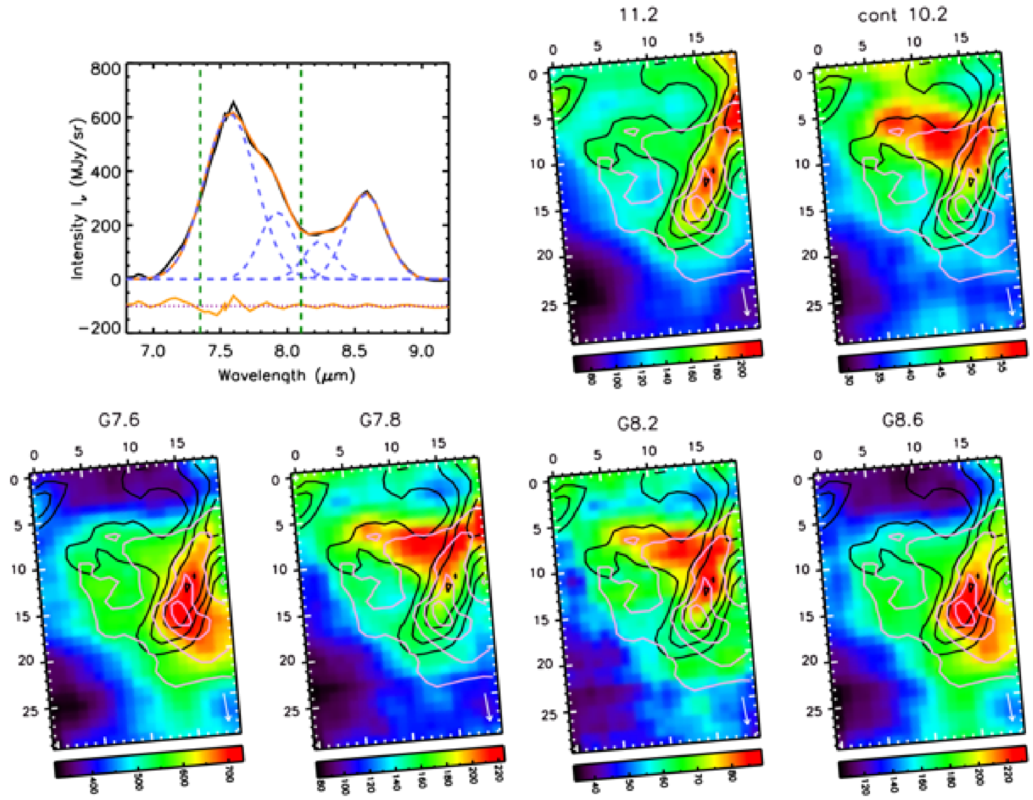

Figure 1 - *The decomposition of the 7 to 9 μm into four Gaussian components and its spatial distribution as well as the 11.2 μm PAH band and the continuum flux at 10.2 μm towards the north of NGC 2023. As a reference, the contours represent the 11.2 and 7.7 μm emission features in respectively black and pink. The maps are orientated so N is up and E is left. The white arrow in the bottom right corners indicates the direction towards the central star.*

To understand this spatial behaviour of the PAH emission in NGC2023, we turned towards theoretical PAH spectra. Given that oval, compact PAHs are underrepresented in the NASA Ames database (PAHdb), we determined the spectra of compact oval PAHs ranging in size from C_{66} to C_{201} computationally using density functional theory. Comparison of the observed 7 to 9 μm relative PAH intensities in NGC2023 with intrinsic relative intensities (from the oval family as well as PAHs present in the PAHdb) reveals that while the astronomical range in individual relative intensities is well represented, very few are consistent with the observed trends (correlation of G7.6 with G8.6, and of G7.8 with G8.2).

Based on the entire PAHdb, we attribute the 7.6 μm emission to compact PAHs with sizes in the range of 50 to 100 C-atoms, the 7.8 μm emission to very large PAHs ($100 \leq \#C < 150$) with bay regions or modified duo CH groups (like adding or removing hydrogens or substituting a N for a CH group), the 8.2 μm emission to PAHs/PAH clusters with multiple bay regions (e.g. PAHs with very irregular structures or corners), and the 8.6 μm emission to very large compact, symmetric PAHs ($96 \leq \#C < 150$). We assigned the plateau emission to very small grains with possible contributions from PAH clusters and hypothesized that the 8.2 μm emission (and possibly the 7.8 μm emission) also originates in these structures. Combine these assignments with the observed spatial sequence, and the photochemical evolution of the interstellar PAH family is revealed as PAHs are more and more exposed to the radiation field of the central star in the evaporative flows associated with the PDRs in NGC 2023 (see the Picture of the Month and its caption).

On a personal level, did you as a scientist have difficulties to balance you career and personal life?

During the last 6 months of my Ph.D., I spend all my time at the office (no, I didn't sleep there) working very hard to finish my thesis on time. Luckily, I was not the only one and I could enjoy the great company of Leticia Martín-Hernández during the lonely hours in the institute. Clearly, not much work-life balance in these months. Aside from that time though, my work-life balance during my Ph.D. and postdoc years was very good. This changed tremendously when I took up a faculty position. The early years were really tough and I worked almost all the time; but it did get better. Luckily. It was important for me to become comfortable with the term 'good enough': for example, at some point, the time it takes to (further) improve a lecture or a talk is not worth the small incremental improvement towards "perfection" obtained. Another important lesson I learnt is to not wait for a bloc of time to do a certain task (they rarely come); take advantage of the small time slots during the day to get started or to continue with a task. Time management is very important.

Did you have a two-body problem and how did you deal with it?

Yes, Jan and I graduated from the same program ('Licentiaat' in Physics) and were fortunate to both be given the opportunity to enroll in the European M.Sc. program in Astronomy. I left Porto earlier to start my Ph.D. research in Physics in Belgium while Jan moved to Leiden Observatory, The Netherlands, for his research project. Luckily, it's only a ~2h drive between Leuven and Leiden and we spend most weekends together. Jan then started his Ph.D. research and resided in Groningen, The Netherlands, for the first two years, doubling the travel time between us (not taking into account rush hour) but still doable for weekend travel. Note that for a typical Belgian (not working in Brussels), a one-hour drive is a long drive (FYI you can cross Belgium in ~1.5 and ~3 hours in respectively the shortest and longest distance). When I switched back to Astronomy, we "re-united" in Groningen. We had another bout of long-distance relationship when Jan moved to paradise (sunny California) 6 months before I did. Here as well, we were fortunate to both have a postdoc position at NASA Ames, thanks to Farid Salama and especially Lou Allamandola. Finally, we moved together to London, Canada, to take up a tenure-track and limited term faculty position at the University of Western Ontario and eventually both got tenure. The University of Western Ontario, as several other universities and organizations these days, has a system in place for spousal/dual appointments and we negotiated a limited term faculty position when the offer was made for the tenure-track position. Thus we did not settle for the worst advice I was given in this respect near the end of my Ph.D. years. It was something like this: "You should be happy when you end up with 1 job for both of you". While I did/do enjoy astronomy and PAHs a lot, I had zero intention to work full-time for half a salary.

Overall, we were very fortunate regarding the distance and length of time we were separated. What helped us along the way is that we were lucky to work in compatible fields (and so both could get a job at NASA Ames for example), we were both competitive enough to be hired, we found jobs in 'big' institutions where several positions were available, and especially, met people along the way that were open to the two body problem and willing to help out where possible.

What was the most important advice somebody gave you?

During my postdoc years at NASA Ames, the results of NASA's Spitzer Space Telescope cycle 1 call for proposals were announced: none of the proposals I was involved in were successful. I was utterly disappointed and, being an observational astronomer, was convinced this was a significant blow to my career. Lou took me for a walk around the building and a very nice, encouraging chat. Bottom-line of his message: ***you need to put everything in perspective (there are more important things in life than approved observing proposals), a rejected proposal doesn't mean you're not a good scientist, it is not the end of the world nor is it the end of your career.***

Do what you really like, work with the people you really like, and have fun. That is something I could daily see in action in my advisors, Xander and Lou. I'm happy to say I still feel like a kid who's playing in the sandbox when I can work on my research, play with data, figure out how the different PAH bands behave, etc.

Abstracts

Identification and discrimination of polycylic aromatic hydrocarbons using Raman spectroscopy

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Polycyclic aromatic hydrocarbons (PAHs) are widely present throughout the solar system and beyond. They have been implicated as a contributor to unidentified infrared emission bands in the interstellar medium, comprise a substantial portion of the insoluble organic matter in carbonaceous chondrites, are expected stable components of organic matter on Mars, and are present in a wide range of terrestrial hydrocarbons and as components of biomolecules. However, PAH structures can be very complicated, making their identification challenging. Raman spectroscopy is known to be especially sensitive to the highly polarizable C-C and C=C bonds found in PAHs, and therefore, can be a powerful tool for PAH structural and compositional elucidation. This study examined Raman spectra of 48 different PAHs to determine the degree to which Raman spectroscopy could be used to uniquely identify different species, factors that control the positions of major Raman peaks, the degree to which induced fluorescence affects the intensity of Raman peaks, its usefulness for PAH discrimination, and the effects of varying excitation wavelength on some PAH Raman spectra. It was found that the arrangement and composition of phenyl (benzene) rings, and the type and position of functional groups can greatly affect fluorescence, positions and intensities of Raman peaks associated with the PAH backbone, and the introduction of new Raman peaks. Among the functional groups found on many of the PAHs that were analyzed, only a few Raman peaks corresponding to the molecular vibrations of these groups could be clearly distinguished. Comparison of the PAH Raman spectra that were acquired with both 532 and 785 nm excitation found that the longer wavelength resulted in reduced fluorescence, consistent with previous studies.

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Icarus, 274, 211 (2016)

http://dx.doi.org/10.1016/j.icarus.2016.03.023

Mid-infrared vibrational study of deuterium-containing PAH variants

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Polycyclic Aromatic Hydrocarbon (PAH) molecules have been long proposed to be a major carrier of Unidentified Infrared (UIR) emission bands that have been observed ubiquitously in various astrophysical environments. These molecules can potentially be an efficient reservoir of deuterium. Once the infrared properties of the deuterium-containing PAHs are well understood both experimentally and theoretically, the interstellar UIR bands can be used as a valuable tool to infer the cause of the deuterium depletion in the ISM. Density Functional Theory (DFT) calculations have been carried out on deuterium-containing ovalene variants to study the infrared properties of these molecules. These include deuterated ovalene, cationic deuterated ovalene, deuteronated ovalene and deuterated-deuteronated ovalene. We present a D/H ratio calculated from our theoretical study to compare with the observationally proposed D/H ratio.

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Planetary and Space Science, in press

http://dx.doi.org/10.1016/j.pss.2016.05.001

Evolution of Chemical Complexity: From simple interstellar molecules to terrestrial biopolymers

Liblice Castle, Czech Republic

13 – 15 September 2016

Organizers:
EU COST Action "Origins and Evolution of Life on Earth and in the Universe"

Rationale: The meeting will try to map the chemical evolution of the molecular building blocks of life from their possible sources in the interstellar medium, the atmospheres of planets and on their surfaces. It also aims to serve to engage the astrochemistry and systems chemistry communities into a dialogue.

The meeting venue is Liblice Castle (http://www.chateau-liblice.com/), a 18th century castle in a wonderful park offers 4 star hotel accommodation, excellent meeting facilities in Baroque settings and excellent meals.

The venue is situated only a 30 minutes drive from Václav Havel airport in Prague. A shuttle service will be provided on the arrival and departure days. Although the venue is very nice the fees for the meeting are fairly low.

Please note: Bursaries are available for scientists and Ph. D. students from countries participating in the European Union COST Action "Origins and Evolution of Life on Earth and in the Universe".

Key dates:
Deadline for registration: July 15th, 2016.
Deadline for abstract submission: July 30th, 2016.

E-mail for contact: cost@jh-inst.cas.cz
Webpage: https://www.jh-inst.cas.cz/tchem/cost2016/

Exploring the Universe with JWST - II

Montreal (Canada)

24 – 28 October 2016

Organizers:
iREx / Université de Montréal

Rationale: The James Webb Space Telescope (JWST), scheduled for launch in October 2018, will be one of the great observatories of the next decade. Its suite of four instruments will provide imaging, spectroscopic and coronagraphic capabilities over the 0.6 to 28.5 micron wavelength range and will offer an unprecedented combination of sensitivity and spatial resolution to study targets ranging from our Solar System to the most distant galaxies. With JWST's launch date approaching rapidly and a first call for proposals scheduled for the end of 2017, it is important to give the astronomical community opportunities to present, highlight and discuss scientific programs that will be made possible by JWST. In this context, we are organizing the scientific conference "Exploring the Universe with JWST - II", which will take place during the week of the 24th to the 28th of October 2016 at the Université de Montréal (Canada). The conference will cover a broad range of scientific topics organized around the main JWST science themes:

- The end of the "dark ages": first light and reionisation.
- The assembly of galaxies.
- The formation and evolution of stars and planets.
- Planetary systems and the origins of life (exoplanets).
- Our Solar System.

This conference is in the same spirit as the one held in the Netherlands at ESTEC (ESA headquarters) in October 2015. The attendance will be limited to approximately 250 persons.

Key dates:
Deadline for registration and abstract submission: July 15th, 2016.

E-mail for contact: jwst16@astro.umontreal.ca
Webpage: http://craq-astro.ca/jwst2016/

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