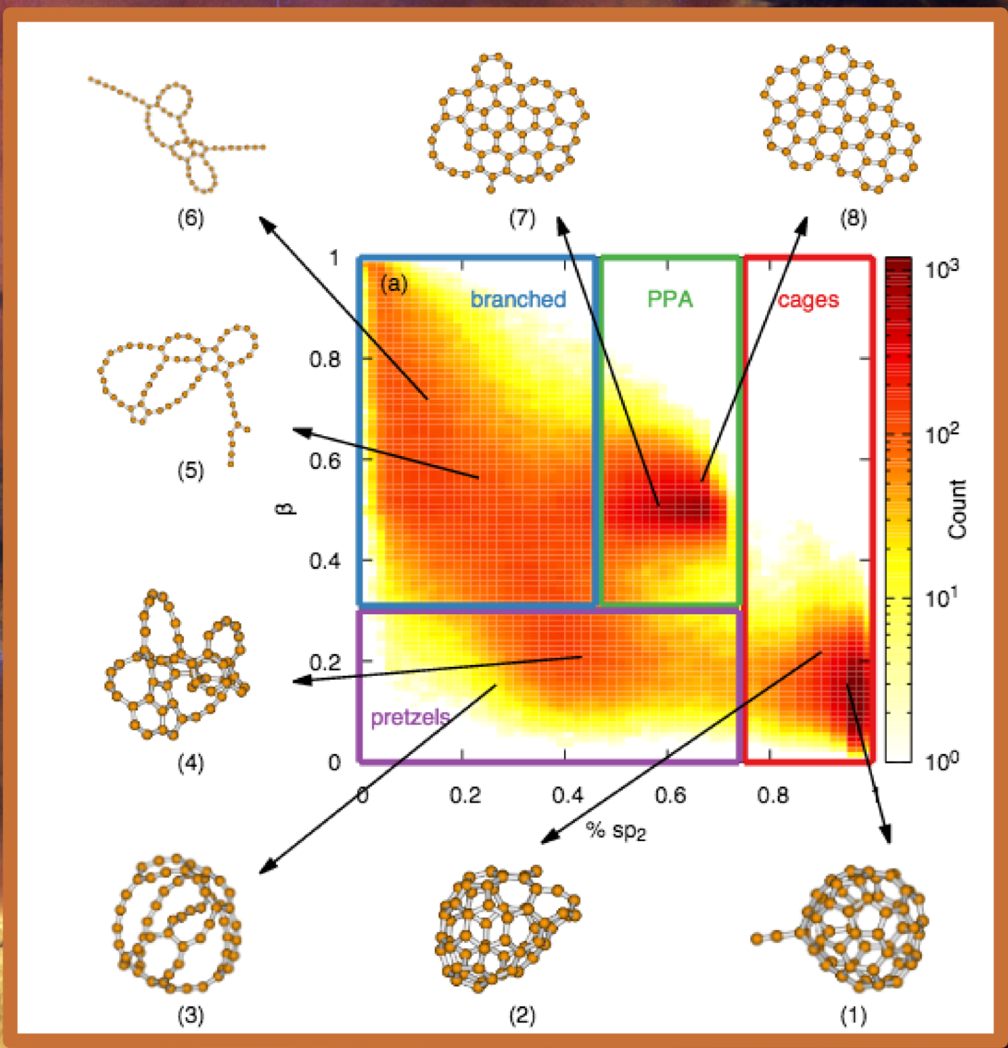
AstroPAH

A Newsletter on Astronomical PAHs

Issue 58 • May 2019



Clusters

Editorial

Dear Colleagues,

We are happy to have you back with us for Issue 58. We are delighted to share with you our In Focus interview with Dr. Ir. Annemieke Petrignani, who was previously part of our AstroPAH Editorial Board and one of its founding editors. Dr. Petrignani now works at the University of Amsterdam and you can learn more about her research and interests in this month's In Focus.

Highlighted Abstracts include recent discoveries and advances on interstellar ionized fulleren C_{60}^{+}, the anharmonicity of pyrene and photochemical production of aromatics in Titan's atmosphere, among others.

We would also like to inform you that the deadlines for abstract submission and Early Bird registration to the 26th International Symposium on Polycyclic Aromatic Compounds (ISPAC) have been extended. More information on the conference website: https://www.oru.se/ISPAC2019. The deadline for oral and poster contributions to the NanoWorld to Stardust Conference have also been extended; they are all detailed in our Meetings section.

We hope you enjoy reading our newsletter and look forward to seeing you again next month.

Enjoy reading our newsletter!

The Editorial Team

Next issue: 20 June 2019.
Submission deadline: 7 June 2019.

Contact us:

astropah@strw.leidenuniv.nl

http://astropah-news.strw.leidenuniv.nl

Click here to Subscribe to AstroPAH

Click here to Contribute to AstroPAH

Contents

PAH Picture of the Month

Two-dimensional distribution of cluster with 60 carbon atoms as a function of the fraction of sp^2 hybridisation and of asphericity β. Four structural families are identified in the plot: cage, planar polycyclic aromatic (PPA), pretzel, and branched and for each family two typical structure are represented. For more details about this theoretical study have a look at the paper by Dubosq et al, A&A Lett., 2019 in the Abstract Section.

Credits: C. Dubosq et al. 2019

Newsletter Design: Isabel Aleman
Background images:
This page: NASA, ESA, and the Hubble Heritage Team (STScI/AURA)
Cover and headers: X-ray by Chandra: NASA/CXC/Univ.Potsdam/L.Oskinova et al; Optical by Hubble: NASA/STScI; Infrared by Spitzer: NASA/JPL-Caltech

An Interview with Dr. Ir. Annemieke Petrignani

Dr. Ir. Annemieke Petrignani works at the University of Amsterdam (UvA) where she leads a research team exploring the organic chemistry in space and the origins of life. Her research focuses on astro-molecular spectroscopy and astrochemistry with an emphasis on the (photo)dynamics and signatures of hydrocarbons in space and on (universal) building blocks of life. She was recently the recipient of a Dutch Astrochemistry Network (DAN) grant as well as a VIDI grant from the Netherlands Organisation for Scientific Research (NWO) to investigate the photofragmentation and the shapes and sizes of hydrocarbons in space. She also received a small joint grant of the Dutch Origins Center to study the role of water and minerals in the ingredients of life. She was one of the founding editors of the AstroPAH newsletter and part of the editorial team until a few months ago. She received her Masters at the Delft University of Technology in Pattern Recognition. She then pursued her PhD at the AMOLF Institute, performing experiments at the ion storage ring CRYRING in Stockholm to investigate the molecular physics of planetary airglow. As a postdoctoral researcher at the Max-Planck Institute for Nuclear Physics, she later investigated the electron recombination and the spectroscopy of small molecular ions using the TSR storage ring and a cryogenic 22-pole trap. Before starting at the UvA, she worked for the Leiden Observatory at the FELIX Laboratory in Nijmegen to investigate the fragmentation of aromatic hydrocarbons using the free electron laser FELICE.

Can you tell us how you got into PAH-related research?

Like with most research, I did not set out to get into this specific research topic. I am actually a trained engineer with a physics background. It was my interest into fundamental issues and applying molecular physics to universal questions that brought me closer to astronomy and eventually also chemistry over the years. After a postdoctoral project at the Max Planck Institute for Nuclear Physics in Heidelberg, I was looking to return to the Netherlands as I had promised my husband. My return coincided with the start of the Dutch Astrochemistry Network programme of NWO. This DAN programme promoted collaboration between observational and theoretical astrochemistry and experimental molecular physics. It was a great fit with my experimental background and the application to astronomy so I ended up working for Xander Tielens. A major difference was that instead of working within physics groups, I found myself being part of a proper astronomy institute, the Leiden Observatory. Suddenly I was also studying huge molecules like PAHs and found myself moving towards experimental astrochemistry.

What did it mean for you to be part of the AstroPAH editorial team? What aspect did you like best?

Being part of this editorial team has been very important to me. AstroPAH was created as a result of a Lorenz Center workshop on interstellar PAHs. This was the first time I organised a big event within the field of astrochemistry. I got to work with two pioneers in the field, Xander Tielens and Lou Allamandola, and thus had a crash course on the history and community of the field. I also met some other young researchers in the field from all over the world, and, at the workshop, we already found ourselves working together to create and co-edit AstroPAH. The creation of AstroPAH was a real result of community building within astrochemistry and I would like to think it is still doing so. Being part of AstroPAH has enriched my academic career immensely, and I have made friends for life.

What, in your opinion, is the most important advancement in PAH research that was accomplished during your time on the AstroPAH board?

That is a difficult question as there has been so much progress accomplished over the years. I think I would have to say that it is the advances in understanding the molecular and photochemical processes at play. We have found out so much more about the underlying molecular physics, such as anharmonic behaviour, photochemistry connecting PAHs with fullerenes, and more. It seems like we are really unravelling the molecular physics at play.

What is your next adventure in PAH research going to be?

I hope the next step will be the identification of individual PAH molecules. I also like to think that my team and I will be able to contribute to this effort. We recently found a really new and exciting way to predict the electronic transitions of PAHs with high accuracy (validated by our own high resolution gas-phase spectroscopy experiments). This is allowing us to narrow down the amount of possible PAH carriers for the diffuse interstellar bands (DIBs). At the moment, I feel very confident that if there are PAH species that are responsible for some of the DIBs, then we will find them this way. I realise though that many scientists have been very optimistic and have tried for many years to identify some of the bands, so it might just be wishful thinking on my part.

Can you tell us about your career path, the difficulties you have faced as a scientist to stay in the field and how you overcame them?

My journey has been a very multidisciplinary one, which has brought me from engineering to physics to astronomy and to chemistry or some combination thereof. This has kept the research always really interesting, and I have learned a lot from all disciplines along the way. It was very difficult from time to time though as I (not always voluntarily) changed fields a couple of times, and it felt like starting all over, especially as an experimentalist. Building up new experiments is - though often satisfyingly challenging - very difficult and time consuming. One spends a lot of time trying to get things to work to only get results in the very end. To then have to move and leave it all behind, can be very frustrating. Getting enough funding to properly expand and/or build experiments is also not an easy task as few grants provide equipment funding. How to overcome these difficulties is not only about being an excellent scientist. It is also partly a matter of being in the right place at the right time. Over the years I have seen many good ideas and researchers being rewarded... or not. Like all scientists I know, you can only get over these barriers through passion, reflection, and perseverance.

Astrochemistry is a very multidisciplinary field. You work with laboratory experiments for applications in Astronomy, which requires you to work amidst scientists in different fields (Physics, Chemistry, Astronomy, Engineering). Can you comment on how you collaborate and communicate with specialists with such different backgrounds, perspectives, jargon, etc... and what you like about such interactions? Do you prefer working in small or large groups and why?

As my journey has led me through many different groups and communities, I am by now feeling a bit like I understand the jargon of the different fields. Though I must admit it still often happens that I notice this is not the case. I have been working in biochemistry recently, and here I feel like a student all over again. I like it a lot though as the multiple disciplines offer many different points of view and a lot of interaction and discussions are needed to understand what is going on to make progress. I like that human interaction is a vital part of this interdisciplinary research. I also find that the best ideas come from interacting with others. My ideal scientific world would be one where teamwork is much more appreciated and stimulated rather than the current focus on the individual efforts.

As for working in small or large groups, it is the diversity that makes it fun. I love working in small groups focusing on more detailed studies as well as working in large groups where it is required to keep the bigger picture in mind. The change of scenery is what I also like most in experimental and interdisciplinary work. You constantly have to approach the problem from different points of view.

What was the most important advice somebody gave you?

I have heard many good pieces of advice throughout my life. The one that comes to mind first and foremost is the one my mother has always given my siblings and me. It translates to ”where there is a will, there is a way”, and it means that if you truly want something, you will be able to find a way to achieve it. As I am very strong-willed, this has helped me get through difficult situations. In my research, I also practice it in the way that if I am truly curious about something, I will find a way to find out what is going on.

How do you balance your professional and personal life?

This has been the most challenging part of my career/life. There have been multiple occasions where I have felt like I needed to choose between family and career, where I felt guilty at home for having to spend so much time at work or being away, or where I felt guilty at work for having to leave earlier or not being able to be at work due to personal situations. I have to be very honest that the births of my children have led to considerable delays and many indirect and unforeseen hindrances because of which I found myself totally out of phase with the typical career path. This diminished my chances to compete in the harsh academic environment dramatically. I was and am however adamant that having a, also larger, family and an academic career is possible. Unfortunately, it is not because the academic world has become women-friendly that it has worked for me. Instead, I took my mothers advice to heart. My passion and strong will have helped a lot. That, and the support of some great female colleagues who always cheered me up and reminded me of the fun in our work.

Abstracts

Confirming interstellar C_{60}^{+} using the Hubble Space Telescope

M. A. Cordiner[1,2], H. Linnartz[3], N. L. J. Cox[4], J. Cami[5], F. Najarro[6], C. R. Proffitt[7], R. Lallement[8], P. Ehrenfreund[3,9], B. H. Foing[10], T. R. Gull[1], P. J. Sarre[11] and S. B. Charnley[1]

[1]NASA Goddard Space Flight Center, 8800 Greenbelt Road, Greenbelt, MD 20771, USA

[2]Department of Physics, Catholic University of America, Washington, DC 20064, USA

[3]Sackler Laboratory for Astrophysics, Leiden Observatory, Leiden University, PO Box 9513, NL 2300 RA Leiden, Netherlands

[4]ACRI-ST, 260 route du Mon Pintard, Sophia Antipolis, France

[5]Department of Physics and Astronomy and Centre for Planetary Science and Exploration (CPSX), The University of Western Ontario, London, ON N6A 3K7, Canada

[6]Departamento de Astrofísica, Centro de Astrobiología (CSIC-INTA), ctra. de Ajalvir km. 4, 28850 Torrejón de Ardoz, Madrid, Spain

[7]Space Telescope Science Institute, 3700 San Martin Drive, Baltimore, MD 21218, USA

[8]GEPI, UMR8111, Observatoire de Paris, 5 Place Jules Janssen, 92195, Meudon, France

[9]George Washington University, Washington DC, USA

[10]ESA ESTEC SCI-S, Noordwijk, The Netherlands

[11]School of Chemistry, The University of Nottingham, University Park, Nottingham, NG7 2RD, UK

Recent advances in laboratory spectroscopy lead to the claim of ionized Buckminsterfullerene (C_{60}^{+}) as the carrier of two diffuse interstellar bands (DIBs) in the near-infrared. However, irrefutable identification of interstellar C_{60}^{+} requires a match between the wavelengths and the expected strengths of all absorption features detectable in the laboratory and in space. Here we present Hubble Space Telescope (HST) spectra of the region covering the C_{60}^{+} 9348, 9365, 9428 and 9577 Å absorption bands toward seven heavily-reddened stars. We focus in particular on searching for the weaker laboratory C_{60}^{+} bands, the very presence of which has been a matter for recent debate. Using the novel STIS-scanning technique to obtain ultra-high signal-to-noise spectra without contamination from telluric absorption that afflicted previous ground-based observations, we obtained reliable detections of the (weak) 9365, 9428 Å and (strong) 9577 Å C_{60}^{+} bands. The band wavelengths and strength ratios are sufficiently similar to those determined in the latest laboratory experiments that we consider this the first robust identification of the 9428 Å band, and a conclusive confirmation of interstellar C_{60}^{+}.

E-mail: martin.cordiner@nasa.gov

ApJL, 875, L28 (2019)

https://arxiv.org/pdf/1904.08821

Spectroscopy of corannulene cations in helium nanodroplets

Michael Gatchell,[1,2] Paul Martini[1], Felix Laimer[1], Marcelo Goulart[1], Florent Calvo[3], and Paul Scheier[1]

[1] Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Technikerstr. 25, A-6020 Innsbruck, Austria

[2] Department of Physics, Stockholm University, 106 91 Stockholm, Sweden

[3] Université Grenoble Alpes, CNRS, LIPhy, Grenoble, France

Helium tagging in action spectroscopy is an efficient method for measuring the absorption spectrum of complex molecular ions with minimal perturbations to the gas phase spectrum. We have used superfluid helium nanodroplets doped with corannulene to prepare cations of these molecules complexed with different numbers of He atoms. In total we identify 13 different absorption bands from corannulene cations between 5500 Å and 6000 Å. The He atoms cause a small, chemically induced redshift to the band positions of the corannulene ion. By studying this effect as a function of the number of solvating atoms we are able to identify the formation of solvation structures that are not visible in the mass spectrum. The solvation features detected with the action spectroscopy agree very well with the results of atomistic modeling based on path-integral molecular dynamics simulations. By additionally doping our He droplets with D_2, we produce protonated corannulene ions. The absorption spectrum of these ions differs significantly from the case of the radical cations as the numerous narrow bands are replaced by a broad absorption feature that spans nearly 2000 Å in width.

E-mail: michael.gatchell@uibk.ac.at

Faraday Discussions, in press (DOI: 10.1039/C8FD00178B)

https://pubs.rsc.org/en/content/articlelanding/2019/fd/c8fd00178b

Experimental approach to the Study of Anharmonicity in the Infrared Spectrum of Pyrene from 14 to 723 K

Shubhadip Chakraborty[1], Giacomo Mulas[1,2], Karine Demyk[1] and Christine Joblin[1]

[1] Institut de Recherche en Astrophysique et Planétologie, Université de Toulouse (UPS), CNRS, CNES, 9 Av. du Colonel Roche, 31028, Toulouse, Cedex 4, France

[2] Istituto Nazionale di Astrofisica (INAF), Osservatorio Astronomico di Cagliari, 09047 Selargius (CA), Italy

Quantifying the effect of anharmonicity on the infrared spectrum of large molecules such as polycyclic aromatic hydrocarbons (PAHs) at high temperatures is the focus of a number of theoretical and experimental studies, many of them motivated by astrophysical applications. We recorded the IR spectrum of pyrene $C_{16}H_{10}$ microcrystals embedded in KBr pellets over a wide range of temperatures (14 – 723 K) and studied the evolution of band positions, widths, and integrated intensities with temperature. We identified jumps for some of the spectral characteristics of some bands in the 423 – 473 K range. These were attributed to a change of phase from crystal to molten in condensed pyrene, which appears to affect more strongly bands involving large CH motions. Empirical anharmonicity factors that quantify

the linear evolution of band positions and widths with temperature for values larger than ∼150 – 250 K, depending on the band, were retrieved from both phases and averaged to provide recommended values for these anharmonicity factors. The derived values were found to be consistent with available gas phase data. We conclude about the relevance of the methodology to produce data that can be compared with calculated anharmonic IR spectra and provide input for models that simulate the IR emission of astro-PAHs.

E-mail: christine.joblin@irap.omp.eu

J. Phys. Chem. A 2019, doi: 10.1021/acs.jpca.8b11016

https://pubs.acs.org/doi/full/10.1021/acs.jpca.8b11016
https://arxiv.org/abs/1904.02899

Mapping the structural diversity of C_{60} carbon clusters and their infrared spectra

C. Dubosq[1], C. Falvo[2,3], F. Calvo[3], M. Rapacioli[1], P. Parneix[2], T. Pino[2], A. Simon[1]

[1] Laboratoire de Chimie et Physique Quantiques LCPQ/IRSAMC, Université de Toulouse and CNRS, UT3-Paul Sabatier, 118 Route de Narbonne, F-31062 Toulouse, France

[2] Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS, Univ. Paris Sud, Université Paris-Saclay, 91405 Orsay, France

[3] Université Grenoble Alpes, CNRS, LIPhy, 38000 Grenoble, France

The current debate about the nature of the carbonaceous material carrying the infrared (IR) emission spectra of planetary and proto-planetary nebulae, including the broad plateaus, calls for further studies on the interplay between structure and spectroscopy of carbon-based compounds of astrophysical interest. The recent observation of C_{60} buckminsterfullerene in space suggests that carbon clusters of similar size may also be relevant. In the present work, broad statistical samples of C_{60} isomers were computationally determined without any bias using a reactive force field, their IR spectra being subsequently obtained following local optimization with the density-functional-based tight-binding theory. Structural analysis reveals four main structural families identified as cages, planar polycyclic aromatics, pretzels, and branched. Comparison with available astronomical spectra indicates that only the cage family could contribute to the plateau observed in the 6–9 µm region. The present framework shows great promise to explore and relate structural and spectroscopic features in more diverse and possibly hydrogenated carbonaceous compounds, in relation with astronomical observations.

E-mail: aude.simon@irsamc.ups-tlse.fr

Astron. Astrophys. Lett., forthcoming article (2019)

https://doi.org/10.1051/0004-6361/201834943

The photochemical production of aromatics in the atmosphere of Titan

J.C. Loison[1], M. Dobrijevic[2], K. M. Hickson[1]

[1] Institut des Sciences Moléculaires (ISM), CNRS, Univ. Bordeaux, 351 cours de la Libration, 33400 Talence, France

[2] Laboratoire d'Astrophysique de Bordeaux, Univ. Bordeaux, CNRS, B18N, allée Geoffroy Saint-Hilaire, 33615 Pessac, France

The photochemical processes at work in the atmosphere of Titan are very complex and lead to a great variety of compounds with aerosols as an end-product. One of the most complex molecules detected so far is benzene (C_6H_6). In the present work, we have updated and improved the chemistry of aromatics in order to better understand the main chemical pathways leading to the production of benzene and determine what other aromatics could be produced efficiently in the atmosphere. This new chemical scheme has been incorporated in our 1D photochemical model corresponding to mean conditions. We confirm the importance of ionic chemistry for benzene production in the upper atmosphere and we have found that excited benzene is an important intermediate in benzene production due to the exothermicity of many production reactions. Among the 24 aromatics included in the model, neutral aromatics like toluene ($C_6H_5CH_3$) and ethylbenzene ($C_6H_5C_2H_5$) are relatively abundant, suggesting in particular that toluene could be detectable in the infrared, and eventually microwave wavelength ranges. However, we obtained large uncertainties on model results highlighting the need for more experiments and theoretical studies to improve the chemistry of aromatics.

E-mail: Michel.Dobrijevic@obs.u-bordeaux1.fr

Icarus 329 (2019) 55-71

https://doi.org/10.1016/j.icarus.2019.03.024

From the NanoWorld to Stardust (NW2SD)

Marseille, France
17 - 19 July 2019

Dear Colleagues,

We are pleased to announce the International Conference “From the NanoWorld to Stardust (NW2SD)”, which will be held in Marseille, France, during July 17-19, 2019. The conference will take place in a scenic location looking over the Mediterranean Sea in central Marseille.

The conference will cover areas like low-dimensional and 2D topological materials, nanostructures for spintronics, quantum computing and neuromorphic computation, nanobio and neuroscience, carbon-based nanomaterials beyond Earth, cosmic dusts, spectroscopy and chemistry on (exo)planets, comets and dust clouds, as well as dusty plasmas etc.

Eminent Plenary Speakers comprise Nobel, Wolf and Kavli Prize Laureates.

Important dates:

- NEW deadline for oral or poster presentations: May 31, 2019
- Early bird registration: May 31, 2019

For further information about the conference, please visit the following website:
https://nw2sd.sciencesconf.org/

Email: nw2sd@sciencesconf.org

Hoping to meeting you next July in Marseille, with our best regards,

Prof. Jean-Marc Layet, Aix-Marseille Univ., France

Celebrating the first 40 Years of Alexander Tielens' Contribution to Science:

THE PHYSICS AND CHEMISTRY OF THE INTERSTELLAR MEDIUM

Centre International des Congrès du Palais des Papes, Avignon, France
September 2 - 6, 2019

Dear colleagues,

We are happy to announce the conference:

****

CELEBRATING 40 YEARS OF ALEXANDER TIELENS' CONTRIBUTION TO SCIENCE:
THE PHYSICS AND CHEMISTRY OF THE ISM
https://tielens2019.sciencesconf.org/

****

Venue
The symposium will be held 2-6 September 2019 in the historical Congrès du Palais des Papes, Avignon, France (http://www.avignon-congres.com/).

Rational
Xander Tielens has been driving research in the fields of interstellar physics and chemistry and the cosmic cycle of matter with outstanding contributions for 40 years. With this meeting, we wish to celebrate his scientific achievements and discuss future research directions opened up by his contributions.

The meeting will focus on the fields strongly influenced by Xander involving the physical and chemical processes that control the interstellar medium and its life cycle: PDRs, interstellar and circumstellar dust, PAHs, ices and astrochemistry. We will especially emphasize future opportunities offered by the powerful telescopes at our disposal such as, for example, ALMA, SOFIA, and JWST. The meeting will consist of invited reviews, invited and contributed talks, and posters.

Key dates

February 11:	Opening of the registration and abstract submission on the symposium website
June 1:	Deadline of Abstract submission for oral contributions
June 15:	Announcement of the selected oral contributions
June 20:	Deadline of registration

Please note that the symposium participation is restricted to 120 persons, based on first-signed first-selected, so do not delay your registration!

Confirmed invited speakers
L. Allamandola, N. Balucani, A. Boogert, F. Boulanger, S. Cazaux, J. Cernicharo,

L. d'Hendecourt, T. de Graauw, J. Goicoechea, D. Hollenbach, C. Joblin, B. Lefloch, M. Kaufman, C. Kemper, M. Meixner, T. Millar, M-E. Palumbo, E. Roueff, K. Schuster, E. van Dishoeck, R. Waters

Scientific Organizing Committee
C. Ceccarelli (chair), A. Candian (co-chair), J. Cami, C. Dominik, L. Hornekaer, K. Justtanont, E. Peeters, M. Wolfire

Local Organizing Committee
B. Lefloch(chair), E. Bianchi,ŁC. Borye, M. Bouvier, M. De Simone, M-H Sztefek

Contacts
loc-XT2019@univ-grenoble-alpes.fr

AstroPAH Newsletter

http://astropah-news.strw.leidenuniv.nl
astropah@strw.leidenuniv.nl

Next issue: 20 June 2019
Submission deadline: 7 June 2019