AstroPAH

A Newsletter on Astronomical PAHs

Issue 12 | October 2014

One Year of AstroPAH

Editorial

Dear Colleagues,

This month marks the **first anniversary of AstroPAH** and we celebrate this landmark with this very special issue and a new design.

In this issue, we look into this past first year of AstroPAH. The Picture of the Month shows a collage of all our past covers, which synthesize the diversity of the PAH topics we covered. Our editor-in-chief, Xander Tielens, begins the newsletter sharing some words on the importance of PAH research.

We have grown to gather a community of more than 200 subscribers from all over the world. The *In Focus* shows this and other numbers to give our readers an idea of the reach of AstroPAH in our research community. We also look at the future of PAHs. We asked our readers what is the PAH-related question you would like to see solved in the next decades. The collection of interesting responses we got from the PAH community can be seen in the extra *In Focus* section on “The Future”.

We do not forget one of the goals of AstroPAH: to keep you updated with the most recent results in PAH research. We have an assortment of interesting abstracts you should not miss: experimental, theoretical and observational studies about PAHs, fullerenes and hydrocarbon molecules and clusters. Two opportunities for students looking for PhD positions are advertised.

We hope you enjoy this special issue, as we have enjoyed editing AstroPAH in this last year. We thank the PAH community for the support so far and welcome your contributions for future issues of AstroPAH.

Best regards

The Editorial Team

Next issue: 18 November 2014.
Submission deadline: 7 November 2014.

Contents

PAH Picture of the Month

A composition of all the covers of AstroPAH in its first year. In the background, the Orion nebula.

Credits for the background image: NASA, ESA, T. Megeath (University of Toledo) and M. Robberto (STScI). **Credits for the images in the covers:** available in the corresponding issue. **Composition:** Isabel Aleman and Alessandra Candian.

CONTACT

astropah@strw.leidenuniv.nl

CLICK HERE TO SUBSCRIBE TO AstroPAH

CONTRIBUTE TO AstroPAH!
http://astropah-news.strw.leidenuniv.nl

Design by Isabel Aleman

Foreword

by A. G. G. M. Tielens

Over the last 20 years, we have learned that we live in a **Molecular Universe** where molecules are omnipresent. Nowhere is this more obvious than in perusing the IRAC/Spitzer gallery of images of astronomical objects The infrared emission of the interstellar medium of galaxies – see, for example, M51 (**Figure 1**) – is dominated, at all scales, by emission from PAHs. It is then immediately obvious that molecules are deeply interwoven in the fabric of the Universe and conversely that if we want to understand the Universe, we have to understand the role of molecules in the evolution of galaxies, the formation of stars and planets, and particularly the prebiotic roots of life.

Figure 1 - False-color composite of 3.6μm (blue), 4.5μm (green), 5.8μm (orange) and 8.0μm (red) emission highlighting the emission from PAHs in M51, the Whirpool galaxy. Credits: NASA/JPL-Caltech/R. Kennicutt (Univ. of Arizona). Click here for more information.

As we wrote in the first issue, astrochemistry is a highly interdisciplinary field where astronomers, molecular physicists, spectroscopists, and quantum chemists meet. AstroPAH was conceived as a way to build an active and involved community, connecting scientists with an interest in interstellar PAHs across disciplinary boundaries. After one year, it is good to step back and make up the balance. From our perspective, AstroPAH has started off well as we published 12 issues packed with abstracts of recent articles, summaries of workshops, news from the field, and even job advertisements. At the same time, we have also experienced this as a fun year and we would like to thank all of you, subscribers and contributors to the AstroPAH newsletter, for your help in making AstroPAH a success.

A Look Back at the First Year of AstroPAH

**E. Sciamma-O'Brien, I. Aleman, A. Candian,
E. Micelotta, A. Petrignani, and A. G. G. M. Tielens**
– the AstroPAH editorial board –

AstroPAH started one year ago with the goal of being a tool to promote constant communication between the different fields working with PAHs in space – Astronomy, Chemistry, and Physics — and to keep the PAH community informed of the latest developments in astronomical PAH research. To celebrate our first anniversary, we want to show you what we have accomplished in this first year.

Our Subscribers

We have now 210 subscribers that come from 27 countries and two international organizations (Gemini Observatory and ESA). **Figure 1** shows the location of the 110 research institutions represented in our subscribers list and **Figure 2** the number distribution of subscribers per country.

Figure 1 - Locations of the 110 research institutions represented in our subscribers list.

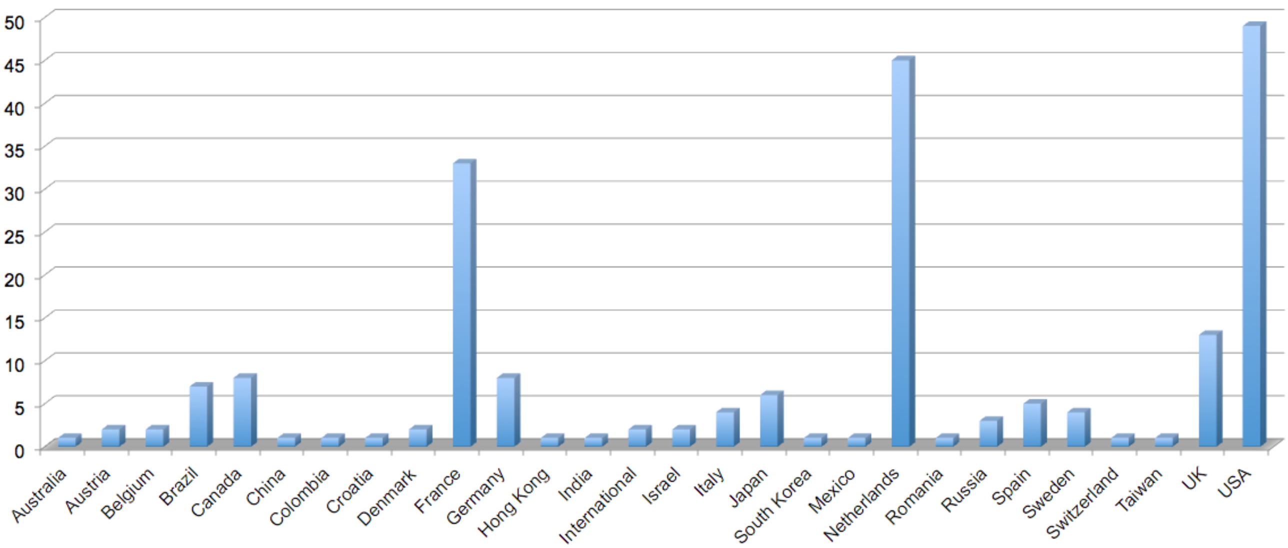


Figure 2 - Distribution of our subscribers per country or International organization.

The Contributions

In this last year, in our 12 editions, we published **84 abstracts of papers** from journals or proceedings and **other 8 contributions** among abstracts of defended thesis, announcement of scientific meetings, and job openings. We also had **12 *In Focus*** original articles, from which four were dedicated to meeting summaries, three to laboratory facilities, and three were interviews.

More than a half of the paper abstracts submitted to AstroPAH were published in astrophysical journals, 20% in physical chemistry journals, 10% in chemistry journals (**Figure 3**).

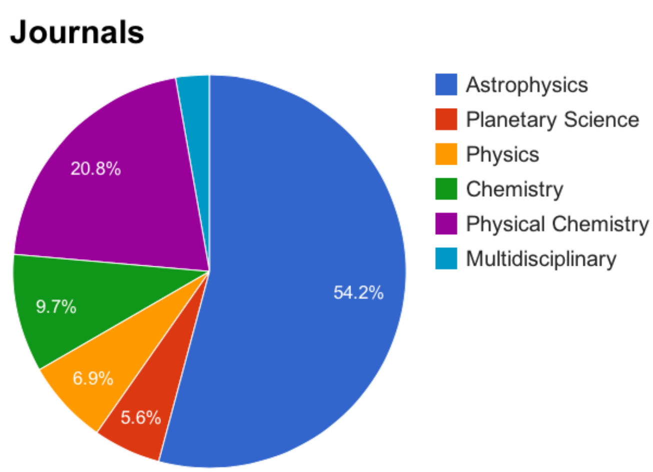
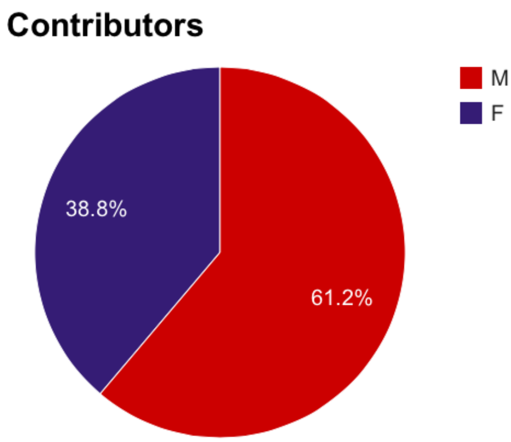


Figure 3 - Topics of the journals where our contributors publish their papers.

The Contributors

The contributions to AstroPAH were submitted by **67 researchers**, from which 38.8% are women and 61.2% are men (**Figure 4, left**). About half of these researchers come from universities, around a third from research institutes, 12% from various space agencies and 9% from astronomical observatories (**Figure 4, right**), for a total of 52 different institutions. The location of these institutions are indicated in the map of **Figure 5**.



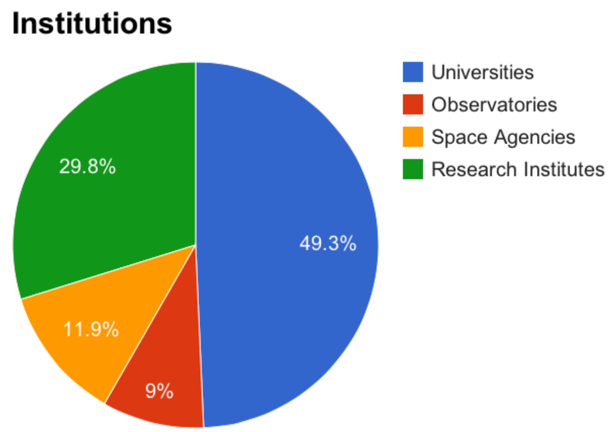
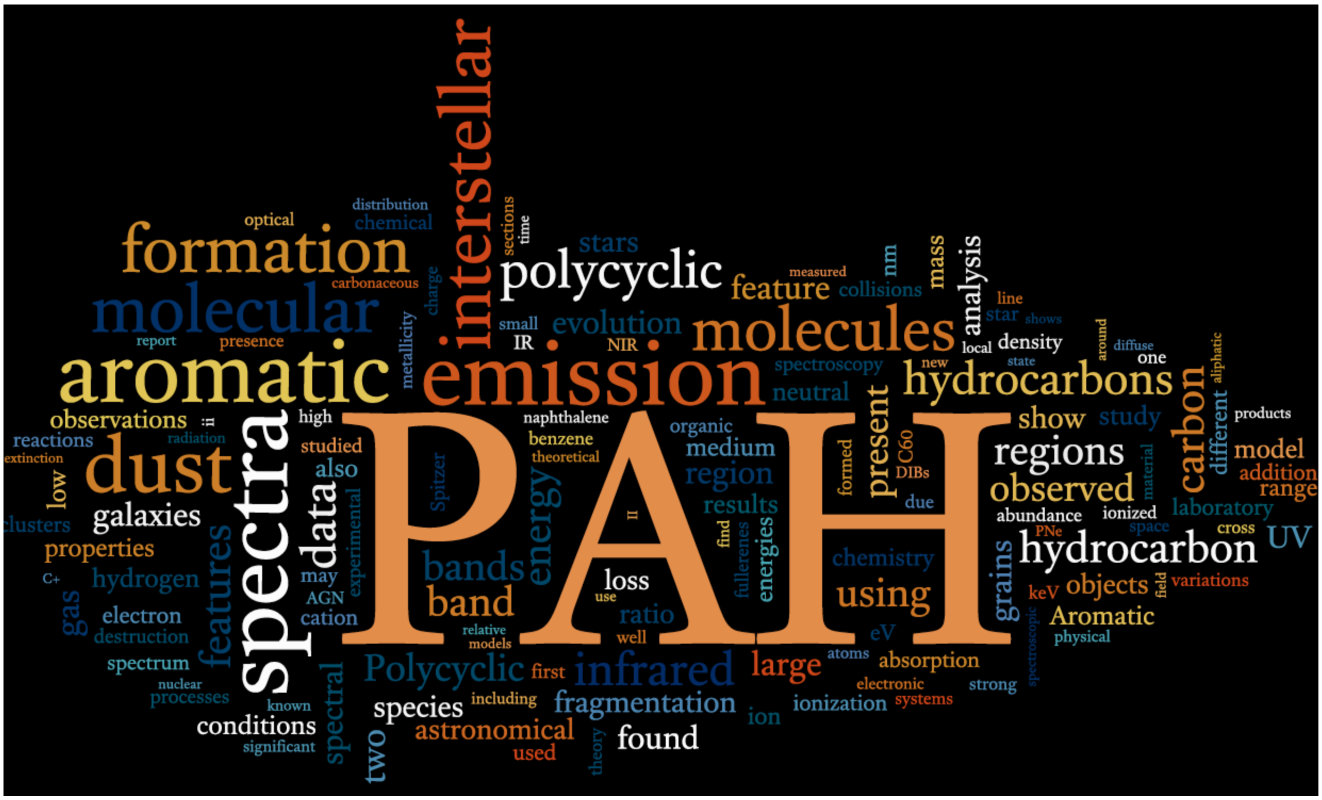


Figure 4 - (Left) Gender distribution of our contributors. (Right) Types of institutions where our contributors work.

Figure 5 - Locations of the research institutes where the 67 researches that contributed to AstroPAH work.

A Fun Way to Look at our Contributors Abstracts: Word Cloud

Taking all the abstracts presented in AstroPAH this past year, we have generated a word cloud that gives greater prominence to words that appear more frequently in the source text (**Figure 6**). Obviously PAH is the most prominent...



A Word of Thank You

This has been a fun year and we, the editorial board of AstroPAH, would like to thank all of you, subscribers and contributors to the AstroPAH newsletter for making it such a wonderful experience.

Please continue to support our newsletter by sending your contributions and telling your colleagues about our newsletter. We have had great feedback from you so far and want to continue to hear from you to improve AstroPAH and to continue supporting the PAH research.

In Focus

The Future

E. Sciamma-O'Brien and Our Subscribers

In our past issue, we posed the question "What is the PAH-related question you would like to see solved in the next decades?" Here are the answers! Please continue to send us your questions, as we will continue compiling them as a gauge of the "health" of the field.

"I would like to see the detection of the signature of astro PAHs (any astro PAH) in a wavelength region other than in the IR (e.g., in the UV, in the Visible, etc..)"

"I would like to see solved the question of the carriers of UIR bands!"

"Are PAHs the carriers of the diffuse interstellar bands? An answer either way would be extremely interesting, but could well take 'decades '!"

"Would be nice to know which - if any - PAHs give rise to the diffuse interstellar bands... Then you would also solve (partly) the question about which PAHs are actually present in interstellar space."

"I'd love to see any given individual PAH conclusively detected in the ISM. It's been done for buckyballs, now for PAHs."

"Given that we have several decades of timeline to work with, I'd like to see directly measured infrared emission spectra of PAH molecules."

"I would like to see data spanning 3-20 microns all in the same direction at the same spatial resolution and with enough spectral resolution to see shifts in the 6.2 micron band. Maps would be very helpful, and I expect JWST to provide this kind of data. It would help a lot with sorting out size and composition variations, maybe even structure. The current data set is just not good enough. To interpret such data properly, we will need a more complete database of PAH spectra and a better understanding of what produces the red (and sometimes blue) wings on the features, but even with the current database and models we would make a lot of progress with better astronomical spectra."

"I would be very interested to see if we can get a real handle on how possibly different PAH mixtures can exhibit the same astronomical PAH emission spectrum, but still reflect local astrophysical conditions. Especially the connection with the (photo)chemistry that is driving the population to this state; think here of chemical reaction networks for hydrogenation and edge group variations - we do mostly understand charge."

"Why, if the ISM is dominated by really large PAHs, don't we see any significant evidence for such large PAHs in primitive meteorites, objects that preserve evidence of plenty of other presolar materials. Much of the carbon in meteorites is aromatic, but it is largely in smaller aromatic units bound together in insoluble organic material."

"Are astronomical PAHs really astronomical PANHs? The question of nitrogen substitutions for several of a PAH's skeletal carbon atoms is important for both astrochemistry and spectroscopy. Astrochemically speaking, having some of the cosmic nitrogen tied up in PANHs instead of N_2 (which is presumed but not really known), means N is chemically accessible because reactions involving PAHs will involve N. If so, some of the cosmic organic compounds containing nitrile and iso-nitrile groups as well as amines might originate in PANHs. There is also the importance of PANHs in biology. From the IR astrospectroscopy perspective, what little we know about PANH IR spectra (Hudgins et al. ApJ 632, 316, 2005) suggests that some key relative band intensities may change dramatically upon nitrogen incorporation. Since astronomers measure relative band intensities in the astronomical spectra to probe fundamental properties such as charge, edge-structure and size of the emitting, astronomical PAH population, this is a critical question."

Abstracts

o-Benzyne fragmentation and isomerization pathways. A CASPT2 study

Giovanni Ghigo[1], **Andrea Maranzana**[1] **and Glauco Tonachini**[1]

[1] Dipartimento di Chimica, Univesità di Torino, via P. Giuria 7, 10125 Torino, Italy

The mechanisms of the fragmentation and isomerization pathways of o-benzyne were studied at the multi-configurational second-order perturbative level [CAS(12,12)-PT2]. The direct fragmentation of o-benzyne to C_2H_2 + C_4H_2 follows two mechanisms: a concerted mechanism and a stepwise mechanism. Although the concerted mechanism is characterized by a single closed-shell transition structure, the stepwise pathway is more complex and structures with a strong diradical character are seen. A third diradicaloid fragmentation pathway of o-benzyne yields C_6H_2 as the final product. As an alternative to fragmentation, o-benzyne can also undergo rearrangement to its $meta$ and $para$ isomers and to the open-chain cis and $trans$ isomers of hexa-3-en-1,6-diyne (HED). These easily fragment to C_2H_2 + C_4H_2 or C_6H_2. Kinetic modelling at several temperatures between 800 and 3000 K predicted that the thermal decomposition of o-benzyne should yield C_2H_2, C_4H_2 and C_6H_2 as the main products. Small amounts of the HED isomers accumulated at temperatures $<$ 1200 K, but they rapidly decompose at higher temperatures. Between 1000 and 1400 K, C_2H_2 + C_4H_2 are formed exclusively from the decomposition of $trans$-HED. At temperatures $>$ 1400 K, C_2H_2 + C_4H_2 also form from the direct fragmentation of o-benzyne. The formation of C_2H_2 + C_4H_2 prevails up to 1600 K but above this temperature the formation of C_6H_2 prevails. At temperatures $>$ 2400 K, the direct fragmentation of o-benzyne again leads to the formation of C_2H_2 + C_4H_2. The formation of hydrogen atoms is also explained by our proposed mechanisms.

E-mail: giovanni.ghigo@unito.it

Phys. Chem. Chem. Phys., 2014, Advance Article

http://pubs.rsc.org/en/content/articlelanding/2014/cp/c4cp02582b#!divAbstract

Dust composition and mass-loss return from the luminous blue variable R71 in the LMC

S. Guha Niyogi[1], M. Min[2], M. Meixner[3], L.B.F.M. Waters[4], J. Seale[3], and A.G.G.M. Tielens[1]

[1] Leiden Observatory, Leiden University, PO Box 9513, NL-2300RA Leiden, The Netherlands

[2] Astronomical Institute "Anton Pannekoek", University of Amsterdam, PO Box 94249, 1090 GE, Amsterdam, The Netherlands

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

[4] SRON, Sorbonnelaan 2, 3584 CA, Utrecht, The Netherlands

Context. We present an analysis of mid- and far-infrared (IR) spectrum and spectral energy distribution (SED) of the luminous blue variable (LBV) R71 in the Large Magellanic Cloud (LMC).

Aims. This work aims to understand the overall contribution of high-mass LBVs to the total dust-mass budget of the interstellar medium (ISM) of the LMC and compare this with the contribution from low-mass asymptotic giant branch (AGB) stars. As a case study, we analyze the SED of R71.

Methods. We compiled all the available photometric and spectroscopic observational fluxes from various telescopes for a wide wavelength range (0.36 – 250 μm). We determined the dust composition from the spectroscopic data, and derived the ejected dust mass, dust mass-loss rate, and other dust shell properties by modeling the SED of R71. We noted nine spectral features in the dust shell of R71 by analyzing *Spitzer Space Telescope* spectroscopic data. Among these, we identified three new crystalline silicate features. We computed our model spectrum by using 3D radiative transfer code MCMax.

Results. Our model calculation shows that dust is dominated by amorphous silicates, with some crystalline silicates, metallic iron, and a very tiny amount of polycyclic aromatic hydrocarbon (PAH) molecules. The presence of both silicates and PAHs indicates that the dust has a mixed chemistry. We derived a dust mass of 0.01 $M_\odot$, from which we arrive at a total ejected mass of $\approx$ 5 $M_\odot$. This implies a time-averaged dust mass-loss rate of 2.5×10^{-6} $M_\odot$ yr^{-1} with an explosion about 4000 years ago. We assume that the other five confirmed dusty LBVs in the LMC loose mass at a similar rate, and estimate the total contribution to the mass budget of the LMC to be $\approx 10^{-5}$ $M_\odot$ yr^{-1}, which is comparable to the contribution by all the AGB stars in the LMC.

Conclusions. Based on our analysis on R71, we speculate that LBVs as a class may be an important dust source in the ISM of the LMC.

E-mail: suklima@strw.leidenuniv.nl

A&A 569, A80 (2014)

http://adsabs.harvard.edu/abs/2014A%26A...569A..80G

C_{60} in Photodissociation Regions

Pablo Castellanos[1], Olivier Berné[2,3], Yaron Sheffer[4], Mark G. Wolfire[4] and Alexander G.G.M. Tielens[1]

[1] Leiden Observatory, P.O. Box 9513, 2300 RA Leiden, The Netherlands

[2] Université de Toulouse, UPS-OMP, IRAP, F-31400 Toulouse, France

[3] CNRS, IRAP, 9 Av. Colonel Roche, BP 44346, 31028 Toulouse Cedex 4, France [4] Department of Astronomy, University of Maryland, College Park, MD 20742, USA

Recent studies have confirmed the presence of buckminsterfullerene (C_{60}) in different interstellar and circumstellar environments. However, several aspects regarding C_{60} in space are not well understood yet, such as the formation and excitation processes, and the connection between C_{60} and other carbonaceous compounds in the interstellar medium, in particular polycyclic aromatic hydrocarbons (PAHs). In this paper we study several photodissociation regions (PDRs) where C_{60} and PAHs are detected and the local physical conditions are reasonably well constrained, to provide observational insights into these questions. C_{60} is found to emit in PDRs where the dust is cool ($T_d = 20 - 40$ K) and even in PDRs with cool stars. These results exclude the possibility for C_{60} to be locked in grains at thermal equilibrium in these environments. We observe that PAH and C_{60} emission are spatially uncorrelated and that C_{60} is present in PDRs where the physical conditions (in terms of radiation field and hydrogen density) allow for full dehydrogenation of PAHs, with the exception of Ced 201. We also find trends indicative of an increase in C_{60} abundance within individual PDRs, but these trends are not universal. These results support models where the dehydrogenation of carbonaceous species is the first step towards C_{60} formation. However, this is not the only parameter involved and C_{60} formation is likely affected by shocks and PDR age.

E-mail: pablo@strw.leidenuniv.nl

ApJ 794, 83 (2014)

http://iopscience.iop.org/0004-637X/794/1/83/

Low-energy vibrational spectra of flexible diphenyl molecules: Biphenyl, Diphenylmethane, Bibenzyl and 2-, 3- and 4-Phenyltoluene

M. A. Martin-Drumel[1,2,*], O. Pirali[1,2], C. Falvo[1], P. Parneix[1], A. Gamboa[1], F. Calvo[4], and Ph. Bréchignac[1]

[1] Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS, Université Paris-Sud , Orsay Cedex, France.

[2] SOLEIL Synchrotron, L'orme des Merisiers, Saint-Aubin, 91192 Gif-Sur-Yvette, France

[3] Laboratoire Interdisciplinaire de Physique (LIPhy), Grenoble, France

[*] Present address: Harvard-Smithsonian Center for Astrophysics, Cambridge MA, USA

Gas phase absorption far-infrared (FIR) spectra of six flexible hydrocarbon molecules containing two phenyl groups –biphenyl, diphenylmethane, bibenzyl and 2-, 3-, 4-phenyltoluene– are reported for the first time, allowing an accurate determination of most of their active low-

frequency vibrational modes. DFT calculations have been carried out at the harmonic and perturbative anharmonic levels to predict the vibrational spectra of these molecules and unambiguously assign observed vibrational modes.

E-mail: mmartin@cfa.harvard.edu

Phys. Chem. Chem. Phys. 16, 22062–22072 (2014)

http://pubs.rsc.org/en/content/articlelanding/2014/cp/c4cp03278k#!divAbstract

AKARI IRC 2.5-5 μm Spectroscopy of Infrared Galaxies Over a Wide Luminosity Range

K. Ichikawa[1], M. Imanishi[2], Y. Ueda[1], T. Nakagawa[3], M. Shirahata[4], H. Kaneda[5], and S. Oyabu[5]

[1] Department of Astronomy, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan

[2] Subaru Telescope, 650 North A'ohoku Place, Hilo, HI 96720, USA

[3] Institute of Space and Astronautical Science (ISAS), Japan Aerospace Exploration Agency, 3-1-1 Yoshinodai, Chuo-ku, Sagamihara, Kanagawa 252-5210, Japan

[4] National Institutes of Natural Science, National Astronomical Observatory of Japan (NAOJ) 2-21-1 Osawa, Mitaka, Tokyo 181-8588, Japan

[5] Graduate School of Science, Nagoya University, Furo-cho, Chikusa-ku, Nagoya, Aichi 464-8602, Japan

We present the result of a systematic infrared 2.5–5 μm spectroscopic study of 22 nearby infrared galaxies over a wide infrared luminosity range ($10^{10}L_\odot < L_{\rm IR} < 10^{13}L_\odot$) obtained from *AKARI* Infrared Camera (IRC). The unique band of the *AKARI* IRC spectroscopy enables us to access both the 3.3 μm polycyclic aromatic hydrocarbon (PAH) emission feature from star forming activity and the continuum of torus-dust emission heated by an active galactic nucleus (AGN). Applying our AGN diagnostics to the *AKARI* spectra, we discover 14 buried AGNs. The large fraction of buried AGNs suggests that AGN activity behind the dust is almost ubiquitous in ultra-/luminous infrared galaxies (U/LIRGs). We also find that both the fraction and energy contribution of buried AGNs increase with infrared luminosity from $10^{10}L_\odot$ to $10^{13}L_\odot$, including normal infrared galaxies with $L_{\rm IR} < 10^{11}L_\odot$. The energy contribution from AGNs in the total infrared luminosity is only $\sim$ 7% in LIRGs and $\sim$ 20% in ULIRGs, suggesting that the majority of the infrared luminosity originates from starburst activity. We investigate the luminosity relation between star formation and AGN. We find that these infrared galaxies exhibit higher star formation rates than optically selected Seyfert galaxies with the same AGN luminosities, implying that infrared galaxies could be an early evolutionary phase of AGN.

E-mail: ichikawa@kusastro.kyoto-u.ac.jp

ApJ, 794, 139 (2014)

http://adsabs.harvard.edu/abs/2014ApJ...794..139I

Structures, stability, and growth sequence patterns of small homoclusters of naphthalene, anthracene, phenanthrene, phenalene, naphthacene, and pyrene

Hiroshi Takeuchi[1]

[1] Division of Chemistry, Graduate School of Science, Hokkaido University, 060-0810, Sapporo, Japan

Growth sequence patterns of molecular clusters have not been well elucidated. To examine structures of planar-molecule clusters, naphthalene, anthracene, phenanthrene, phenalene, naphthacene, and pyrene clusters with up to 10 molecules were theoretically investigated with the all-atom OPLS potential. The global-minimum geometries of the naphthalene dimer, trimer, and tetramer are consistent with the experimental data, suggesting that the model potential is useful for predicting the cluster geometries. The growth sequence patterns of the naphthalene, anthracene, phenanthrene, and naphthacene clusters are based on herringbone structures whereas the structures of the phenalene and pyrene clusters are amorphous. The magic numbers of the clusters are 7 or 8 except for the phenalene clusters. These numbers are used to discuss structural motifs of the clusters.

E-mail: takehi@sci.hokudai.ac.jp

Comput. Theoret. Chem. 1021, 84 (2013)

http://www.sciencedirect.com/science/article/pii/S2210271X13002661

PhD Positions at Leiden Observatory

Leiden University, The Netherlands

http://www.strw.leidenuniv.nl

The Leiden Observatory invites applications for ~**10 PhD positions 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, 2014** will receive full consideration.

For more detail, see http://www.strw.leidenuniv.nl/jobs/index.php?node=6

Elena M. Rossi
Ignas Snellen

Chairs of the PhD admission committee

Ph.D Position at Paris 6 University

Study of photo-induced and radical reactions between CH_4 and NH_3: astrochemical applications

Advertised by: Prof. Lahouari KRIMY

We have an opening for up to 3-year Ph.D position at University Pierre et Marie Curie-Paris 6 in experimental physical chemistry. The important focus of the research group is laboratory experiments simulating the processes that may occur on the surface of interstellar dust grains. The experimental side consists in generating a controlled environment for the study of heterogeneous or condensed-phase cold chemical reactions, essentially based on the well-mastered technique of rare gas matrix isolation coupled to Fourier-transformed infrared spectroscopy. We are looking for a Ph.D candidate who will use and develop an experimental device coupling state-of-the-art cold chemistry and state-of-the-art gas and solid phase spectroscopy dedicated to the study of processes in an astrochemical context.

The candidate should be specialized in physical chemistry with a solid background in infrared spectroscopy and previous experience with low temperatures and low pressures.

The candidate should submit a CV, an application letter, 2 letters of recommendation and the names and contact emails of 2 referees to lahouari.krim@upmc.fr

Contact:

Lahouari KRIM, Professeur UPMC
Laboratoire MONARIS ”de la Molécule aux Nano-objets: Réactivité, Interactions et Spectroscopies”
Université Pierre & Marie Curie (UPMC-Paris VI)
UMR CNRS-UPMC 8233, Boîte 49, Bât F 74
4 place Jussieu 75252 PARIS CEDEX 05
Tel: +33 (0)1. 44. 27. 30. 23
Fax: +33 (0)1. 44. 27. 30. 21
E-mail contact: lahouari.krim@upmc.fr

AstroPAH Newsletter

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

Next issue: 18 November 2014
Submission deadline: 7 November 2014