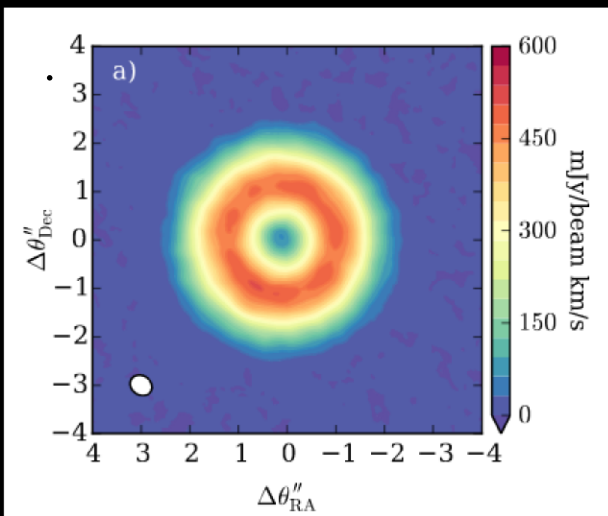
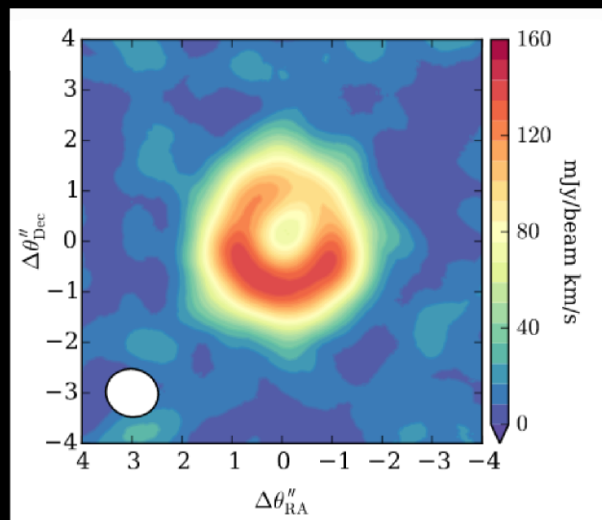
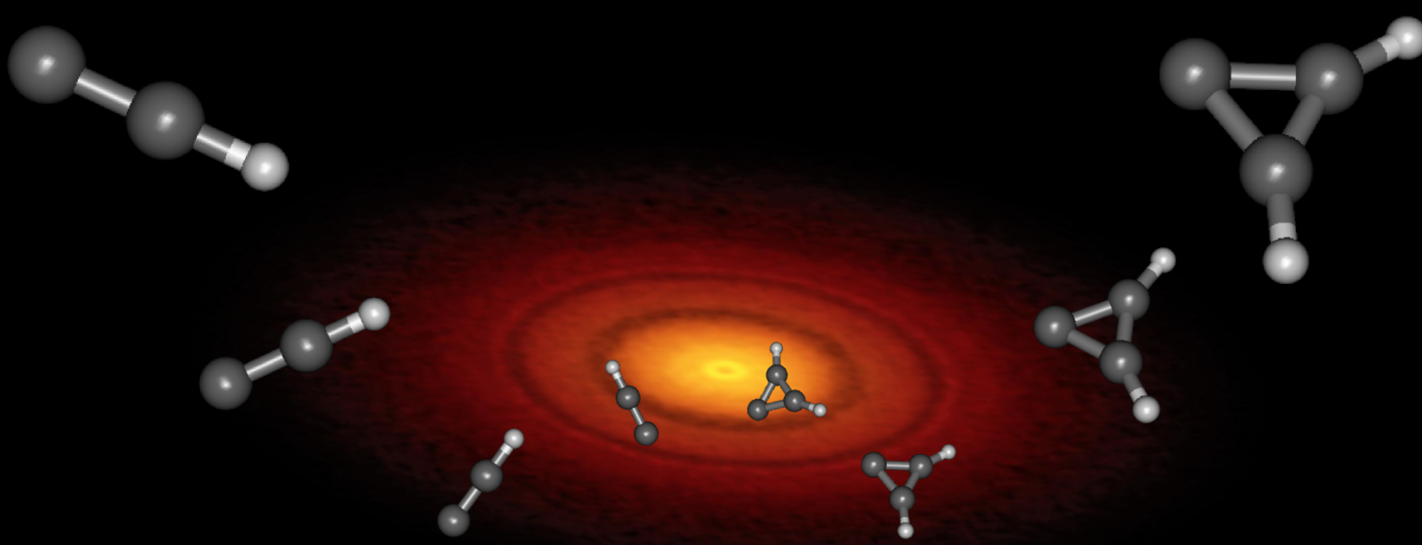
AstroPAH

A Newsletter on Astronomical PAHs

Issue 35 | February 2017







HYDROCARBONS

Editorial

Dear Colleagues,

After our traditional January break, AstroPAH is back!

We start by introducing our newest editorial board member, **Amanda Steber**. Welcome, Amanda! You can read about her in the *In Focus*, together with an update of the ins and outs of our editorial board since its creation.

The cover of this first AstroPAH of 2017 celebrates the recent discovery of small hydrocarbons (C_2H and c-C_3H_2) in a protoplanetary disk. Other many interesting discoveries in a wide range of topics are presented in our abstracts section. Studies on PAHs and hydrocarbons in protoplanetary disks, PAH emission features in NGC 2023, and the connection between the PAH band profiles and the radiation field strength are just a few of the topics covered in this newsletter. Other topics presented include the role of fullerene C_{24} and of PAHs with aliphatic side groups as possible carriers of some of the unidentified infrared bands, the formation of pentagonal rings in the dissociation of polyaromatics, the characterisation of clusters of coronene with rare gas atoms, a principal component analysis of the diffuse interstellar bands and finally the characterisation of three stable noble gas molecules including $NeCCH^+$ whose formation proceeds more efficiently through adsorption of the reactants on a PAH surface.

We have good news from the Netherlands, where the Dutch Astrochemistry Network of the Dutch Science Foundation was renewed. This entails 5 more years of dedicated funding for our field. See our second *In Focus*! With this network also comes funding for many PhD positions of which several in the field of astronomical PAHs. The announcement of these vacancies can be found at the end of the newsletter as well as with several other positions.

Two meetings are coming up with fast approaching deadlines, the Laboratory Astrophysics Division meeting at AAS in June (deadline for abstract is March 2nd) and the Molecules in Spaces symposium at ACS in August.

AstroPAH can help you promote your science! Have you published a paper recently? Do you have an interesting picture for our cover? A topic or text for the In Focus? Are you organising an upcoming meeting? Has your thesis been approved? Do you want to advertise an open position? Please let us know! Visit our webpage or contact us for more information. You can send us your contributions anytime. For publication in March, see the deadlines below.

We thank you all for your contributions so far!

The Editorial Team

Next issue: 21 March 2017.
Submission deadline: 10 March 2017.

AstroPAH Newsletter
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PAH Picture of the Month

Stacked images of all transitions of the small hydrocarbons C_2H (left) and cyclic C_3H_2 (right), detected by ALMA in the gas-rich protoplanetary disks around the young star TW HYa. See the paper by Bergin et al. (2016) in the Abstract section of this issue for more details.

Credits: Image of TW HYa: S. Andrews (CfA); B. Saxton (NRAO/AUI/NSF); ALMA (ESO/NAOJ/NRAO). Composition by Alessandra Candian.

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

In Focus

The AstroPAH Editorial Team New Member and Update

It has been more than three years since the AstroPAH newsletter was created to bridge the gap in communication between scientists working on different aspects of the PAH model (laboratory, theory, astronomical observation) and in different fields (e.g. Astronomy, Physics, Chemistry), to promote further developments. In October 2013, in our first issue, we introduced the five editors, Isabel Aleman, Alessandra Candian, Elisabetta Micelotta, Annemieke Petrignani and Ella Sciamma-O'Brien, and we took a look at where each of us was in their professional career. Now looking back at the three first years of AstroPAH, the newsletter is a success, and we have more than 300 subscribers. A lot of things have happened in the last three years both professionally and on a personal level for all of the AstroPAH editors, and as we have all advanced in our careers, we have decided to expand our team of editors. We are very happy to welcome Amanda Steber as the newest addition to our editorial team.

In this In Focus, we first want to introduce Amanda, followed by an update on all the editors. Thank you for your support and your continued interest in the AstroPAH newsletter. We are looking forward to the coming years being part of this community.

The AstroPAH editorial team:

Ella Sciamma-O'Brien
Amanda Steber
Isabel Aleman
Alessandra Candian
Elisabetta Micelotta
Annemieke Petrignani
Xander Tielens

Dr. Amanda Steber

I am a Postdoc in Melanie Schnell's group in Hamburg, Germany. I am excited to be joining the editorial board for AstroPAH. I am originally from Illinois, USA. After obtaining my bachelor's degree in both Chemistry and Biology, I went on to obtain my Ph.D. from the University of Virginia in November 2014. There I worked under Brooks Pate, who has been a pioneer not only in instrument development for microwave spectroscopy but also in developing new techniques and applications using microwave spectroscopy. My primary focuses were developing a chirped pulse Fourier transform instrument that operated in the millimeter wave regime and using the broadband reaction screening process to learn more about the chemical composition and potential reaction pathways occurring in the interstellar medium. After my time in the Pate lab, I moved to the Schnell lab. Here we also use broadband chirped pulse Fourier transform microwave spectroscopy to elucidate the molecular structure of molecules and complexes alike.

How did you get into PAH research?

PAHs are a hard subject to get interested in when doing microwave spectroscopy. Most of them do not have a dipole moment, and combined with the fact that larger PAHs are hard to get into the gas phase, we have limited hope of being able to measure them. However, shortly after joining the Schnell group in late 2014, we decided to measure the rotational spectrum of Corannulene ($C_{20}H_{10}$) again. Corannulene is a special PAH in that it has a fairly large dipole moment due its curvature, and thus we can measure it using rotational spectroscopy. Following this study, I wanted to micro-solvate the surface of PAHs in order to begin to understand how water would build up molecule by molecule.

What are you working on right now?

I am currently working on a paper about the complexation of acenaphthene with water. We have been able to observe the complexation of acenaphthene with up to four waters, and complexes that involve two acenaphthene molecules with water. Using isotopically enriched water, we have been able to determine the experimental structure of the structures of acenaphthene $-$ $(H_2O)_{1-3}$. Later, this system will be compared to the results of those for acenaphthylene$-$water in order to understand how water builds up on these PAH surfaces, molecule by molecule.

What has changed in your career/life since the beginning of AstroPAH?

In the last three years, I have had several life changes, and I have become involved in PAH research. In November 2014, I defended my dissertation at the University of Virginia, where I was working under Brooks Pate. I then moved to Hamburg, Germany because I was awarded a Louise Johnson Fellowship at the Universität Hamburg. I started working with Melanie Schnell's group in December 2014, during which time I have been working on the PAH project, instrument development in the laboratory, and the study of small organic molecules that might play a role in interstellar reactions. Just recently, I was invited to become an editor for the AstroPAH newsletter, and I am excited to work more closely with the community and the other editors. I believe that this publication offers a great service to our community, and I look forward to being a part of this team.

What was the most important advice somebody gave you?

Over the years I have had a great deal of mentors so it is very hard to pick out the most important advice that someone has given me. However, through their examples I have learned that it is important to be passionate about what you do and to never settle for anything less than your personal best. It will take a lot of perseverance and fortitude, but the end result is something you can be proud of.

What do you do outside of work?

When I am not in the lab or traveling for work, I can be found traveling around Europe to take in the various cultures. Beyond that, I enjoy baking and cross stitching blankets for my nieces and nephews.

Dr. Isabel Aleman

How did you get into PAH research?

My main research interest is molecules in gaseous nebulae. My first contact with PAH research was during my PhD, where I improved a photoionization code to include the detailed microphysics of molecular hydrogen, dust and PAHs. These molecules have a very important effect in physics and chemistry of gaseous nebulae and therefore they called my attention very early in my career.

What are you working on right now?

I am working on several projects at the moment. One you may find interesting is an unpublished work on the analysis of optical observations of Tc 1, a planetary nebula (PN) where fullerenes have been detected. I am also working on a few other projects involving small molecules in PNe, most of them consist of models to analyze observations or in preparation for observations in present (Gemini) and future (JWST and LLAMA) facilities.

What has changed in your career/life since the beginning of AstroPAH?

Since we launched AstroPAH, over three years ago, several things have changed in my life. For example, I was working at the Leiden Observatory at that time. After spending three amazing years there, I am back to my alma matter, the University of São Paulo, Brazil, as senior postdoc.

But the biggest changes in my life and carrier are related to the experiences I have had, which helped me growing as a person and as a scientist. Moving to different countries and meeting people from different cultures, including many scientists, have added immensely to my personal culture and have improved significantly my knowledge and thinking.

What was the most important advice somebody gave you?

I got two advices that I found invaluable along my career. The first was given by my late father: "Always do your best". The other, which I have heard from a few professors along my career (including Xander, see his answer below!), is that you must have fun while doing your research. Being passionate about your work helps producing great results, while maintaining a fun life in this very demanding career.

What do you do outside of work?

Two of my passions are travelling and attend to music concerts. Putting both of them together is perfect! In 2015, for example, I celebrate my birthday in the season opening concert of the Koninklijk Concertgebouworkest (Netherlands) featuring Yo Yo Ma. Unforgetable! Paul McCartney, Ringo Starr, Mark Knopfler, Rolling Stones, Sting+Paul Simon, a-ha, Bon Jovi, Kaiser Chiefs, Lionel Richie, and Simply Red were some other concerts I enjoyed in the last years.

Dr. Alessandra Candian

How did you get into PAH research?

During my master project in cosmology, I had to model the contribution of several foreground signals to the polarization of the cosmic microwave background as measured by Planck. One of the foreground was due to the presence of dust, so I got interested in dust properties such as size, shape and composition, which in turn awoke my interest for chemistry. Once I received my master thesis, I decided to pursue a doctoral degree abroad on an astronomy-chemistry related topic. I was then taken to work on the IR astronomical spectra of PAHs at the University of Nottingham (UK).

What are you working on right now?

I am characterizing the fragmentation behavior of PAHs and nanodiamonds using quantum chemistry, in particular Density Functional Theory. I would like to understand better which products are formed and if their abundances are relevant in the ISM and/or in protoplanetary disks. Also, I am looking into how much anharmonicity affects the vibrational spectrum of neutral and charged PAHs. Ideally, the outcome of these studies would be of help in interpreting the soon-to-come amazing spectra obtained by the James Webb Space Telescope!

What has changed in your career/life since the beginning of AstroPAH?

Several things changed in both my career and life since September 2013. Last year, I obtained a VENI grant, which is a fellowship awarded by the Netherlands Organisation for Scientific Research (NWO) to conduct independent research for three years on PAHs. As I have been enjoying working at the Leiden Observatory, I decided to conduct my research here.

In the meantime, I also got married and became the proud mum of a 1-year-old baby girl, Viola.

What was the most important advice somebody gave you?

That is a difficult choice! "Work on topics you like with people you have fun with" is a simple but very powerful advice I got at the beginning of my postdoc carrier. Very recently I read in a thesis the following statement "Just do it and hope nature is kind" which I found inspiring.

What do you do outside of work?

I love spending time with my family. I also very much like travelling, cooking, reading and photography, not always in this order.

Dr. Elisabetta Micelotta

How did you get into PAH research?

During my Master I studied cosmic rays. A consistent fraction of these energetic particles originates from large dust grains when these latter are sputtered by supernova shocks. For my PhD, I was therefore very thrilled to move to the other side of the table and investigate in details the processing of dust by shocks. Shortly after having started I learned about the different dust components including the smallest ones, PAHs, and I realized that not that much was known about the processing of PAHs by shocks and cosmic rays. In both these cases, the molecules are bombarded by ions and electrons instead of photons. That was my thing: the perfect occasion to combine atomic physics and astrophysics. Everything started from there.

What are you working on right now?

Different projects: the relationship between matter and dust polarization in star forming regions, where the polarization is used as a proxy for the magnetic field; the stability of C_{60} in space; the photoprocessing of PAHs and carbonaceous nanoparticles in HII regions. On top of this, I am working on a review article about dust in supernova remnants. A bit of variety.

What has changed in your career/life since the beginning of AstroPAH?

The first issue of AstroPAH (October 2013) coincided with me moving out from Canada to start an Individual Marie Curie Fellowship at the Institut d'Astrophysique Spatiale in Orsay, near Paris. Right now, I am celebrating a year into my 'new' research position at the University of Helsinki, in Finland. In Orsay I started to work on hydrocarbon nanoparticles, and in Helsinki I got interested in dust polarization. Moving to another country is always a big change in life, and these are only those that happened since October 2013! In my case, any moving allowed me to expand my scientific interests as well.

What was the most important advice somebody gave you?

Hard to choose. Let me mention this one: "There are no sealed compartments in (astro)physics". It comes from Constantinos Paizis, my professor of Cosmic Ray Physics when I was a Master student at the University of Milano, in Italy. I have been following this advice since then. If you have read so far, you probably noticed that.

What do you do outside of work?

I have many interests: literature, music, visual arts, dance, cooking... But something that I really like to do whenever it's possible is to listen to people. Everybody has a story to tell.

Dr. Annemieke Petrignani

How did you get into PAH research?

As usual, it was a combination of factors, professional and personal. At the time, I was working at the Max-Planck Institute for Nuclear Physics (MPI-K) in Heidelberg, Germany. My husband and I had decided to only go abroad for 2 years, which ended up to be 5 years. Our time in Heidelberg was really nice and our son was even born there, but after these 5 years we wanted to go back to the Netherlands again. My focus at the MPI-K was on the smallest molecules (from a physics point of view). I studied the IR to UV spectroscopy of cold H_3^+ and the dissociative electron recombination of cold molecular ions in storage rings. Through my former PhD supervisor I met Jos Oomens, a chemistry professor at the FELIX Laboratory in Nijmegen. He was working on a project together with Xander Tielens (whom I had never heard of) and they were looking for an experimentalist to work on PAHs. So after years of working in physics groups, I ended up working for astronomers at the Leiden Observatory. It was quite the transition to suddenly find myself studying astronomy and chemistry and trying to figure out huge molecules like PAHs.

What are you working on right now?

Since last year, I have been working in the chemistry department of the University of Amsterdam (UvA), where Wybren Jan Buma welcomed me within his molecular photonics group. I am very happy to be able to say that I was awarded a VIDI grant from the Dutch Science Organisation NWO to start my own small research team in Laboratory Astrochemistry. Recently, I was also awarded a grant within the NWO Dutch Astrochemistry Network programme (with many PhD vacancies, including one of mine, so please see the announcement at the end of this newsletter). My team consists of a (soon 2) PhD student and a postdoc. My research focuses on large PAHs, both ionic and neutral, and by large, I mean astronomically sized. We are developing methods to produce and study these large species in the gas phase, which is very challenging as these big monsters resist gas-phase techniques. Additionally, we are focusing on the dynamics and kinetics of the photochemistry of these large PAHs.

What has changed in your career/life since the beginning of AstroPAH?

A lot of things have changed. Where basic PAH spectroscopy and chemistry sufficed before, we have now entered an era where the underlying molecular physics and photochemistry of these species have become essential. Amongst other, I am now involved in a successful project on molecule specific anharmonic behaviour. Additionally, I now work for the University of Amsterdam and started my own research team. In my personal life things change continuously with growing children going to school for the first time, learning to read and write and do math, (re)challenging their parents all the time, sharing joys and sorrows, so I'll just mention the biggest highlight: the birth of our 3^{rd} child.

What was the most important advice somebody gave you?

It may sound cliché, but the best advice I ever received is from my mother. She had several life mottos; like "seize the day", but the one closest to my heart is the saying "where there is a will, there is a way". I naturally forward this advice to my children. If they really want something, they should make an effort.

What do you do outside of work?

My family is my first passion, then my work. I love spending time with my children, doing what they love to do, teaching them things, playing, reading, trying out new stuff (I try to live by example), and more. Although it doesn't happen as much as we would like, my husband and I like going out to the cinema, for dinner or spend time with friends. And although we don't manage to travel a lot as a family, we do like to travel; gaining new experiences and visit our friends abroad whenever we can.

Dr. Ella Sciamma-O'Brien

How did you get into PAH research?

Not at all a straight way. After pursuing a Master of Sciences in Electrical Engineering in France, I did an internship at the University of Texas at Austin in a Physics/Engineering laboratory where I discovered what it was to do fundamental research (I worked on a Laser Ablation of Microparticles experiment). I loved it and got into the PhD program at UT to pursue a PhD in plasma physics, where I entered, as my PhD advisor called it, "the Wonderful World of Physics". I used plasma emission spectroscopy to optimize the performances of a plasma propulsion system. At the end of my PhD, I looked for a postdoc that would link my expertise in plasma physics to planetary science. I found one at LATMOS, a CNRS lab near Paris, where I worked on an experiment simulating Titan's atmospheric chemistry by plasma discharge. Because of the complex organic molecules, including aromatics, produced in Titan's N_2-CH_4 chemistry, I was already dealing with PAHs then, but that wasn't really the focus of my research. In 2011, I returned to the US to work with Farid Salama on the Titan Haze Simulation (THS) experiment developed at NASA Ames COSmIC facility. That's when I really started being part of the PAH research community, by studying the chemical pathways that link the simple molecules resulting from the first steps of the N_2-CH_4 chemistry to benzene, and to PAHs and nitrogen-containing PAHs (PANHs) as precursors to the production of solid aerosols. My involvement in the AstroPAH newsletter in 2013 further connected me to the field.

What are you working on right now?

My research project on the COSmIC/THS experiment was first to characterize the gas phase products in the plasma discharge and I demonstrated that the THS experimental setup was a unique tool to probe the first and intermediate steps of Titan's atmospheric chemistry. In the last three years, I have also been studying the solid phase produced in the THS. We just got a paper accepted (that will be in the next issue of AstroPAH :)) where we present the first results of the solid phase analysis of the Titan aerosol analogs generated in the THS experiment: in particular we present an infrared spectroscopy studies of THS solid aerosols produced in four gas mixtures: N_2-CH_4, N_2-CH_4-C_2H_2, N_2-CH_4-C_6H_6 and N_2-CH_4-C_2H_2-C_6H_6. This IR analysis has highlighted changes in the nitrogen chemistry, and the abundance of aromatic compounds depending on the initial gas mixture.

What has changed in your career/life since the beginning of AstroPAH?

In my professional life, I received two grants to fund my research, and I developed the solid phase study on the THS experiment, which adds a new dimension to the amazing potential of the COSmIC platform. I have used scanning electron microscopy, infrared spectroscopy, mass spectrometry and X-ray Absorption Near Edge Structure spectroscopy to characterize the aerosols produced in the THS.

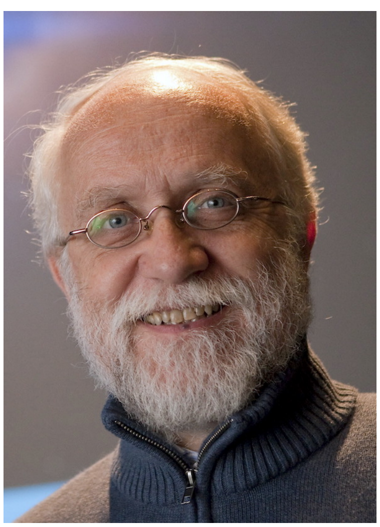
In my personal life, I had a second child, Nina, who will turn 3 in two months. I was actually 1 week pregnant when I accepted the invitation by Annemieke to become an editor of AstroPAH in August 2013. My husband, Dan, who had been taking care of our son, Liam, when we moved to the US, got a job in a start up in 2014 and started working the day I was going back to work and Nina was starting daycare. We are now a family with two kids and two working parents which makes for a crazy busy but wonderful life.

What was the most important advice somebody gave you?

"Work with people you like, not just on a subject you like". That is a very important advice when choosing a PhD subject and advisor/research group, but it is also extremely important when finding a postdoc, and later a more permanent position. I feel very lucky to work in my group at Ames. The scientists I have interacted with in the last 6 years have been fantastic mentors and friends and have helped me a lot to go through the little struggles and frustrations both in the lab and in my personal life, as a working parent.

What do you do outside of work?

I am passionate about my work but I also am passionate about my family and try to find a good balance between the two. I love reading books with my kids and playing outside with them, but I am also grateful they are good sleepers and go to bed early enough for my husband and I to have some 'us time' in the evening too, talking or watching one of our favorite shows. We also like to talk about our day and exchange ideas or pick each other's brains when we have issues in our respective labs. I also have been dancing argentine tango for the last 20 years and, now that Nina finally sleeps through the night and that I am not as sleep deprived, I have started dancing tango again.



Dr. Xander Tielens

How did you get into PAH research?

I did my PhD in Leiden in a group focused on laboratory astrophysics, graduating in 1982. Afterwards, I joined David Hollenbach at NASA Ames Research Center for a postdoc. At NASA Ames, I became aware of the opportunities of observing with the Kuiper Airborne Observatory (KAO). That was a unique facility that gave access to the mid IR range and produced the first spectra of the UIR bands in the late 70s using a circular variable filterwheel spectrometer. At Ames, Fred Witteborn together with David Rank and Jesse Bregman had built a mid-IR grating spectrometer for the KAO and we started to take spectra of the UIR bands. When Lou Allamandola joined NASA ARC in 1984 (?), we got inspired by discussions with Kris Sellgren and Mike Werner to investigate PAH molecules as the UIR band carriers. Lou and I hooked up with John Barker an expert in the field of molecular physics at SRI in Menlo Park.

What are you working on right now?

We still have a very active program on the physics and chemistry of PAHs in space but we have also branched out to study the ”largest atoms” (about 100 micron in size) in space using low frequency radio waves. When I say we, it should be understood that I just ride the coattails of a group of students and postdocs. I have always been blessed by talented students and postdocs who provided me with their unique view of the molecular universe.

I am not really working on an article but I am writing a new textbook ”Molecular Astrophysics” (and I am hopelessly behind).

What has changed in your career/life since the beginning of AstroPAH?

When this field started, molecules in general and PAHs specifically were a curiosity. Now it is clear that molecules are deeply interwoven into the fabric of the universe. Molecules are abundant, ubiquitous, and play an important role in the evolution of the interstellar medium of galaxies.

What was the most important advice somebody gave you?

The advice I give my students is to do fun things with fun people. I learned over my career that this keeps me interested and focused but most of all happy. At least, it is what makes me tick.

What do you do outside of work?

I love to go to a Giants baseball game with my daughters and enjoy the smell of freshly mowed grass, the cracking of the bat, the excitement of the game, but most of all, the quality time with them.

Dutch Astrochemistry Network II

by Xander Tielens

The Netherlands Organisation for Scientific Research, NWO, has renewed the Dutch Astrochemistry Network with, among others, exciting research projects on PAHS and related compounds.

The field of molecular astrophysics is a highly interdisciplinary field where molecular physics, laboratory spectroscopy, surface science, theoretical chemistry, astrochemistry, astronomical observations, and astronomical modeling intersect. Progress in this area can only come through a close collaboration between scientists in these diverse fields. The Netherlands Organisation for Scientific Research, NWO, started Dutch Astrochemical Network, DAN, in 2010 as an integrated and coherent program of astrochemical and astrophysical experiments, quantum chemical calculations, and laboratory spectroscopy of astronomically relevant species in combination with an active program on modeling and observations of astronomical sources. This highly interdisciplinary network combines the astronomical and chemical expertise in the Netherlands with the goal of understanding the origin and evolution of molecules in space and their role in the Universe.

NWO has decided to renew the Dutch Astrochemical Network, DAN, for another five years and has made 2.5 million euros available for astrochemistry research. Twelve, deeply interwoven, interdisciplinary research projects have been selected for funding in the Dutch Astrochemistry Network II program (DAN II). DAN II, focuses on three major astrochemical themes where Dutch astronomy and chemistry have particular strong expertise and experience as well as access to unique observational or experimental facilities. The three themes are 1) The Gaseous Molecular Universe where formation and destruction as well as the excitation of simple molecules are studied; 2) The Icy Universe where the role of ices is studied in the origin of molecular complexity in the Universe; 3) The Aromatic Universe, which studies the contribution of aromatic species to the molecular inventory and their evolution in space. The three themes are complementary with projects addressing common science questions from different perspectives including the photostability of small and large hydrocarbons and their reaction products, the interaction of water with grains and with PAHs, and photodissociation in the gas phase and in ice environments. Within the aromatic Universe theme, projects have been approved on high-resolution vibrational and electronic spectroscopy of PAH molecules in the gas phase, on quantum studies of PAHs and the route towards chemical complexity, on the photoprocessing, reactivity and spectroscopic characteristics of large PAHs and their derivatives, and on the reaction dynamics of ionic and neutral PAHs.

The DAN II network is now actively soliciting applications for graduate students and one postdoc. Details on the projects and the application procedure can be found n the Annoucements Section below and on the website: http://www.nwo.nl/en/research-and-results/programmes/Astrochemistry.

Abstracts

Polycyclic Aromatic Hydrocarbon in Protoplanetary Disks around Herbig Ae/Be and T Tauri Stars

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A distinct set of broad emission features at 3.3, 6.2, 7.7, 8.6, 11.3, and 12.7 µm, is often detected in protoplanetary disks (PPDs). These features are commonly attributed to polycyclic aromatic hydrocarbons (PAHs). We model these emission features in the infrared spectra of 69 PPDs around 14 T Tauri and 55 Herbig Ae/Be stars in terms of astronomical-PAHs. For each PPD, we derive the size distribution and the charge state of PAHs. We then examine the correlations of the PAH properties (i.e., sizes and ionization fractions) with the stellar properties (e.g., stellar effective temperature, luminosity, and mass). We find that the characteristic size of PAHs shows a tendency of correlating with the stellar effective temperature ($T_{\rm eff}$) and interpret this as the preferential photodissociation of small PAHs in systems with higher $T_{\rm eff}$ of which the stellar photons are more energetic. In addition, the PAH size shows a moderate correlation with the red-ward wavelength-shift of the 7.7 µm PAH feature that is commonly observed in disks around cool stars. The ionization fraction of PAHs does not seem to correlate with any stellar parameters. This is because the charging of PAHs depends on not only the stellar properties (e.g., $T_{\rm eff}$, luminosity) but also the spatial distribution of PAHs in the disks. The mere negative correlation between the PAH size and the stellar age suggests that continuous replenishment of PAHs via the outgassing of cometary bodies and/or the collisional grinding of planetesimals and asteroids is required to maintain the abundance of small PAHs against complete destruction by photodissociation.

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Accepted for publication in ApJ

https://arxiv.org/abs/1612.09454

Comparative investigation of pure and mixed rare gas atoms on coronene molecules

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Clusters formed by the combination of rare gas (RG) atoms of He, Ne, Ar and Kr on coronene have been investigated by means of a basin-hopping algorithm and path integral Monte Carlo calculations at T= 2 K. Energies and geometries have been obtained and the role played by the specific RG-RG and RG-coronene interactions on the final results is analysed in detail. Signatures of diffuse behaviour of the He atoms on the surface of the coronene are in contrast with the localization of the heavier species, Ar and Kr. The observed coexistence of various geometries for Ne suggests the motion of the RG atoms on the multi-well potential energy surface landscape offered by the coronene. Therefore, the investigation of different clusters enables a comparative analysis of localized versus non-localized features. Mixed Ar-He-coronene clusters have been also considered as well as the competition of the RG atoms to occupy the docking sites on the molecule is discussed. All the obtained information is crucial to assess the behavior of coronene, a prototypical polycyclic aromatic hydrocarbon clustering with RG atoms at a temperature close to that of interstellar medium, which arises from the critical balance of the interactions involved.

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A principal component analysis of the diffuse interstellar bands

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We present a principal component analysis of 23 line of sight parameters (including the strengths of 16 diffuse interstellar bands, DIBs) for a well-chosen sample of single-cloud sightlines representing a broad range of environmental conditions. Our analysis indicates that the majority (∼93%) of the variations in the measurements can be captured by only four parameters The main driver (i.e., the first principal component) is the amount of DIB-producing material in the line of sight, a quantity that is extremely well traced by the equivalent width of the λ5797

DIB. The second principal component is the amount of UV radiation, which correlates well with the λ5797/λ5780 DIB strength ratio. The remaining two principal components are more difficult to interpret, but are likely related to the properties of dust in the line of sight (e.g., the gas-to-dust ratio). With our PCA results, the DIBs can then be used to estimate these line of sight parameters.

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The PAH emission characteristics of the reflection nebula NGC 2023

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We present 5-20 µm spectral maps of the reflection nebula NGC 2023 obtained with the Infrared Spectrograph SL and SH modes on board the Spitzer Space Telescope which reveal emission from polycyclic aromatic hydrocarbons (PAHs), C_{60}, and H_2 superposed on a dust continuum. We show that several PAH emission bands correlate with each other and exhibit distinct spatial distributions revealing a spatial sequence with distance from the illuminating star. We explore the distinct morphology of the 6.2, 7.7 and 8.6 µm PAH bands and find that at least two spatially distinct components contribute to the 7–9 µm PAH emission in NGC 2023. We report that the PAH features behave independently of the underlying plateaus. We present spectra of compact oval PAHs ranging in size from C_{66} to C_{210}, determined computationally using density functional theory, and investigate trends in the band positions and relative intensities as a function of PAH size, charge and geometry. Based on the NASA Ames PAH database, we discuss the 7–9 µm components in terms of band assignments and relative intensities. We assign the plateau emission to very small grains with possible contributions from PAH clusters and identify components in the 7–9 µm emission that likely originates in these structures. Based on the assignments and the observed spatial sequence, we discuss the photochemical evolution of the interstellar PAH family as they are more and more exposed to the radiation field of the central star in the evaporative flows associated with the PDRs in NGC 2023.

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Facile pentagon formation in the dissociation of polyaromatics

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Energetic processing of gaseous polycyclic aromatic hydrocarbons (PAHs) plays a pivotal role in the chemistries of inter- and circumstellar environments, certain planetary atmospheres, and also in the chemistry of combustion and soot formation. Although the precursor PAH species have been extensively characterized, the products from these gaseous breakdown reactions have received far less attention. It has been particularly challenging to accurately determine their molecular structure in gas-phase experiments, where comparisons against theoretical modeling are best made. Here we report on a combined experimental and theoretical study of the dissociative ionization of two nitrogen containing polycyclic aromatic hydrocarbons of $C_{13}H_9N$ composition, acridine and phenanthridine. The structures of HCN-loss fragments are resolved by infrared multiple-photon dissociation (IRMPD) spectroscopy of the mass-isolated products in an ion trap mass spectrometer. Quantum-chemical computations as well as reference IRMPD spectra are employed to unambiguously identify the molecular structures. Furthermore, the computations at the density functional level of theory provide insight into chemical pathways leading to the observed products. Acenaphthylene$^{\cdot+}$ and benzopentalene$^{\cdot+}$ two aromatic species containing pentagons are identified as the main products, suggesting that such species are easily formed and may be abundant in regions where thermal or photoprocessing of polyaromatics occurs.

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http://pubs.rsc.org/en/content/articlelanding/2016/cp/c6cp08349h#!divAbstract

Polycyclic Aromatic Hydrocarbons with Aliphatic Sidegroups: Intensity Scaling for the C–H Stretching Modes and Astrophysical Implications

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The so-called unidentified infrared emission (UIE) features at 3.3, 6.2, 7.7, 8.6, and 11.3 µm ubiquitously seen in a wide variety of astrophysical regions are generally attributed to polycyclic aromatic hydrocarbon (PAH) molecules. Astronomical PAHs may have an aliphatic component as revealed by the detection in many UIE sources of the aliphatic C-H stretching feature at 3.4 µm. The ratio of the observed intensity of the 3.4 µm feature to that of the 3.3 µm aromatic C-H feature allows one to estimate the aliphatic fraction of the UIE carriers. This requires the knowledge of the intrinsic oscillator strengths of the 3.3 µm aromatic C-H stretch ($A_{3.3}$) and the 3.4 µm aliphatic C-H stretch ($A_{3.4}$). Lacking experimental data on $A_{3.3}$ and $A_{3.4}$ for the UIE candidate materials, one often has to rely on quantum-chemical computations. Although the second-order Moller-Plesset (MP2) perturbation theory with a large basis set is more accurate than the B3LYP density functional theory, MP2 is computationally very demanding and impractical for large molecules. Based on methylated PAHs, we show here that, by scaling the band strengths computed at an inexpensive level (e.g., B3LYP/6-31G*) we are able to obtain band strengths as accurate as that computed at far more expensive levels (e.g., MP2/6-311+G(3df,3pd)). We calculate the model spectra of methylated PAHs excited by starlight of different spectral shapes and intensities. We find (I3.4/I3.3)mod, the ratio of the model intensity of the 3.4 µm feature to that of the 3.3 µm feature, is insensitive to the spectral shape and intensity of the exciting starlight. We derive a straightforward relation for determining the aliphatic fraction of the UIE carriers (i.e., the ratio of the number of C atoms in aliphatic units $N_{\rm C,ali}$ to that in aromatic rings $N_{\rm C,aro}$) from the observed band ratios $(I_{3.4}/I_{3.3})_{\rm obs}$: $N_{\rm C,ali}/N_{\rm C,aro} \approx 0.57 \times (I_{3.4}/I_{3.3})_{\rm obs}$ for neutrals and $N_{\rm C,ali}/N_{\rm C,aro} \approx 0.26 \times (I_{3.4}/I_{3.3})_{\rm obs}$ for cations.

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Coronene molecules in helium clusters: Quantum and classical studies of energies and configurations

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Coronene-doped helium clusters have been studied by means of classical and quantum mechanical (QM) methods using a recently developed He-$C_{24}H_{12}$ global potential based on the use of optimized atom-bond improved Lennard-Jones functions. Equilibrium energies and geometries at global and local minima for systems with up to 69 He atoms were calculated by means of an evolutive algorithm and a basin-hopping approach and compared with results from path integral Monte Carlo (PIMC) calculations at 2 K. A detailed analysis performed for the smallest sizes shows that the precise localization of the He atoms forming the first solvation layer over the molecular substrate is affected by differences between relative potential minima. The comparison of the PIMC results with the predictions from the classical approaches and with

diffusion Monte Carlo results allows to examine the importance of both the QM and thermal effects.

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A Small Fullerene (C_{24}) may be the Carrier of the 11.2 micron Unidentified Infrared Band

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We analyze the 11.2 µm unidentified infrared band (UIR) spectrum from NGC 7027 and identify a small fullerene (C_{24}) as a plausible carrier. The blurring effects of lifetime and vibrational anharmonicity broadening obscure the narrower, intrinsic spectral profiles of the UIR band carriers. We use a spectral deconvolution algorithm to remove the blurring, in order to retrieve the intrinsic profile of the UIR band. The shape of the intrinsic profile, a sharp blue peak and an extended red tail, suggests that the UIR band originates from a molecular vibration-rotation band with a blue band head. The fractional area of the band-head feature indicates a spheroidal molecule, implying a non-polar molecule and precluding rotational emission. Its rotational temperature should be well approximated by that measured for non-polar molecular hydrogen, $\sim$825 K for NGC 7027. Using this temperature, and the inferred spherical symmetry, we perform a spectral fit to the intrinsic profile that results in a rotational constant implying C_{24} as the carrier. We show that the spectroscopic parameters derived for NGC 7027 are consistent with the 11.2 µm UIR bands observed for other objects. We present density functional theory (DFT) calculations for the frequencies and infrared intensities of C_{24}. The DFT results are used to predict a spectral energy distribution (SED) originating from absorption of a 5 eV photon, and characterized by an effective vibrational temperature of 930 K. The C_{24} SED is consistent with the entire UIR spectrum and is the dominant contributor to the 11.2 and 12.7 µm bands.

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Polycyclic Aromatic Hydrocarbon emission in *Spitzer*/IRS maps II: A direct link between band profiles and the radiation field strength

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We decompose the observed 7.7 µm polycyclic aromatic hydrocarbon (PAH) emission complexes in a large sample of over 7000 mid-infrared spectra of the interstellar medium (ISM) using spectral cubes observed with the *Spitzer*/IRS-SL instrument. In order to fit the 7.7 µm PAH emission complex we invoke four Gaussian components which are found to be very stable in terms of their peak positions and widths across all of our spectra, and subsequently define a decomposition with fixed parameters which gives an acceptable fit for all the spectra. We see a strong environmental dependence on the inter-relationships between our band fluxes – in the HII regions all four components are inter-correlated, while in the reflection nebulae (RNe) the inner and outer pairs of bands correlate in the same manner as previously seen for NGC 2023. We show that this effect arises because the RNe maps are dominated by strongly irradiated PDR emission, while the much larger HII region maps are dominated by emission from regions much more distant from the exciting stars, leading to subtly different spectral behavior. Further investigation of this dichotomy reveals that the ratio of two of these components (centered at 7.6 and 7.8 µm) is linearly related to the UV field intensity (log G_0). We find that this relationship does not hold for sources consisting of circumstellar material, which are known to have variable 7.7 µm spectral profiles.

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Hydrocarbon emission rings in protoplanetary disks induced by dust evolution

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We report observations of resolved C_2H emission rings within the gas-rich protoplanetary disks of TW Hya and DM Tau using the Atacama Large Millimeter Array (ALMA). In each case the emission ring is found to arise at the edge of the observable disk of mm-sized grains (pebbles) traced by (sub)mm-wave continuum emission. In addition, we detect a C_3H_2 emission ring with an identical spatial distribution to C_2H in the TW Hya disk. This suggests that these are hydrocarbon rings (i.e. not limited to C_2H). Using a detailed thermo-chemical model we show that reproducing the emission from C_2H requires a strong UV field and C/O > 1 in the upper disk atmosphere and outer disk, beyond the edge of the pebble disk. This naturally arises in

a disk where the ice-coated dust mass is spatially stratified due to the combined effects of coagulation, gravitational settling and drift. This stratification causes the disk surface and outer disk to have a greater permeability to UV photons. Furthermore the concentration of ices that transport key volatile carriers of oxygen and carbon in the midplane, along with photochemical erosion of CO, leads to an elemental C/O ratio that exceeds unity in the UV-dominated disk. Thus the motions of the grains, and not the gas, lead to a rich hydrocarbon chemistry in disk surface layers and in the outer disk midplane.

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http://adsabs.harvard.edu/abs/2016ApJ...831..101B

The Carriers of the Unidentified Infrared Emission Features: Clues from Polycyclic Aromatic Hydrocarbons with Aliphatic Sidegroups

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The unidentified infrared emission (UIE) features at 3.3, 6.2, 7.7, 8.6, 11.3 and 12.7 µm are ubiquitously seen in a wide variety of astrophysical regions in the Milky Way and nearby galaxies as well as distant galaxies at redshifts $z \gtrsim 4$. The UIE features are characteristic of the stretching and bending vibrations of aromatic hydrocarbon materials. The 3.3 µm feature which results from the C–H stretching vibration in aromatic species is often accompanied by a weaker feature at 3.4 µm. The 3.4 µm feature is often thought to result from the C–H stretch of aliphatic groups attached to the aromatic systems. The ratio of the observed intensity of the 3.3 µm aromatic C–H feature ($I_{3.3}$) to that of the 3.4 µm aliphatic C–H feature ($I_{3.4}$) allows one to estimate the aliphatic fraction (e.g., $N_{\rm C,aliph}/N_{\rm C,arom}$, the number of C atoms in aliphatic units to that in aromatic rings) of the carriers of the UIE features, provided that the intrinsic oscillator strengths (per chemical bond) of the 3.3 µm aromatic C–H stretch ($A_{3.3}$) and the 3.4 µm aliphatic C–H stretch ($A_{3.4}$) are known. In this review we summarize the computational results on $A_{3.3}$ and $A_{3.4}$ and their implications for the aromaticity and aliphaticity of the UIE carriers. We use density functional theory and second-order perturbation theory to derive $A_{3.3}$ and $A_{3.4}$ from the infrared vibrational spectra of seven polycyclic aromatic hydrocarbon (PAH) molecules with various aliphatic substituents (e.g., methyl-, dimethyl-, ethyl-, propyl-, butyl-PAHs, and PAHs with unsaturated alkyl chains). The mean band strengths of the aromatic ($A_{3.3}$) and aliphatic ($A_{3.4}$) C–H stretches are derived and then employed to estimate the aliphatic fraction of the carriers of the UIE features by comparing the ratio of the intrinsic band strength of the two stretches ($A_{3.4}/A_{3.3}$) with the ratio of the observed intensities ($I_{3.4}/I_{3.3}$). We conclude that the UIE emitters are predominantly aromatic, as revealed by the observationally-derived mean ratio of $\langle I_{3.4}/I_{3.3}\rangle \approx 0.12$ and the computationally-derived mean ratio of $\langle A_{3.4}/A_{3.3}\rangle \approx 1.76$ which

suggest an upper limit of $N_{\rm C,aliph}/N_{\rm C,arom} \approx 0.02$ for the aliphatic fraction of the UIE carriers.

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Note from the authors: A considerable fraction of this article is concerned with the computational techniques and results, readers who are mainly interested in astrophysics may wish to only read ”Introduction”, and ”Astrophysical Implications”.

http://arxiv.org/abs/1702.03438

Vibrational Frequencies and Spectroscopic Constants of Three, Stable Noble Gas Molecules: $NeCCH^+$, $ArCCH^+$, and $ArCN^+$

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The search for possible, natural, noble gas molecules has led to quantum chemical, spectroscopic analysis of $NeCCH^+$, $ArCCH^+$, and $ArCN^+$. Each of these systems has been previously shown to be a stable minimum on its respective potential energy surface. However, no spectroscopic data are available for laboratory detection or interstellar observation of these species, and the interstellar medium may be the most likely place in nature where these noble gas cations are found. The bent shape of $NeCCH^+$ is confirmed here with a fairly large dipole moment and a bright C−H stretching frequency at 3101.9 cm^{-1}. Even if this molecule is somewhat unstable, it is likely observable now that the spectral ranges of where to look have been established. $ArCCH^+$ is much more stable but has dim double harmonic intensities for the vibrational fundamentals and a dipole moment below 0.5 D making its rotational transitions likely buried in the astronomical weeds. Even so, $ArCCH^+$ cannot be excluded as a possibility in laboratory experiments of hydrocarbons in argon-rich environments. $ArCN^+$, on the other hand, has a dipole moment of greater than 3.5 D, an observable C−N stretching fundamental at 2189.6 cm^{-1} (4.567 microns), and a viable formation pathway through HCN, a highly-abundant interstellar molecule. Consequently, these molecules containing noble gas atoms are spectroscopically classified at high-level for the first time and may be present in observable regions of outer space.

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PCCP, 19, 5230 (2017)

http://pubs.rsc.org/en/content/articlelanding/2017/cp/c6cp08140a#!divAbstract

Molecules in space:
Linking the interstellar medium to (exo)planets

Fall National Meeting of the American Chemical Society

http://ism2planets.strw.leidenuniv.nl/

Washington DC, USA
20-24th August, 2017

Science Organizing Committee:

Prof. Alexander Tielens (Leiden University)
Dr. Partha P. Bera (NASA Ames Research Center).

Rationale: Molecules from simple to as complex as fullerenes have been identified in various astrophysical environments such as the interstellar media, dark clouds, hot cores, outflows of carbon stars, protoplanetary disks, and in the atmospheres of (exo)planets. We are only beginning to understand by sustained laboratory experimental, spectroscopic, computational, modeling, and observational efforts how these molecules are synthesized in the gas phase and on grain surfaces, evolve in those exotic conditions, and become incorporated in to planetary bodies. With the advent of new and upcoming capabilities such as the Atacama Large Millimeter Array (ALMA) and the James Webb Space Telescope (JWST), the scope of molecular exploration will increase many folds over the next decade.

We are organizing a five-day symposium “Molecules in Space: Linking the Interstellar Medium to (exo)planets” at the American Chemical Society’s Fall National Meeting to be held in Washington DC from 20-24th August, 2017 to address the exploration of the molecular universe. The symposium will cover a wide breadth of subjects that will include organic inventory of the gas phase, the chemistry of the dark clouds, interplay of gas and dust, hot-cores and corinos, organic inventory of proto-planetary disks, high-resolution spectroscopy, the diffuse interstellar bands, the chemistry of atmospheres of stars and planets, and present and future opportunities such as ALMA, SOFIA, and JWST. Each session will begin with an overview talk by an eminent scholar in the field, followed by talks on astronomical observation, laboratory experiment, quantum chemistry calculations, and modeling.

The sessions will be introduced by overview talks followed by invited talks on specific aspects of the session and contributed papers. In addition, there are poster sessions.

Abstracts can be submitted for consideration for contributed talks and posters through the ACS Fall 2017 National Meeting webpage between the following dates.

Key dates:
Abstract submission window opened on **23rd January, 2017**. https://abstracts.acs.org
Abstract submission window closes on **6th April, 2017**.

Sessions:
Session I: Organic inventory of the gas phase: from small molecules to PAHs
Session II: Chemistry of dark clouds: the interplay of gas and dust
Session III: Hot cores and corinos: Observations, theory and experiments
Session IV: Organic inventory of protoplanetary disks
Session V: Spectroscopy: Meeting the needs of astronomers with experiments and theory
Session VI: The DIBs: solving a century old problem
Session VII: Chemistry of atmospheres of stars and planets

Summer 2017 Laboratory Astrophysics Division Meeting

230th meeting of the American Astronomical Society

Austin TX, USA

4-8th June, 2017

Abstract submission & Registration Open!

Dear colleague,

Abstract submission (and registration) for the 2017 LAD meeting, held with the 230th AAS meeting (June 4-8th, 2017, in Austin TX) are now open! Please go to https://aas.org/meetings/aas230 for all the details.

Key dates:
Early Registration Deadline: **22 February, 2017**.
Abstract Submission Deadline: **2 March, 2017, 9 pm ET**.

The LAD meeting will begin in the afternoon of Monday June 5th and end with a morning session on Thursday June 8th, with morning and afternoon sessions Tuesday and Wednesday. There will also be a LAD plenary talk on Tuesday morning by Dr. Bonnie Buratti of JPL on results from the ROSETTA mission, with a focus on the importance of laboratory measurements to our understanding. Session topics & confirmed invited speakers include:

Dust & Ices - with invited speaker Dr. Christine Joblin (IRAP)
Plasmas - with invited speaker Dr. R. Paul Drake (UMich) on upcoming major challenges and opportunities in plasma physics studies in the lab
Molecular Physics - with invited speaker Dr. Catherine Walsh (Leeds), speaking on chemical complexity in protoplanetary disks in the era of ALMA and Rosetta
Planetary Physics - with invited speaker Dr. Michael A'Hearn (UMd), speaking on studies of comet 67P/Churyumov-Gerasimenko
Atomic Physics - with invited speaker Dr. Stuart Loch (Auburn) speaking on methods for generating error estimates for theoretical calcuations
Nuclear/Particle Physics - with invited speakers Dr. Annika Peter (OSU) talking about Dark Matter searches and detection techniques

This will also be your chance to meet, hear, and congratulate the LAD prize winners for 2017:
Dr. James Lawler (LAD Prize)
Dr. Carolyn Kuranz (Early Career LAD Prize)
Dr. Kyle Walker (LAD Dissertation Prize)

Substantial room has been left in the schedule for contributed talks (and posters), so please plan to attend and present your latest results at what will be a top meeting for Laboratory Astrophysics in 2017!

For the LAD Executive Committee,

Randall Smith
LAD Vice Chair
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Announcements

Post-doctoral position in Observational Infrared Astronomy at the University of Western Ontario

Advertised by Prof. Els Peeters

Applications are invited for a post-doctoral position in observational infrared astronomy in the Department of Physics and Astronomy at The University of Western Ontario. The successful candidate will pursue projects with Prof. Els Peeters. These projects will be related to studies of Polycyclic Aromatic Hydrocarbons (PAHs) and dust in various environments, with an emphasis on (galactic and extragalactic) star-forming regions and photodissociation regions (PDRs), and will utilize Spitzer, SOFIA, ground-based and future JWST observations. The successful applicant will be expected to participate in the preparation for the upcoming JWST mission and in the analysis of JWST Early Release Science data.

Candidates must have a PhD in astrophysics or related fields. Preference will be given to candidates with a strong background in IR astronomy and astronomical data reduction. Prior research experience with PAHs and dust is desirable but not required. The appointment is for 2 years with an additional year dependent upon performance and continued funding. The start date is flexible but is expected to be summer 2017.

Applicants should send (preferably electronically) a cover letter, CV, a statement of research interests, and arrange for three letters of recommendation to be send directly to Dr. Peeters by March 1, 2017. The University of Western Ontario is committed to employment equity.

Application deadline: March 1, 2017.

Contact: Prof. Els Peeters
Department of Physics & Astronomy
University of Western Ontario
London, Ontario, N6A 3K7, Canada
E-mail: epeeters@uwo.ca
Telephone: 1 519 661 2111

http://www.astro.uwo.ca/~epeeters/
http://www.physics.uwo.ca/
https://jobregister.aas.org/node/58693

Post-doctoral position in Interstellar Optical Spectroscopy at the University of Western Ontario

Advertised by Prof. Jan Cami

Prof. Jan Cami invites applications for a post-doctoral research position in interstellar optical spectroscopy in the Department of Physics and Astronomy and the Centre for Planetary Science and Exploration (CPSX) at the University of Western Ontario. The successful applicant will work on the Diffuse Interstellar Band (DIB) problem and lead much of the data analysis efforts to exploit the EDIBLES (ESO DIB Large Exploration Survey) data set, an unprecedented collection of high signal-to-noise and high spectral resolution observations obtained with VLT/UVES. He or she will also have the possibility to participate in other research programs as well as carrying out independent research.

Candidates must have a PhD in astrophysics or related fields, and preferably a background in astronomical spectroscopy and/or data analysis. Expertise in studies of the interstellar medium or in data analysis using advanced statistical methods and/or machine learning techniques would be advantageous.

The initial appointment is for 1 year with the expectation of one or two additional years dependent upon performance and continued funding. The start date is flexible, but preferably not later than the summer of 2017.

Support for research and observing travel as well as publications will be provided.

Applicants should send a cover letter, CV with bibliography, a brief statement of research interests, and arrange for three letters of recommendation to be sent directly to Prof. Cami. The position will remain open until filled. For full consideration, complete applications should be received by March 1, 2017. The University of Western Ontario is committed to employment equity.

Application deadline: March 1, 2017.

Contact: Prof. Jan Cami
Department of Physics & Astronomy
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Webpage: https://jobregister.aas.org/node/58926

12 PhD (and a Postdoctoral) positions within the Dutch Astrochemistry Network (DAN II)

Advertised by Harold Linnartz on behalf of the DAN II consortium

We currently have 12 vacancies for 4-yrs PhD positions and a 3-yrs Postdoc position within the framework of DAN II (www.nwo.nl/astrochemistry). DAN II is funded by The Netherlands Organisation for Scientific Research, NWO, with the aim to study the origin and evolution of molecules in space. This interdisciplinary programme combines astrochemical and astrophysical experiments, quantum chemical calculations, laboratory spectroscopy of astronomically relevant species and modeling and observations of astronomical sources. DAN II has defined a highly integrated and coherent science programme on gas-phase chemistry, solid-state chemistry, and interstellar polycyclic aromatic hydrocarbon molecules.

There are three 'universes' with each 4 projects. We are looking for enthusiastic individuals with a (recent) Master degree in astronomy, physics or chemistry, who are interested in astrochemistry and with the specific backgrounds as indicated with the project titles listed below. Good communication skills in English are essential. Interested students can request more details by contacting the PI and co-Is of a specific project. The application for that position should be sent directly to the corresponding PI/Co-Is, and contain a short letter of motivation, CV and names of two persons who are willing to provide letters of recommendation. Applications are accepted until the vacancies are filled. Depending on the project, we aim for starting dates as early as Spring 2017, but not later than September 1st 2017.

Application deadline PhD positions: starting as soon as possible
Application deadline PD position: starting in 2018

The Gaseous Molecular Universe

Project 1: 4 yrs PhD position
Photo-Absorption and Dissociation of CH and Carbon Based Radicals
Prof. Wim Ubachs (Free University Amsterdam), w.m.g.ubachs@vu.nl in collaboration with Prof. Harold Linnartz (Leiden Observatory), linnartz@strw.leidenuniv.nl
The candidate is an experimental physicist or physical chemist, preferably with a background in molecular/laser spectroscopy.

Project 2: 3 yrs Postdoc position (starting 2018)
Protostellar and Protoplanetary Disk Chemistry; from Basic Data to Astrochemical Models
Prof. Ewine van Dishoeck (Leiden Observatory), ewine@strw.leidenuniv.nl
The candidate has experience with astrochemical and radiative transfer models and/or is an expert on photodissociation processes.

Project 3: 4 yrs PhD position
Rotation-Vibration Inelastic Collision Rates of Polyatomic Molecules
Prof. Gerrit Groenenboom (Radboud University Nijmegen), gerritg@theochem.ru.nl
The candidate is a computational chemist/physicist

Project 4: 4 yrs PhD position
It Takes Two to Tango; Bi-Molecular (Half) Collisions of Astrochemical Relevance)
Prof. David Parker (Radboud University Nijmegen), parker@science.ru.nl in collaboration with Prof. Bas van de Meerakker (Radboud University Nijmegen), B.vandeMeerakker@science.ru.nl
The candidate is an experimental physicist or physical chemist.

The Icy Universe

Project 5: 4 yrs PhD position
Circumstellar Ice and Snow Lines - Photochemistry at the Edge
Dr. Michiel Hogerheijde (Leiden Observatory), michiel@strw.leidenuniv.nl in collaboration with Prof. Harold Linnartz (Leiden Observatory), linnartz@strw.leidenuniv.nl
The candidate has an experimental background in physics or chemistry or astronomical instrumentation and has interest to spend 50% of his/her time on astronomical observations (ALMA).

Project 6: 4 yrs PhD position
Molecular Complexity in Interstellar Ices - A Combined Experimental / Theoretical Study
Prof. Harold Linnartz (Leiden Observatory), linnartz@strw.leidenuniv.nl in collaboration with Dr. Herma Cuppen (Radboud University Nijmegen), h.cuppen@science.ru.nl.
The candidate has an experimental background, preferably experience with UHV, molecular spectroscopy and mass spectrometry, with strong interest in astrochemical modeling.

Project 7: 4 yrs PhD position
Mobility and Restructuring in Interstellar Ices
Dr. Herma Cuppen (Radboud University Nijmegen), h.cuppen@science.ru.nl in collaboration with Dr. Britta Redlich (Radboud Universiy Nijmegen), b.redlich@science.ru.nl
The candidate is a computational chemist/physicist.

Project 8: 4 yrs PhD position
Velocity Map Imaging at Icy Surfaces
Prof. David Parker (Radboud University Nijmegen), parker@science.ru.nl
The candidate is an experimental physicist or physical chemist.

The Aromatic Universe

Project 9: 4 yrs PhD position
High Resolution Vibrational and Electronic Spectroscopy of the Isolate Aromatic Universe
Prof. Wybren-Jan Buma (University of Amsterdam), W.J.Buma@uva.nl, in collaboration with Dr. Anouk Rijs (Radboud University Nijmegen), a.rijs@science.ru.nl.
The candidate is an experimental physicist or physical chemist.

Project 10: 4 yrs PhD position
Reaction of PAHs: A Route to Chemically Complex Molecules?
Prof. Matthias Bickelhaupt (Free University, Amsterdam), f.m.bickelhaupt@vu.nl, in collaboration with Dr. Ingmar Swart (University Utrecht), I.Swart@uu.nl.
The candidate is a theoretical chemist, computational chemist/physicist.

Project 11: Two 4 yrs PhD positions
Photo-processing, Reactivity and Spectroscopic Characteristics of Large PAHs and their Derivatives
Prof. Jos Oomens, (Radboud University Nijmegen), J.Oomens@science.ru.nl Prof. Xander Tielens (Leiden Observatory), tielens@strw.leidenuniv.nl
The candidate is an experimental physicist, physical chemist with interests in astrochemical modeling.

Project 12: 4 yrs PhD position
The Reaction Dynamics of Ionic and Neutral PAHs
Dr. Annemieke Petrignani (University of Amsterdam), a.petrignani@uva.nl
The candidate is an experimental physicist or physical chemist.

For further information, see: http://www.nwo.nl/astrochemistry

The EUROPAH Network is Currently Hiring

Advertised by Alexander Tielens on behalf of the network

The EUROPAH network was funded by the Marie Curie Innovative Training Network program. EUROPAHs' scientific research goal is to understand the role that polycyclic aromatic hydrocarbons play in the physics and chemistry of the interstellar medium.

Polycyclic aromatic hydrocarbons (PAHs) are universally ubiquitous and lock-up close to 15% of the elemental carbon in space. They play a key role in maintaining the ionization balance and in the heating of interstellar gas; hence controlling the phase structure of the interstellar medium (ISM) of galaxies and regulate star formation. PAHs are also central to the chemical complexity of space and the organic inventory of regions of star and planet formation. On Earth, PAHs are pernicious pollutants affecting the atmosphere and aquatic environments. Understanding PAHs and their multitude of roles in the Universe is thus a key question in both astrophysics and terrestrial chemistry.

While several positions have been filled, EUROPAH is still actively recruiting graduate positions. Each ESR will be enrolled in a PhD program and complete a specially designed training schedule in tandem with performing research and innovation projects at their host organisation. This will be a highly multidisciplinary network that combines astronomy, molecular physics, molecular spectroscopy, environmental science, quantum chemistry, surface sciences, plasma physics and scientific communication. The training program is aimed at developing a research-oriented, creative and innovative mindset and will place you well for a future career in academia or in industry.

Details can be found on http://europah.eu/Recruitment/index.html

AstroPAH Newsletter

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

Next issue: 21 March 2017
Submission deadline: 10 March 2017