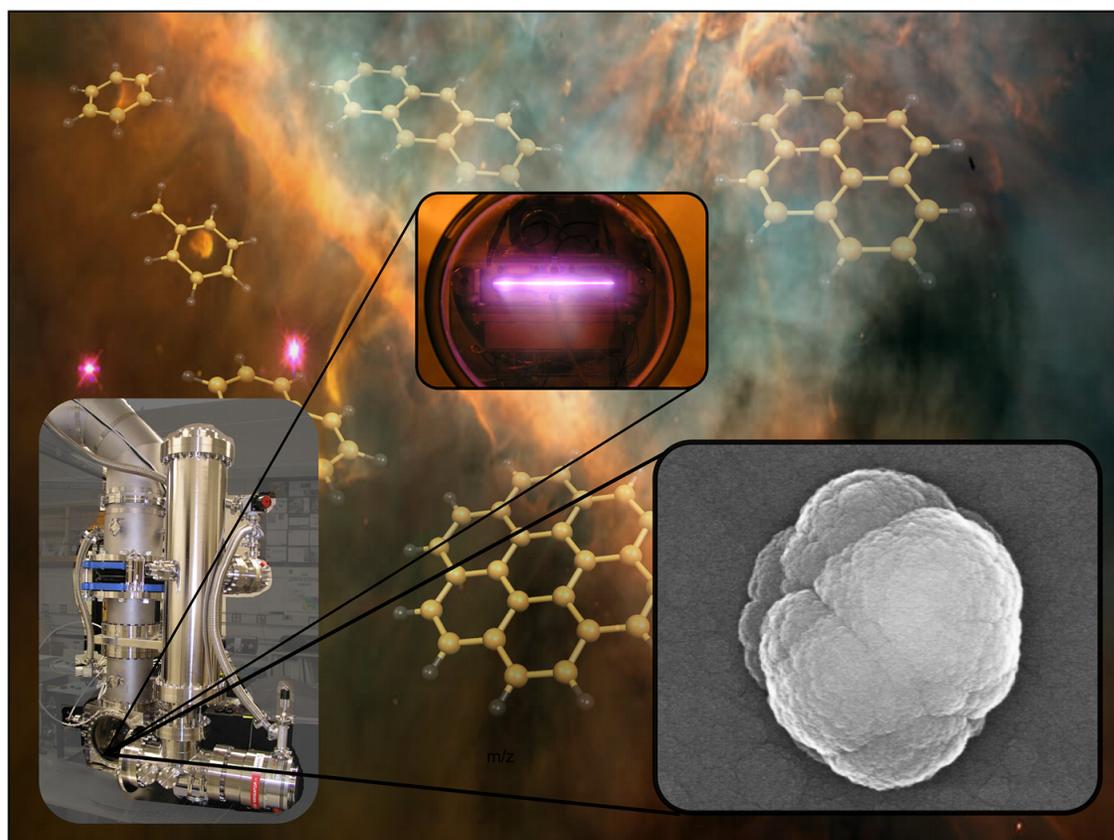


Issue 8 | June 2014

# AstroPAH

A Newsletter on Astronomical PAHs



## COSMIC dust

# Editorial

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**Dear Colleagues,**

Welcome to the 8th release of AstroPAH!

The Picture of the Month features a recent NASA press release presenting the laboratory results obtained by a team of scientists at NASA Ames Research Center who has successfully reproduced the processes that occur in the atmosphere of a red giant star and has produced nanoscale grains, analogs of interstellar dust.

In Focus presents an (astro)chemically excited interview given by Prof. Alan Rowan, specialist in the field of electronic and crystalline materials, catalysis, and single molecule studies. We thank Alan for his time and enthusiasm in giving us his insight as a chemist.

In this issue, we have abstracts featuring laboratory studies on proton-PAH collisions, anionic PAHs, and spectroscopy of PAHs. You can also find a study of the PAH emission in nearby tidal streams, and a statistical analysis comparing theoretical and observational PAH spectra. Do not miss the abstract of Koen Maaskant's thesis, where, among other subjects, he studied PAHs in protoplanetary disks.

In our previous newsletter, we published the abstracts of three PAH-related papers presented during the 168th Faraday Discussion on Astrochemistry of Dust, Ice and Gas. During the meeting, the paper presentations were followed by very interesting discussion sessions, in particular for some of the abstracts we presented in the previous issue of AstroPAH. The transcripts of these discussion sessions will be included in the FD 168 volume, making the lively opinion-exchange available to everybody interested.

We would like to thank you all for your contributions and please keep them coming. You can send your contributions to AstroPAH any time – abstracts, in-focus suggestions, awards, future events, or other information you would like to share with the community. Also, we encourage you to contact us with any feedback or questions you may have on our various sections, such as the In Focus.

The deadline for contributions to appear in the next issue is 4 July 2014. The next issue of AstroPAH will be out on 22 July 2014.

For more information on AstroPAH, visit our website:

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

Best regards

**The Editorial Team**

# AstroPAH Newsletter

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## PAH Picture of the Month

Using the Cosmic Simulation Chamber (COSmIC) facility designed and built at Ames, scientists now are able to recreate and study in the laboratory dust grains similar to the grains that form in the outer layers of dying stars. They plan to use the dust to gather clues to better understand the composition and the evolution of the universe. The new findings are expected to help scientists better understand the formation of planets, including Earth-like planets.

Credits: NASA/Ames/Farid Salama.

### NASA Press Release

[NASA Simulator Successfully Recreates Space Dust](#)

[NASAs COSmIC Simulator Helps Fingerprint Unknown Matter in Space](#)

# In Focus:

## Interview with Prof. Alan Rowan

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### Please introduce yourself. Which were your first steps into science and/or chemistry?

"I am from England; I did my studies in Chemistry at the University of Liverpool while I was being trained to be a jet pilot for the Royal Air Force. Once I got my degree, I had to choose between chemistry and being a pilot. As I was not very good with taking orders, I went into the PhD program in Liverpool, where I obtained a prestigious scholarship to work on whatever project I liked. I decided to study the properties of assembling and orientation of chlorophylls, which are in fact large aromatic molecules. After finishing my PhD in three years, I moved to New Zealand for my first post-doc, to study how molecules assemble via aromatic-aromatic interactions. After two and half years, I came to work at the University of Nijmegen, first as a Marie-Curie fellow and then as an assistant professor. I am now Professor of Molecular Materials here in Nijmegen, Netherlands.



**Prof. Alan Rowan**

I consider myself an intuitive chemist. Naturally I read literature and I hear other people, but you know when something's worth investigating more and yet, you can't tell why. Some of our biggest discoveries are from experiments where people say that it won't work, but you go 'no, there's something here'. I've been very lucky to have the funds and the people to take the time and follow as the Americans say 'a hunch'. This feeling together with a lot of hard work have nearly always produced our Nature and Science papers. My students and staff often make the complaint 'I came into your office with a question and I left with ten ideas'. I really rely on a team to sometimes extract some of the creativeness and then in discussions to pin it down."

### Tell us about your line of research.

"My interest is in physical organic chemistry. I make molecules and try to understand the relation between their architectures and physical properties. I use synthesis techniques, which

advanced a little from the old days but basically are the same, similar to cooking. It is a long process: first the molecule is synthesized and then examined by means of every available technique to study its physical characteristics – structure, magnetic and optical properties, chirality etc. The group of which I am part comprises 40 people and we have many international students and collaborators and also joint PhD projects with other institutes with the Institute for Molecules and Materials (IMM). It is curiosity-driven science. I study what takes my interest: conductive materials, polymers for solar cells, and molecules of interest for biomedicine.”

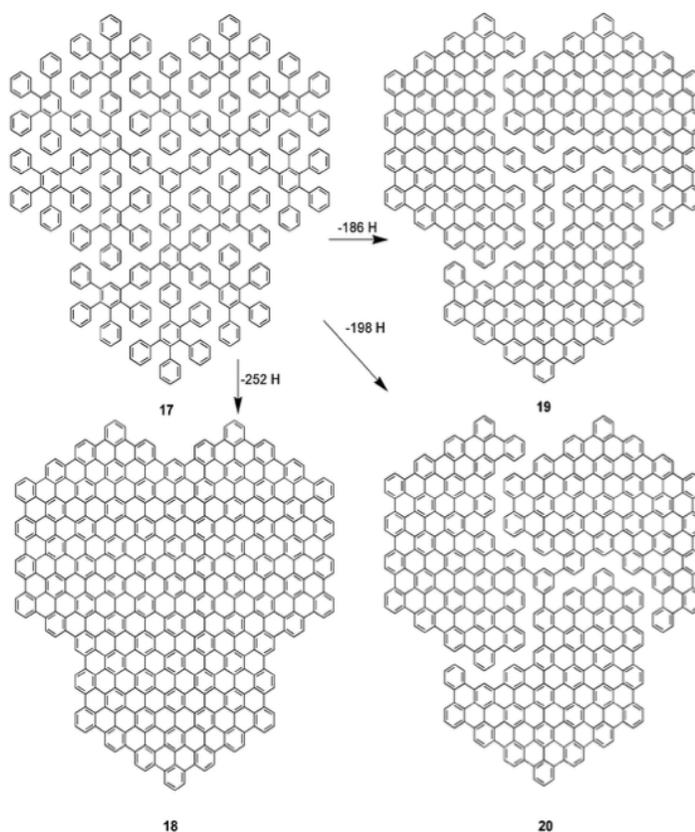
## Do you also study PAHs or related species?

“We have been working on how to order and self-assemble large aromatic molecules such as PAHs to create conductive material, in particular for molecular electronic applications. We try to control the assembling configuration, but it is a complex balance between the electronic properties, the shape, and the functionality of the molecule, which finally govern the assembled architecture and ultimately the properties. Actually my first post-doc project was on trying to quantify the ‘interaction of aromatic molecules’.”

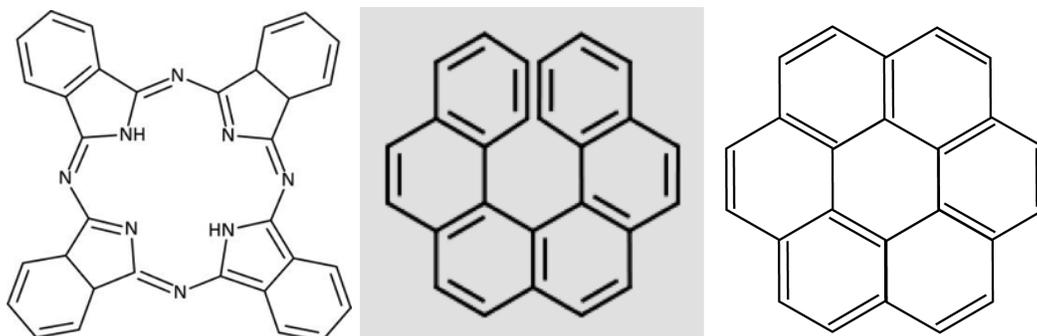
## Can you synthesize large PAHs?

“It is difficult but doable. The two main problems are size and amount you can create. As soon as PAHs grow in size, they become insoluble so it is difficult to do chemistry on them. Moreover, in the lab you create very small quantities ( $\mu\text{g}$  rather than kg), which are not enough to study from a chemical point of view. For physics applications though, the amounts are enough. If you need a specific molecule we can help you or at least tell you who can.

**Figure 1** shows examples of PAHs that are relatively easy to make and accessible. These are probably in the direction you see things in space. The chemistry to make these types of molecules is relatively straightforward. They are probably all made in a different way than they are made in space. We can make them locally or I would ask the people who’ve already done it before. It is synthetically possible to make a myriad of these molecules. From chiral to non-



**Figure 1:** The state of art in large aromatic molecules is highlighted above. This work developed by Prof. Klaus Muellen (Max Planck Institute for Polymer Research, Mainz) has been used in molecular electronics within several EU networks Prof. Rowan’s group participate in.



**Figure 2:** Chemical structures of a phthalocyanine, helicene, and coronene

chiral to charged or not charged. It's very possible.

To start getting into the realm of large aromatic molecules, phthalocyanines (**Figure 2**) are easy to make, even the bigger ones. They are basically stable aromatic molecules, fully aromatic, and can hold different metals. They are used from the food industries through to CD production (the green colour on your CD is a phthalocyanine). We make phthalocyanines ourselves. So they are one route, helicenes are also an interesting route, giving you chiral aromatic PAHs and then of course the most famous family of PAHs, coronenes (**Figure 2**)."

## How pure are they?

"The purity will not be an issue, when you want to do small quantities and laser spectroscopy. The structure is easy to separate by mass using mass spectrometry time of flight experiments and then immediately into the laser. You can basically, even if you had a mixture, do laser ablation. You can then run it through a vacuum with a mass separator, a sort of combined mass spectrometry. Depending on the magnetic field you apply, you can selectively choose the mass you want to look at. You can then do many molecules at the same time with different mass. Effectively, by combining the fact that the heavy ones will move more in the magnetic field, you should be able to control it."

## What are the possibilities of studying large aromatics in the gas phase?

"These species have extensively been studied by gas-phase mass spectrometry. They are too big to do in solution chemistry, because they don't dissolve. They want to self-assemble, forming large aromatic stacks. It's like saying you've got a bit of glitter band. If it's big enough it's just impossible to pull apart. As the surface area increases, the van-der-Waals interactions dominate and the molecules form co-facial stacks. The surface area is too much; the van-der-Waals forces are too strong. However, if you put them in an aromatic/organic solvent, though they're not really dissolved in it, you could perform laser excitation, direct them into the mass spectrometer and measure the respective mass spectra. If you can measure the mass spectra, then in principle you can apply laser excitation and so measure their infrared spectra. It may be a challenge, but it should be possible.

What is the size-limit is the first question; at what point can you not see anything anymore? The second question is if different shapes do different things. Do you see it because of the triangular, square, or circular, helical, none helical structures and such? Would you see it if there is a hydroxide on the outside, or some other functional group. These are all things that can be studied.”

## On a current topic: what does your intuition tell you about meteorites versus interstellar-matter chemistry?

“The reason you possibly don’t see large aromatics on meteorites is because other chemistry can happen. If we say that space is primarily full of PAHs, than the most likely event to occur is for two aromatic hydrocarbons to come together. If one is a radical by photo excitation as soon as they come in contact, they’re going to react and form a bond with each other. This may not be flat; it may be at an angle. So if the most likely chemical reaction is with another PAH, then after a period of time, you’re going to see a distribution of bigger PAHs. If you go back in time and look at places that are earlier in time you would see smaller PAHs and as you come out in time, you start seeing the bigger ones. The chemistry changes when the chances of hitting water or other molecules increases, e.g., on a meteorite or on dust grains. If you have other species, you don’t get large aromatics. The small PAHs do other chemistry. That would be my completely unscientific intuition.”

## Do you investigate transitions between different types of hydrocarbons?

“We’ve never really been involved in that because that was never a driving force for organic chemistry. We do see that you may get cross-linking of aromatic molecules. Anthracene is an example; it will form a dimer if you photo-activate it. These are however problems we try to prevent when trying to make organic devices. We don’t want those things. Also, we do everything in solution at mg concentration. It’s a completely different chemistry. The interstellar processes are side reactions for us. Nonetheless, they may play a big role, because they can reduce our yields. When we start making molecules like this, we wrap everything in aluminium foil to stop light getting in, because any radical will cause unwanted side reactions. In many organic molecular devices, one of the biggest problems is that when you excite PAHs, you get this excited state and it starts reacting with itself. In our systems, where there are many molecules, it can easily lead to decomposition or it leads to electric current.

I think a lot of this behaviour goes back to research carried out 20 to 30 years ago, where they looked at photochemistry and they looked in the interactions upon photo-excitation. It’s always something to come back to now with modern technology. If PAHs are deposited on a surface and you would do excitation, you could use a vacuum scanning tunneling microscope (STM) to look at them on an atomic level, or even sub-atomic level depending on the resolution. You may start seeing radicals, broken bonds. Maybe you start to see a reaction occurring in certain positions on, e.g., a C<sub>60</sub> or a coronene. Will there be any holes? Do bonds start splitting and reactions occurring? That would be an interesting thing to come across. Also try to see

how their shape and size will affect things. This is an idea.

You could also have mixing chambers afterwards, where you might mix with very small percentages of water or oxygen or nitrogen. What happens if you fire in some dust particles? Or have  $C_{60}$  to act as a template. There are all these interesting things to do, which would sort of make sense to. We do a lot of STM, together with Dr. Elemans, on our molecules and we look at molecules. We look at their very dilute order on a surface. For astrochemistry, one could do likewise, to give an idea of what's going on. These are things we can help with."

## What is astrochemistry to you as a chemist?

"I think that it's a fascinating topic and I think you have also a whole different type of chemistry in there. The difference of the long times and low concentrations of the reactions conditions is interesting. This leads to stochastic and rare events in astrochemistry. We, on the other hand, are confined to a flask and large concentrations in solution. We may miniaturize it and maybe change some of the thermodynamics, but its pretty much the same thing. We would always do reactions in  $\mu\text{g}$  to  $\text{mg}$ , so astrochemistry is really in the noise. We're really talking bulk chemistry compared to your stochastic chemistry. However, the chemistry is at some point similar, because you break the bond, you make a radical, and then the radical reacts with something. So the basic principles from both chemistries should apply.

To account for long time scales and low concentrations in the lab, you have to have extremely high sensitivity, where you can look at one or two molecules and you're basically taking into account time. We're talking about stochastic events. So you'll have to look at these stochastic events and determine the anomalies. They only happen one in a million but over a period of a billion years that's a lot of molecules. You must have the technology and sensitivity to see this. That's the trick. It's really about sensitivity."

## What in astrochemistry could give you new insights in chemistry?

"That's a very interesting question. We certainly found when we do these experiments that a particular aromatic ring may be far more chemically reactive in a certain position. This may all help us to likewise reactions in space-like conditions and tell us something about selectivity. Though in many cases, a lot of the molecular dynamics, or high-resolution molecular density of states calculations of small molecules, which are fairly accurate, would give very valuable reactions. Still, it may be that suddenly you learn one or two things about particular aromatic molecules, about some stochastic processes, which may be important in optical devices in the future. These are unexpected side reactions and it's very difficult to study them. You have a whole new chemistry when you start looking at  $C_{60}$ , how it unfolds, and starts giving you surfactants. I think that's very fascinating. This might uncover a whole new way to design some of those things or tell us to rethink how we already thought about it. The similarities are that it's all chemistry that is all bond-bond formation.

Practically wise it does no harm for astrochemistry to look at alternative chemistry reactions.

You're using extremely expensive equipment to study things in unnatural conditions. You may argue that there's a lot of money going in, but that it is fundamental science. We can however learn new things; we found  $C_{60}$ , which gave us graphene and nanotubes. All of these things may give us new routes to how to modify graphene or may show some of the ways graphene behaves which may help the future electronic industry. Those things all have knock-on effects. One piece of knowledge helps two people and they generate eight and that's how it goes on. You could never predict that somebody with a piece of sellotape pulling of graphene would get a Nobel price so few years later."

## Do you have any specific questions to the astronomical PAH community?

"I would like to raise the question about helicenes. Has anybody seen helicenes in space? I have a strong believe that if you're looking for life, by definition you've got to look for chirality. Chirality by definition doesn't mean that there is life, but I think you will never get life without it. Is life chiral because of a purely stochastic event? By definition it will always have to go down one route.

What would be another question is if one can determine formation routes to larger PAHs at e.g. the free electron laser (FEL) facility. You can put different PAH concentrations together, small ones like coronenes, and look into the formation of larger PAHs. If I take two of them and set them in a more sort of concentrated gas phase and excite them with a certain frequency, which I know will split a bond and create radicals, do I see a dimer starting to appear? Do I see that chemistry happening?"

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

"I have had conflicts. If you go in academia as it is now, with limited funding for research, you need first to get money and/or grants, competing internationally. As in other jobs, if you want to be top class in what you do, you have to make sacrifices. It is naive to think the contrary. Of course you can also have an academic career that can be rewarding enough without having to sacrifice too much. In this, balance is really important. Universities could do better in helping people doing their job and maintaining their life/work balance. For example, a larger support network would reduce the amount of administrative work a scientist has to endure and that takes time out of research. At the end of the day, the government pays us to teach and innovate and we should be evaluated on that."

## What advice do you have for the younger scientists?

"One of the criticisms I have with the current system is that there's such a pressure to produce that maybe there's a lot less flexibility because of the funding to take risks. Sometimes the younger scientists really pre-plan everything because they can't fail. We try and rationalize everything. After all science is all about rational and logical decisions. We underestimate the

intuitive network we possess. I think we'll discover more things by listening to our intuition. If something feels right, give it a go. You can have many ideas. Good ones keep on coming back in your mind. You discuss those with people and then it evolves from that point. You have to put that seed into the ground and let it grow. You also have to create a fertile ground of different people. As example, someone might be talking about astrochemistry and I'm thinking about drug delivery. There may be a connection or there may not be yet a real connection. But the thought might create something. It's the unusual things that lead to complete discoveries or as we say disruptive science.

Also, science is a passion and it's about creativity. We have to embrace and express that a lot more. We've lost the connection between science and the public. Sometimes we're a bit in our own worlds. We should try and express how much we love it, get people to understand there's a real passion. Invention and innovation, it is creativity, as much as a painting or an art or a play. You might make something that has never existed, a sculpture in the nano-science, a molecular sculpture. In that case, you should go home to your parents; you just built something that never existed before. If you can't be proud of that, what can you be proud of? You've made a baby, a new molecule. It never existed. If that's not exciting, I don't know what is. It is extremely creative."

## If you could, what would you change in the current system?

"I would personally split off the teaching and the research completely. Go to Institutes of Research and Centres of Teaching. I was in South Africa and one of the universities there had just gone and contacted a big company to plan the future of university. They said it's not teaching, because in the future university will not be the source of information. Information will be on the web and everywhere else. So the teaching at universities will change. The only thing that will not change at university, which is the heart of university, is innovative research. If you look at the future of universities, it's not as we're trying to do in the Netherlands now, focus on education. Obviously, educating your people is incredibly important. The question is, does university play a role in that in the future? I would argue to move education to Centres of Teaching with guest lectures from Institutes of Research. That will be the more efficient route.

This will also enable outreach more. Outreach is a long overdue topic. We are experts in science and we have to take responsibility in doing something for society and try and reach out to the people in it. I do think we do more outreach now, but there is more to do and we can no longer sit in our ivory towers. We are trained as highly elite scientists, but we're also employed to teach (whether we can or not) and students are right to demand better and better teaching. So we're putting a round peg in a square hole sometimes. The truth is that our funding, our face to the outside world, our impact on the rest of the world is based primarily on our scientific output. Society needs this research to create innovative science, spin-off companies, and create jobs. On the other side of the coin, universities are the source of the young people of the future. This is the difficult balance. For me, the key role of the university is to inspire young people to want to change the world and it's as simple as that!"

# Recent Papers

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## Laboratory infrared spectroscopy of gaseous negatively charged polyaromatic hydrocarbons

Juehan Gao<sup>1</sup>, Giel Berden<sup>1</sup>, and Jos Oomens<sup>1,2</sup>

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Based largely on infrared spectroscopic evidence, polycyclic aromatic hydrocarbon (PAH) molecules are now widely accepted to occur abundantly in the interstellar medium. Laboratory infrared spectra have been obtained for a large variety of neutral and cationic PAHs, but data for anionic PAHs are scarce. Nonetheless, in regions with relatively high electron densities and low UV photon fluxes, PAHs have been suggested to occur predominantly as negatively charged ions (anions), having substantial influence on cloud chemistry. While some matrix spectra have been reported for radical anion PAHs, no data is available for even-electron anions, which are more stable against electron detachment. Here we present the first laboratory infrared spectra of deprotonated PAHs ( $[\text{PAH} - \text{H}]^-$ ) in the wavelength ranges between 6 and 16  $\mu\text{m}$  and around 3  $\mu\text{m}$ . Wavelength-dependent infrared multiple-photon electron detachment is employed to obtain spectra for deprotonated naphthalene, anthracene, and pyrene in the gas phase. Spectra are compared with theoretical spectra computed at the density functional theory level. We show that the relative band intensities in different ranges of the IR spectrum deviate significantly from those of neutral and positively charged PAHs, and moreover from those of radical anion PAHs. These relative band intensities are, however, well reproduced by theory. An analysis of the frontier molecular orbitals of the even- and odd-electron anions reveals a high degree of charge localization in the deprotonated systems, qualitatively explaining the observed differences and suggesting unusually high electric dipole moments for this class of PAH molecules.

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ApJ, 787, 170 (2014)

<http://iopscience.iop.org/0004-637X/787/2/170/article>

# Velocity dependence of fragmentation yields in proton - naphthalene collision and comparison with electronic energy loss calculation

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We investigate the interaction of a high velocity proton projectile (velocity between 1.41 and 2.68 au) with a gaseous naphthalene target. Fragmentation as well as multiple ionization yields are measured from the resulting mass spectra. The total fragmentation yields decrease with an increase in projectile velocity, which is in accordance with decreasing electronic stopping. *Monte Carlo* simulations have been performed within the framework of local density approximation to calculate the mean electronic energy loss. The theoretical cross sections are calculated from the energy loss distribution using a lower limit to internal energy deposition. The latter has been estimated from the resonant capture process measured concurrently for the same system. The velocity dependence of fragmentation yields obtained from the experiment is consistent with the modelled theoretical cross sections. Measurements of singly and doubly charged He projectiles with naphthalene show the effects of charge state equilibration and projectile charge screening.

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J. Phys. B: At. Mol. Opt. Phys. 47, 085202 (2014)

<http://iopscience.iop.org/0953-4075/47/8/085202>

# Random mixtures of polycyclic aromatic hydrocarbon spectra match interstellar infrared emission

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The mid-infrared (IR; 5-15  $\mu\text{m}$ ) spectrum of a wide variety of astronomical objects exhibits a set of broad emission features at 6.2, 7.7, 8.6, 11.3 and 12.7  $\mu\text{m}$ . About 30 years ago it was proposed that these signatures are due to emission from a family of UV heated nanometer-sized carbonaceous molecules known as *polycyclic aromatic hydrocarbons* (PAHs), causing them to be referred to as aromatic IR bands (AIBs). Today, the acceptance of the PAH model is far from settled, as the identification of a single PAH in space has not yet been successful and physically relevant theoretical models involving “true” PAH cross sections do not reproduce the

AIBs in detail. In this paper, we use the NASA Ames PAH IR Spectroscopic Database, which contains over 500 quantum-computed spectra, in conjunction with a simple emission model, to show that the spectrum produced by any random mixture of at least 30 PAHs converges to the same *'kernel'-spectrum*. This kernel-spectrum captures the essence of the PAH emission spectrum and is highly correlated with observations of AIBs, strongly supporting PAHs as their source. Also, the fact that a large number of molecules are required implies that spectroscopic signatures of the individual PAHs contributing to the AIBs spanning the visible, near-infrared, and far infrared spectral regions are weak, explaining why they have not yet been detected. An improved effort, joining laboratory, theoretical, and observational studies of the PAH emission process, will support the use of PAH features as a probe of physical and chemical conditions in the nearby and distant Universe.

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<http://arxiv.org/abs/1405.5383>

## Valence Shell Photoelectron Spectroscopy of Pyrene and Fluorene: Photon Energy Dependence in the Far - Ultraviolet Region

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Inner and outer valence photoelectron spectra (PES) of pyrene and fluorene, two members of the polycyclic aromatic hydrocarbon (PAH) family, were recorded with a high-resolution synchrotron photoelectron spectrometer. Relative photoelectron emission cross sections were measured at photon energies between 15 and 40 eV. Several bands observed in the experimental PES were assigned with the help of OVGf/cc - pVDZ calculations. The first ionization potentials were estimated to be  $7.436 \pm 0.015$  and  $7.944 \pm 0.055$  eV for pyrene and fluorene, respectively. Photoelectron emission cross sections show a clear difference in trend for inner ( $\sigma$  - dominated) and outer ( $\pi$  - dominated) bands. Contrary to the expectation from the trend observed in benzene, the inner bands significantly dominate in the photon energy region from 15 to 27 eV and then are found to contribute uniformly. A pronounced peak in the cross sections is observed at a photon energy of approximately 17 eV for both molecules (irrespective of the difference in symmetry and structure), particularly for the inner valence bands. The feature is observed to be independent of the details of the molecular orbital associated with the outgoing electron. These observations are correlated to a collective excitation in the far-ultraviolet region.

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<http://pubs.acs.org/doi/abs/10.1021/jp502445d>

## Electron emission and electron transfer processes in proton-naphthalene collisions at intermediate velocities

P. M. Mishra<sup>1</sup>, J. Rajput<sup>2</sup>, C. P. Safvan<sup>3</sup>, S. Vig<sup>4</sup> and U. Kadhane<sup>1</sup>

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We investigate the fragmentation and ionization of naphthalene by protons at intermediate velocities (between 1.41 and 2.68 a.u.). Relative cross sections for electron capture (EC), electron emission (EE), and capture ionization are measured. The EC cross sections decrease rapidly over the energy range under consideration (50 - 150 keV) and are lower than EE cross sections. The EE cross sections, on the other hand, change very slowly in this energy range. The energetics of interactions is quantified by comparing the mass spectra with the photodissociation breakdown curves from literature. In the case of single capture, resonant electron transfer to  $n = 1$  state in  $H^+$  is seen to dominate the interaction but is shown to be accompanied by a small amount of electronic energy loss. In the EE mode, two mechanisms are shown to be active in the collision process: large impact parameter plasmon excitation mode, and closer encounters with higher amounts of electronic energy loss.

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## Reflectance spectroscopy (350–2500 nm) of solid-state polycyclic aromatic hydrocarbons (PAHs)

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Polycyclic aromatic hydrocarbons (PAHs) are organic compounds based on fused aromatic rings, and are formed in a variety of astrophysical, solar nebula and planetary processes. Polycyclic aromatic hydrocarbons are known or suspected to occur in a wide variety of planetary settings including icy satellites, Titan's hazes, carbonaceous meteorites, comet nuclei, ring par-

ticles; and terrestrial organic-rich lithologies such as coals, asphaltites, and bituminous sands. Relatively few measurements of the visible and near-infrared spectra of PAHs exist, yet this wavelength region (350–2500 nm) is widely used for remote sensing. This study presents detailed analyses of the 350–2500 nm reflectance spectra of 47 fine-grained powders of different high-purity solid-state PAHs. Spectral properties of PAHs change with variations in the number and connectivity of linked aromatic rings and the presence and type of side-groups and heterocycles. PAH spectra are characterized by three strong features near  $\sim 880$  nm,  $\sim 1145$  nm, and  $\sim 1687$  nm due to overtones of CH fundamental stretching vibrations. Some PAHs are amenable to remote detection due to the presence of diagnostic spectral features, including: N—H stretching overtones at 1490–1515 nm in NH- and NH<sub>2</sub>-bearing PAHs, aliphatic or saturated bond C—H overtone vibrations at  $\sim 1180$ –1280 nm and  $\sim 1700$ –1860 nm; a broad asymmetric feature between  $\sim 1450$  nm and  $\sim 1900$  nm due to O—H stretching overtones in aromatic alcohols, C—H and C=O combinations near  $\sim 2000$ –2010 nm and  $\sim 2060$ –2270 nm in acetyl and carboxyl-bearing PAHs. Other substituents such as sulphonyl, thioether ether and carboxyl heterocycles, or cyano, nitrate, and aromatic side groups, do not produce well-resolved diagnostic spectral features but do cause shifts in the positions of the aromatic C—H vibrational overtone features. Fluorescence is commonly suppressed by the presence of heterocycles, side-groups and in many non-alternant PAHs. The spectral characteristics of PAHs offer the potential, under suitable circumstances, for remote characterization of the classes of PAH present and in some cases, identification of particular heterocyclic or side-group substituents.

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## Star Formation and the Interstellar Medium in Nearby Tidal Streams (SAINTS): Spitzer Mid-infrared spectroscopy and Imaging of Intergalactic Star-forming Objects

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A spectroscopic analysis of 10 Tidal Star Forming Objects (TSFOs) and a photometric analysis of 67 TSFOs in a sample of 14 interacting systems is presented. The majority of the TSFOs have relative PAH band strengths similar to those of nearby spiral and starburst galaxies. In contrast to what is observed in Blue Compact Dwarfs (BCDs) and local giant HII regions in the Milky Way (NGC 3603) and the Magellanic Clouds (30 Doradus and N 66), the relative PAH band strengths in TSFOs correspond to models with a significant PAH ion fraction ( $< 50\%$ ) and bright emission from large grains ( $\sim 100$  carbon atoms). The [Ne III]/[Ne II] and [S IV]/[S III] line flux ratios indicate moderate levels of excitation with an interstellar radiation field that is harder than the majority of the SINGS and starburst galaxies, but softer than BCDs and local giant HII regions. The TSFO neon line flux ratios are consistent with a burst of star formation  $\lesssim 6$

million years ago. Most of the TSFOs have  $\sim 10^6 M_{\odot}$  of warm  $H_2$  with a likely origin in PDRs. Infrared Array Camera (IRAC) photometry shows the TSFOs to be bright at  $8 \mu\text{m}$ , with one third having  $[4.5] - [8.0] > 3.7$ , i.e., enhanced non-stellar emission, most likely due to PAHs, relative to normal spirals, dwarf irregulars and BCD galaxies. The relative strength of the  $8 \mu\text{m}$  emission compared to that at  $3.6 \mu\text{m}$  or  $24 \mu\text{m}$  separates TSFOs from dwarf galaxies in Spitzer two color diagrams. The infrared power in two thirds of the TSFOs is dominated by emission from grains in a diffuse interstellar medium. One in six TSFOs have significant emission from PDRs, contributing  $\sim 30 - 60\%$  of the total power. TSFOs are young knots of intense star formation.

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## Tracing the Evolution of Protoplanetary Disks

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The evolution of young massive protoplanetary disks towards planetary systems is expected to correspond to changes in their morphology, including the formation of gaps. We have focused our attention on the depletion of dust and gas in the disk gaps seen in the disks around six key Herbig Ae/Be stars (HD97048, HD169142, HD135344B, Oph IRS 48, HD100453 and HD34282). By modeling spatially resolved Q-band images, we find that the property responsible for the absence of mid-infrared silicate emission ( $\sim 10 \mu\text{m}$ ) is the depletion of dust grains in the  $\sim 300\text{-}500 \text{ K}$  temperature regime. We speculate that many, if not all Herbig disks with disk classification group I are disks with large gaps and can be characterized as (pre-)transitional. An evolutionary path from the observed group I to the observed group II sources seems no longer likely. Instead, both might derive from a common ancestor (Maaskant et al. 2013). In a follow up study targeting on the same transitional Herbig Ae/Be disks, we have characterized how the charge state of PAHs can be used as a probe of flows of gas through protoplanetary gaps. Ionized PAHs trace low-density optically thin disk regions where the UV field is high and the electron density is low. Such regions are characteristic of gas flows through the gaps of transitional disks. While in optically thick disks, PAHs are predominantly neutral. The PAH spectra of transitional disks can thus be understood as superpositions of neutral PAH emission from the optically thick disk, and ionized PAHs from the ‘gas flows’ through the gap. In a larger sample of Herbig stars, we find a correlation between PAH ionization (traced by the 6.2/11.3 PAH feature ratio) and the disk mass (traced by the 1.3 mm luminosity). This may imply that lower-mass disks have larger gaps. Ionized PAHs in gas flows through these gaps contribute strongly to their spectra (Maaskant et al, 2014). Finally, a modeling study is presented to understand the location and sizes of the crystalline silicate ‘forsterite’ in protoplanetary disks. We characterize how the 23 and 69  $\mu\text{m}$  features, as observed by the Spitzer



and Herschel telescopes, can be used to constrain the physical locations of forsterite in disks. We check for consistency between two independent forsterite temperature measurements: the 23/69 feature strength ratio and the shape of the 69  $\mu\text{m}$  band. We find that for disks with low upper limits of the 69  $\mu\text{m}$  feature (most notably in flat, self-shadowed disks), the forsterite must be hot, and thus close to the star. We find no correlation between disk gaps and the presence or absence of forsterite features. We argue that the 69  $\mu\text{m}$  feature of the evolved transitional disks HD141569 and Oph IRS 48 is most likely a tracer of larger (i.e.  $>10 \mu\text{m}$ ) forsterite grains (Maaskant et al, 2014, accepted).

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