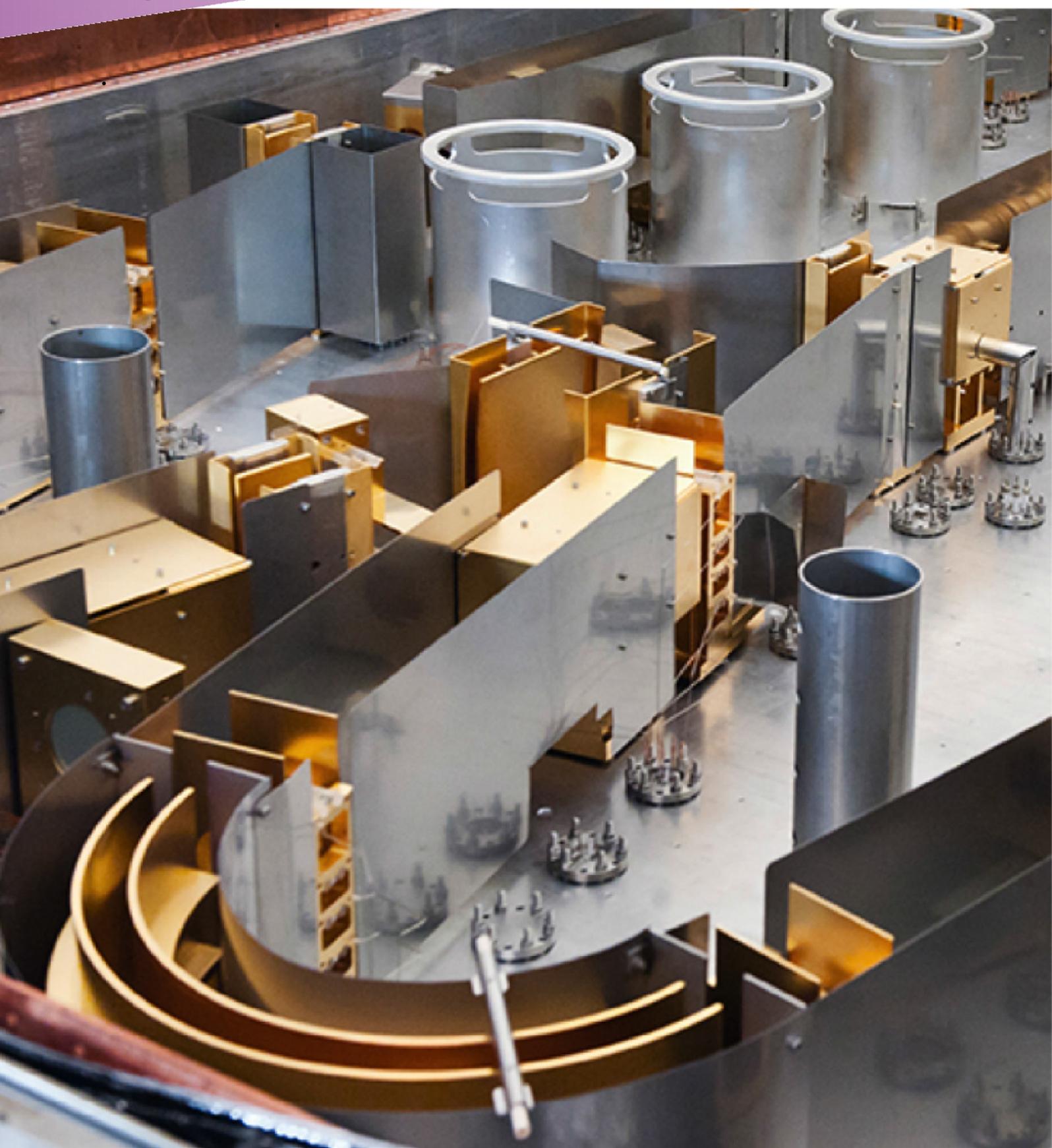


# AstropAH

A Newsletter on Astronomical PAHs

Issue 21 | September 2015



# Editorial

**Dear Colleagues,**

This issue of AstroPAH showcases the capabilities of the DESIREE Infrastructure at the Stockholm University for experimental studies of PAHs and other molecules.

We also have a diverse collection of paper abstracts covering observation, theory, and experiment on PAHs, deuterated PAHs, PAHs with functional groups, ionic PAHs, dust, and more.

The new journal Molecular Astrophysics was officially launched at the IAU General Assembly in Honolulu, Hawaii in August. We have some pictures of this celebration!

Next month is our 2nd anniversary! If you would like to see your abstract or announcement in our October anniversary issue, send us your contribution before the deadlines below. Naturally, you can also send us your contributions anytime for publication in a later issue. Contributions can be sent for any of our sections: Picture of the Month, In Focus, Abstracts, Thesis, Announcements (meetings, jobs, etc...).

Best regards,

**The Editorial Team**

**Next issue: 20 October 2015.  
Submission deadline: 9 October 2015.**

# AstroPAH Newsletter

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## PAH Picture of the Month

Detail of the Double ElectroStatic Ion-Ring ExpEriment (DESIREE) at the Stockholm University, Sweden. It offers rich opportunities for studies of PAHs.

**Credits:** H. Schmidt, H. Zettergren, and H. Cederquist.

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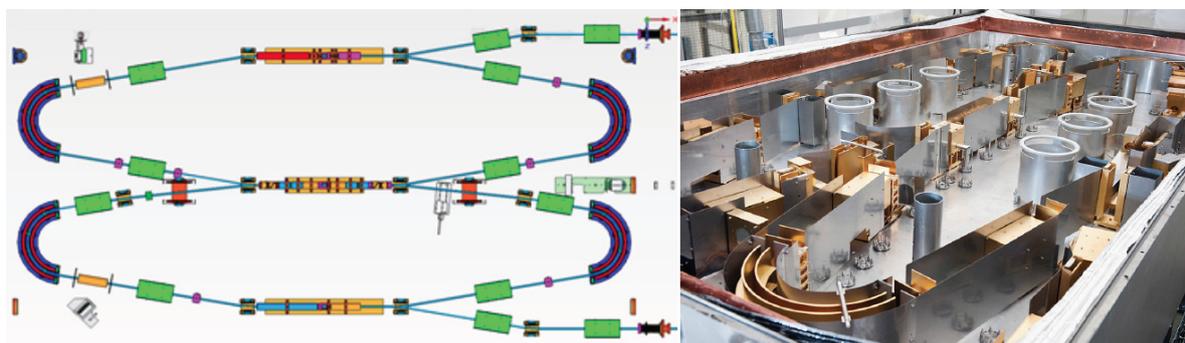
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*Design by Isabel Aleman*

## The DESIREE Infrastructure at Stockholm University: Present and Future Studies of PAHs and Other Molecules

by Henning Schmidt, Henning Zettergren, and Henrik Cederquist

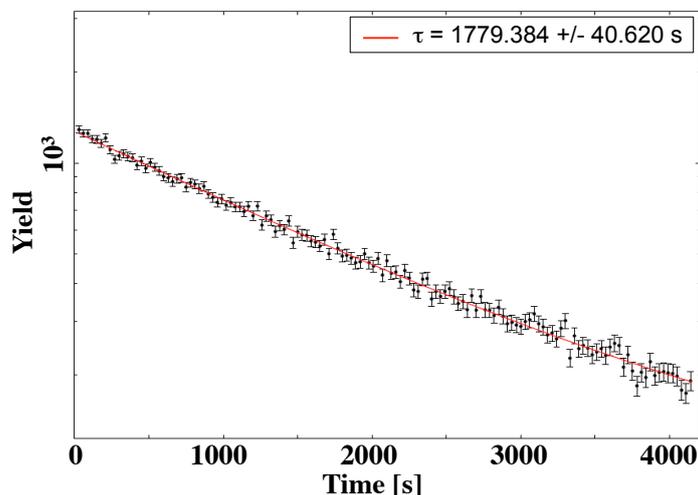
The DESIREE infrastructure at Stockholm University (SU) in Stockholm, Sweden, has recently been taken into operation<sup>[1–4]</sup>. **It offers rich opportunities for studies of various properties of, for example, Polycyclic Aromatic Hydrocarbon (PAH) molecules.** The name DESIREE is an abbreviation for the **D**ouble **E**lectro**S**tatic **I**on-**R**ing **E**xp**E**riment. These twin storage rings make up the main instrument of the facility. A schematic as well as a picture of the setup are shown in Figure 1.



**Figure 1** - Schematic (left) and picture (right) of the DESIREE setup.

In addition, the facility has a stand-alone beam line for single pass experiments, which at present is equipped with an ElectroSpray Ion (ESI) source. The ESI can be used to produce beams of, for examples, cationic or protonated PAH molecules. So far, a range of collision induced dissociation experiments at PAH-atom center-of-mass collision energies of roughly 10–1000 eV have been performed. It has been suggested that such collisions, and the specific fragmentation pathways that they favor, could be of relevance for stellar wind interactions with regions containing PAHs<sup>[5–7]</sup>. The PAH chemistry in these regions is likely to differ from that found in areas with low particle fluxes as ion or atom impact, or impact by heavy particles in general, leads to other PAH fragments than the ones resulting from photo-absorption. Photo-absorption typically favors the lowest energy dissociation channels. On the other hand, heavy particle impact, under certain conditions, may lead to exotic fragmentation channels – in particular removal of single carbon atoms. Such fragmentation leads to the efficient formation of pentagons in PAHs that initially consist of only hexagonal structures<sup>[8]</sup>. In turn, this may favor the transformation from two- to three-dimensional PAH-fragment structures and possibly also the formation of fullerenes from very large PAHs (compare the discussion by Berné and Tielens<sup>[9]</sup> and their suggestion of fullerene formation from large PAHs irradiated by UV-photons).

In the following, we will briefly describe the double ion storage ring, which, since it is cryogenically cooled to about 13 K, opens up for so-called action spectroscopy<sup>[10]</sup> of PAH anions with internal temperatures typical of the interstellar medium. We will also describe the ElectroSpray beam line and single pass experiment together with some of the results obtained with this apparatus. These latter results will also be related to results from Molecular Dynamics (MD) simulations and experimental results on ion collisions at much higher kinetic energies (typically tens of keV) obtained at the ARIBE facility in Caen, France (with Patrick Rousseau, Alicja Domaracka, Bernd Huber, Lamri Adoui and coworkers).

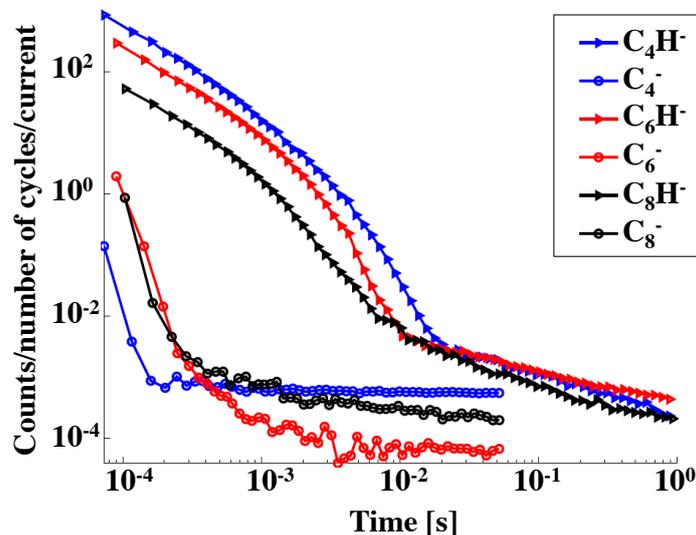


**Figure 2** - Yield of neutral Te atoms from laser photo-detachment of  $\text{Te}^-$  stored in DESIREE at 12 K as a function of time after injection. The data set is fitted to the sum of a constant (due to detector background) and a single exponential function. The 1/e storage lifetime was determined to be  $1779 \pm 41$  s.

The DESIREE double ring structure has two 8.6-meters circumference-, purely electrostatic ion storage rings (cf. Figure 1). The rings may be operated separately, but they do share a common straight section where two stored co-moving ion beams may be merged. **This will allow us to perform studies of individual reactions between positively charged ions stored in one ring and negatively charged ions stored in the other ring.** The two beams travel together in the same direction with typical laboratory frame kinetic energies of tens of keV in the ion-beams merging section and are enclosed in a tube electrode system. By biasing the voltage of one or several of these tubes, one of the beams will be accelerated and the other decelerated such that one can reach nominally zero collision energy in the center-of-mass system. Thus there is the possibility to study collisions between internally cold ions (as they can be stored for very long times – minutes and beyond<sup>[3]</sup>) at collision energies ranging from meV- to keV-energies, thus covering regimes of particular interest for astrophysics. It is important that the ions in the rings are guided by only electric fields. This means that all ions with the same kinetic energy, irrespective of their mass, will require the same voltage settings on all lenses and deflectors for storage. The masses of the ions to be stored are instead selected by two large, high-resolution, bending magnets on the two ion-injection lines. The residual gas density has been estimated<sup>[2]</sup> to be a few times  $10^4$   $\text{H}_2$  molecules per cubic centimeter at 13 K (all other gases, except He, are frozen out at this temperature). This low residual-gas density is key to the long storage times – we have demonstrated an 1/e-storage lifetime of a 10 keV  $\text{Te}^-$  beam of  $\sim 30$  minutes ( $1779 \pm 41$  seconds) which means that circulating ions can be observed (by means of laser detachment of the additional electron) for more than an hour after injection (cf. Figure 2).

These excellent vacuum conditions also allow us to store complex molecular ions for extended periods of time – minutes and beyond – and this gives ample time for such ions to equilibrate with the 13 K environment through the blackbody radiation field. Typically this means that the ions reach their electronic and vibrational ground states and low-lying rota-

tional states on time scales (milliseconds to seconds depending of the particular ion) much shorter than the ion storage time. We have performed ion storage- and cooling experiments in one of the rings. Examples include the inherent lifetimes of bound long-lived metastable states in  $S^-$ ,  $Se^-$  and  $Te^-$  [3], and Ni- [manuscript in preparation] and  $Cu_n^-$ ,  $C_n^-$ , and  $C_nH^-$  clusters or molecules ( $n$  being the number of Cu atoms in the clusters or the number of C atoms in the molecules).

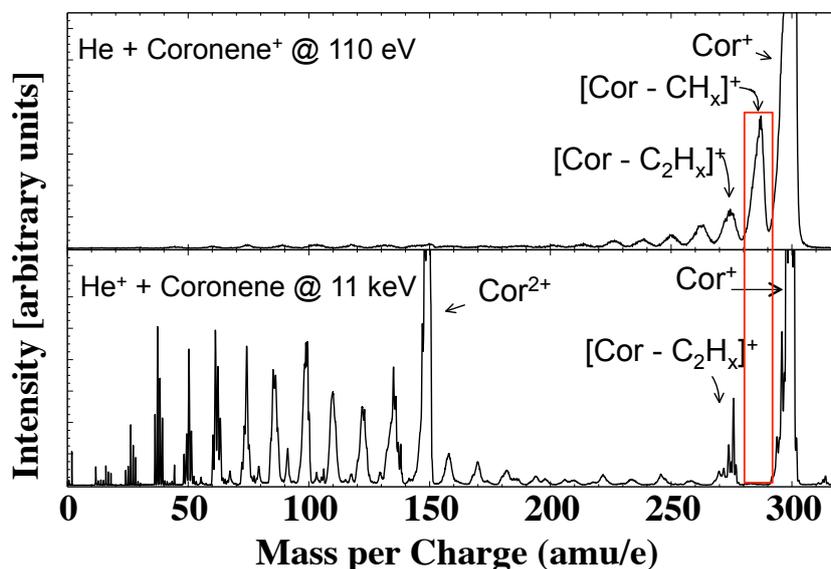


**Figure 3** - Yields of neutrals as functions of time for stored beams of  $C_n^-$  and  $C_nH^-$  ions.

In Figure 3, we compare the cooling rates of  $C_n^-$  and  $C_nH^-$  ions for  $n = 4, 6,$  and  $8$ . Here we see some large differences – the  $C_n^-$  ions cool much faster than the corresponding  $C_nH^-$  ions. A specific  $C_n^-$  or  $C_nH^-$  ion beam is selected by the magnet on the injection line and injected and stored in the ring. Then we record, as a function of time after injection, the rate of neutrals produced in spontaneous electron detachment or fragmentation processes of the hot molecular ions. The rate of neutrals will decrease with time due to two different effects. The hotter the ions, the faster their spontaneous decay and therefore we get a depletion of the ion beam in which the hot ions decay first. Therefore the rate of decay of the remaining ions will be lower on average. This characteristic behavior leads to a power-law decay of the recorded signal<sup>[11]</sup>. The other effect is that the ions may cool by radiative processes. For the  $C_nH^-$  ions, infrared emission related to vibrational cooling make the decay curves deviate from their initial power-law behavior on a ms time scale. For the  $C_n^-$  ions, it is clear that a much faster cooling process is involved. The reason is that  $C_n^-$  ions have low lying electronically excited states that may be reached through inverse internal conversion between vibrational excited states belonging to the electronic ground state potential and low lying vibrational states of the first electronically excited state<sup>[12]</sup>. This is then followed by the emission of a photon, which is a fast process. This relates to the issue on how molecular anions are formed in space. For the formation cross sections of anions to be large, it is important that excited states may relax efficiently.

One very appealing option is to use action spectroscopy to measure the photo-absorption spectra of internally cold PAH anions stored in DESIREE. The strength of this technique is that it allows absorption spectroscopy on very small samples of ions using the fact that they are moving with high speed in the ring such that the effect of any ‘action’ – detachment or fragmentation – giving neutral products can be detected for nearly every photo-absorption event. By recording the signal as a function of laser wavelength the photo-absorption cross section is obtained. An equally appealing option is to study charge exchange experiments involving PAH ions in the merged beams section. This section is at the moment being commissioned with test beams of  $C^-$  and  $Ar^+$ , and so far we have successfully operated test experiments at center-of-mass energies in the keV range. The test results are very promising – mutual neutralization count rates of hundreds of Hz. This is far above the background

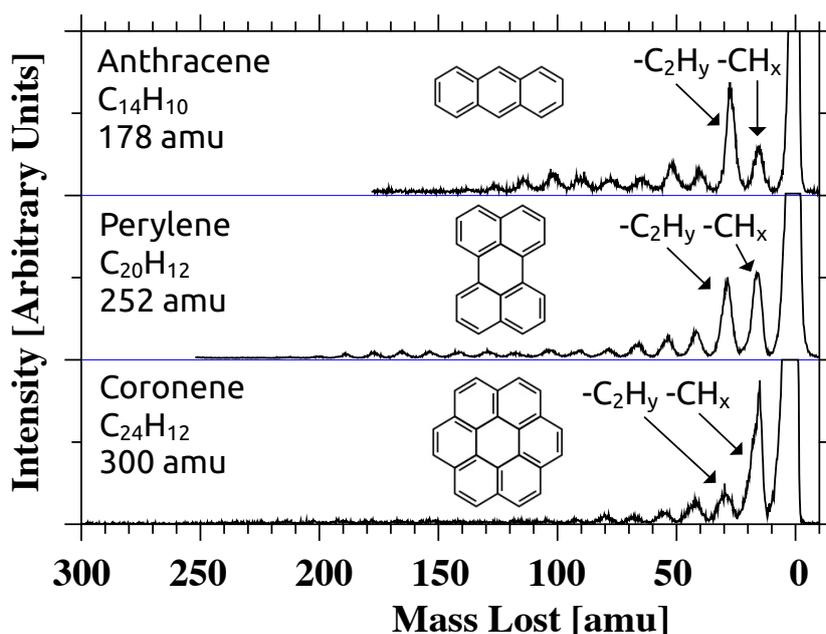
due to neutralization in the residual gas. The next step here is to use a multi-dynode detector which will allow us to separate two mutual neutralization products arriving within nanoseconds of each other, and thus to go to very low center-of-mass collision energies (meV) of direct interest for astrophysics. Here, experiments with atomic and molecular ions will be possible.



**Figure 4** - Mass spectra from 110 eV  $C_{24}H_{12}^+ + He$  (upper panel) and 11 keV  $He^+ + C_{24}H_{12}$  (lower panel) collisions. The energy transfer is dominated by interactions with the molecular electron cloud in the high energy collisions. The coronene molecule is then strongly heated resulting in a rich fragment mass spectrum. At the lower energy, the energy transfer is mainly to the vibrational degrees of freedom. One atom may then be promptly knocked out in the collision, which gives a new peak in the mass spectrum corresponding to  $CH_x$ -loss.

In our experiments at the ElectroSpray beam-line, we have thus far focused on collision-induced dissociation of PAH cations colliding with helium at center-of-mass (CoM) energies between about 10 and 200 eV. The lowest-energy dissociation channels of PAHs and their cations are typically  $H^-$  and  $C_2H_2$ -loss, which lie in the range of 5-7 eV as shown by Holm *et al.*<sup>[13]</sup> for example. In Figure 4, we show a comparison of fragmentation spectra for anthracene cations,  $C_{14}H_{10}^+$ , colliding with He at about 100 eV (CoM), and higher energy collisions between He-ions and neutral anthracene molecules as measured at the ARIBE facility. The difference is striking. At the higher energy, one of the lower energy dissociation channels, that of  $C_2H_2$ -loss is clearly important. There are also smaller fragments that could result from secondary fragmentation following initial  $C_2H_2$ -loss if the fragment is sufficiently hot - and/or so called multi-fragmentation processes. For keV collisions, the energy transfer is mainly to the electronic degrees of freedom. This is followed by a very rapid redistribution of energy to vibrational degrees of freedom such that the lowest energy dissociation channels are favored (for example  $C_2H_2$ -loss). At the lower collision energy we still have contributions from electronic excitation processes, but as the 'projectile' (He) now is slower it has more time to interact with individual atoms in the PAH molecule and may transfer sufficient amounts of energy to one (or several) of them to promptly knock them out and a new peak appears corresponding to  $CH_x$ -loss. The timescale for this is given by the time it takes the projectile to traverse the molecule, and is in this example in the range of femtoseconds. Typical energies transferred in such collisions are a few tens of eV, which are shared between kinetic energy of the atom that is knocked out, and internal excitation of the fragment. The fragment may then go through further fragmentation steps. As demonstrated in figure 5, such secondary fragmentation processes following knockout become less important for larger PAHs with larger heat capacities. In this context, it should be noted that the energy

transferred in collisions leading to knockout are similar for PAHs of different sizes<sup>[8]</sup>.



**Figure 5** - Mass spectra from 110 eV  $C_{14}H_{10}^+ + He$  (upper panel),  $C_{20}H_{12}^+ + He$  (middle panel), and  $C_{24}H_{12}^+ + He$  (lower panel) collisions. The peak corresponding to single carbon knockouts ( $-CH_x$ ) becomes more prominent with increasing PAH size (heat capacity) as the decay rate for secondary fragmentation processes after knockout decreases.

As the knockout process is very fast (fs) – the fragmentation happens already before the excitation energy has time to distribute over all vibrational degrees of freedom – we refer to the fragmentation step as being non-statistical. Recently, we have performed a detailed study of the threshold behavior of the knockout process for anthracene, pyrene, and coronene colliding with He. The cross sections for knockout have been measured as functions of center-of-mass collision energy, and we have derived threshold energies for single carbon knockout from the experiment and from parallel MD-simulations using the Tersoff potential to describe C-C and C-H bonds in these molecules. The experiment and the simulations are in good agreement, and we have shown that it is possible to use an analytical expression by Chen *et al.*<sup>[14]</sup> for the absolute cross section for knockout from PAHs to describe the data. This expression should thus be useful for good estimates of knockout cross section in arbitrary large PAHs which cannot be easily studied in the laboratory.

We have performed a range of additional PAH collision studies which may be of interest for the Astro-PAH community including fragmentation studies of nitrogen-containing PAHs, PANHs<sup>[15]</sup>, an investigation of the formation of  $H_2$  from non-hydrogenated PAHs showing that this may be an efficient process at sufficiently large internal energies<sup>[16]</sup>, and a study of carbon-backbone fragmentation of native and superhydrogenated PAHs showing that superhydrogenation of pyrene increases backbone fragmentation for a given internal energy. Thus superhydrogenation seems not to be a way to explain large abundances of PAHs in certain astrophysical regions, at least not from the point of view of our study. It should be noted, though, that a different conclusion is reached by the Groningen group<sup>[17]</sup>. They, however, used a different excitation method and a different molecule – coronene instead of pyrene. This is an interesting issue requiring more studies from both sides – and such studies are now indeed underway. Finally it has been mentioned before that the knockout process gives other and more reactive fragments than for example photo-fragmentation processes. Effects of this is clearly seen in studies of ion impact on clusters of fullerenes<sup>[18]</sup> and clusters of the PAH molecule pyrene<sup>[19]</sup> as well as in mixed PAH-fullerene clusters<sup>[20]</sup>.

Finally, let us take this opportunity to announce a short meeting on PAHs, fullerenes, and small hydrocarbon molecules in the laboratory and in space. The purpose is, similar to last year's meeting in Leiden, to define common research goals on these topics. Next year's meeting will be organized from April 11 to 13, 2016 at Stockholm University, Sweden. More information about the meeting will follow shortly but please make a note for your planning.



**Henning Schmidt:** Full professor at the University of Stockholm. Studies of structure and dynamics of (primarily atomic) ions and their interactions with neutral atoms or molecules, with laser light and with other ions. The experimental studies are mostly performed with ions stored in electrostatic storage rings and traps. Developments of ion storage instrumentation. E-mail: [schmidt@fysik.su.se](mailto:schmidt@fysik.su.se).



**Henning Zettergren:** Associate professor at the University of Stockholm. Experimental and theoretical studies of complex molecules such as PAHs, fullerenes, biomolecules and their clusters. Charge transfer, cooling dynamics, molecular fusion processes, and the effect of a surrounding environment in interactions with ions or photons. E-mail: [henning@fysik.su.se](mailto:henning@fysik.su.se).



**Henrik Cederquist:** Full professor at the University of Stockholm. Studies of atomic and molecular reaction processes using ion storage devices, measurements of lifetimes of metastable states, cluster relaxation processes, reactions inside excited clusters, molecular growth processes. Experiments on fullerenes, Polycyclic Aromatic Hydrocarbon molecules, clusters, diatomic molecules, anions etcetera. Development of ion storage instrumentation. E-mail: [cederq@fysik.su.se](mailto:cederq@fysik.su.se).

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# Abstracts

## A Tale of Three Galaxies: Deciphering the Infrared Emission of the Spectroscopically Anomalous Galaxies: IRAS F10398+1455, IRAS F21013-0739 and SDSS J0808+3948

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The *Spitzer*/Infrared Spectrograph spectra of three spectroscopically anomalous galaxies (IRAS F10398+1455, IRAS F21013-0739 and SDSS J0808+3948) are modeled in terms of a mixture of warm and cold silicate dust, and warm and cold carbon dust. Their unique infrared (IR) emission spectra are characterized by a steep  $\sim 5\text{--}8\ \mu\text{m}$  emission continuum, strong emission bands from polycyclic aromatic hydrocarbon (PAH) molecules, and prominent silicate emission. The steep  $\sim 5\text{--}8\ \mu\text{m}$  emission continuum and strong PAH emission features suggest the dominance of starbursts, while the silicate emission is indicative of significant heating from active galactic nuclei (AGNs). With warm and cold silicate dust of various compositions (“astronomical silicate,” amorphous olivine, or amorphous pyroxene) combined with warm and cold carbon dust (amorphous carbon, or graphite), we are able to closely reproduce the observed IR emission of these galaxies. We find that the dust temperature is the primary cause in regulating the steep  $\sim 5\text{--}8\ \mu\text{m}$  continuum and silicate emission, insensitive to the exact silicate or carbon dust mineralogy and grain size  $a$  as long as  $a \sim 1\ \mu\text{m}$ . More specifically, the temperature of the  $\sim 5\text{--}8\ \mu\text{m}$  continuum emitter (which is essentially carbon dust) of these galaxies is  $\sim 250\text{--}400\text{K}$ , much lower than that of typical quasars which is  $\sim 640\text{K}$ . Moreover, it appears that larger dust grains are preferred in quasars. The lower dust temperature and smaller grain sizes inferred for these three galaxies compared with that of quasars could be due to the fact that they may harbor a young/weak AGN which is not maturely developed yet.

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Astrophysical Journal, in press, 2015

<http://arxiv.org/abs/1507.03280>

# Dust and Polycyclic Aromatic Hydrocarbon in the HD 34700 Debris Disk

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The debris disk around the Vega-type star HD 34700 is detected in dust thermal emission from the near infrared (IR) to millimeter (mm) and submm wavelength range. Also detected is a distinct set of emission features at 3.3, 6.2, 7.7, 8.6, 11.3 and 12.7  $\mu\text{m}$ , which are commonly attributed to polycyclic aromatic hydrocarbon (PAH) molecules. We model the observed dust IR spectral energy distribution (SED) and PAH emission features of the HD 34700 disk in terms of porous dust and astronomical-PAHs. Porous dust together with a mixture of neutral and ionized PAHs closely explains the dust IR SED and PAH emission features observed in the HD 34700 disk. Due to the stellar radiation pressure and Poynting-Robertson drag together with the photodissociation of PAHs, substantial removal of dust and PAHs has occurred in the disk, and continuous replenishment of these materials is required to maintain their current abundances. This implies that these materials are not primitive but secondary products probably originating from mutual collisions among planetesimals, asteroids, and comets.

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The Astrophysical Journal 2015, in press

<http://arxiv.org/abs/1507.06627>

## Dissociative Photoionization of Polycyclic Aromatic Hydrocarbon Molecules Carrying an Ethynyl Group

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The life cycle of the population of interstellar polycyclic aromatic hydrocarbon (PAH) molecules depends partly on the photostability of the individual species. We have studied the dissociative photoionization of two ethynyl-substituted PAH species, namely, 9-ethynylphenanthrene and 1-ethynylpyrene. Their adiabatic ionization energy and the appearance energy of fragment ions have been measured with the photoelectron photoion coincidence (PEPICO) spectroscopy technique. The adiabatic ionization energy has been found at  $7.84 \pm 0.02$  eV for 9-ethynylphenanthrene and at  $7.41 \pm 0.02$  eV for 1-ethynylpyrene. These values are similar to those determined for the corresponding non-substituted PAH molecules phenanthrene and pyrene. The appearance energy of the fragment ion indicative of the loss of a H atom following photoionization is also similar for either ethynyl-substituted PAH molecule and its non-substituted counterpart. The measurements are used to estimate the critical energy for the loss of a H atom by the PAH cations and the stability of ethynyl-substituted PAH molecules upon photoionization. We conclude that these PAH derivatives

are as photostable as the non-substituted species in H I regions. If present in the interstellar medium, they may play an important role in the growth of interstellar PAH molecules.

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<http://dx.doi.org/10.1088/0004-637X/810/2/114>

<http://arxiv.org/abs/1508.00259>

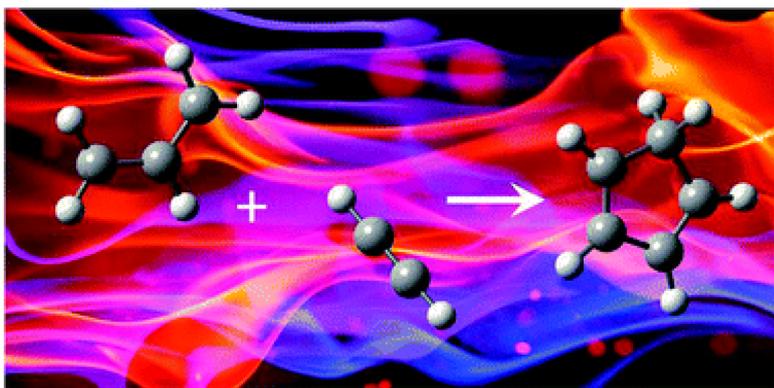
## On the formation of cyclopentadiene in the $C_3H_5 + C_2H_2$ reaction

Jordy Bouwman<sup>1</sup>, Andras Bodi<sup>2</sup>, Jos Oomens<sup>1,3</sup> and Patrick Hemberger<sup>2</sup>

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The reaction between the allyl radical ( $C_3H_5$ ) and acetylene ( $C_2H_2$ ) in a heated microtubular reactor has been studied at the VUV beamline of the Swiss Light Source. The reaction products are sampled from the reactor and identified by their photoion mass-selected threshold photoelectron spectra (ms-TPES) by means of imaging photoelectron photoion

coincidence spectroscopy. Cyclopentadiene is identified as the sole reaction product by comparison of the measured photoelectron spectrum with that of cyclopentadiene. With the help of quantum-chemical computations of the  $C_5H_7$  potential energy surface, the  $C_2H_2 + C_3H_5$  association reaction is confirmed to be the rate determining step, after which H-elimination to form  $C_5H_6$  is prompt in the absence of re-thermalization at low pressures. The formation of cyclopentadiene as the sole product from the allyl + acetylene reaction offers a direct path to the formation of cyclic hydrocarbons under combustion relevant conditions. Subsequent reactions of cyclopentadiene may lead to the formation of the smallest polycyclic aromatic molecule, naphthalene.

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Phys.Chem.Chem.Phys., 2015, 17, 20508

<http://pubs.rsc.org/en/content/articlepdf/2015/cp/c5cp02243f>

# Probing the ionization states of polycyclic aromatic hydrocarbons via the 15-20 $\mu\text{m}$ emission bands

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We report new correlations between ratios of band intensities of the 15-20  $\mu\text{m}$  emission bands of polycyclic aromatic hydrocarbons (PAHs) in a sample of fifty-seven sources observed with Spitzer/IRS. This sample includes Large Magellanic Cloud point sources from the SAGE-Spec survey, nearby galaxies from the SINGS survey, two Galactic ISM cirrus sources and the spectral maps of the Galactic reflection nebulae NGC 2023 and NGC 7023. We find that the 16.4, 17.4 and 17.8  $\mu\text{m}$  band intensities are inter-correlated in all environments. In NGC 2023 and NGC 7023 these bands also correlate with the 11.0 and 12.7  $\mu\text{m}$  band intensities. The 15.8  $\mu\text{m}$  band correlates only with the 15-18  $\mu\text{m}$  plateau and the 11.2  $\mu\text{m}$  emission. We examine the spatial morphologies of these bands and introduce radial cuts. We find that these bands can be spatially organized into three sets: the 12.7, 16.4 and 17.8  $\mu\text{m}$  bands; the 11.2, 15.8  $\mu\text{m}$  bands and the 15-18  $\mu\text{m}$  plateau; and the 11.0 and 17.4  $\mu\text{m}$  bands. We also find that the spatial distribution of the 12.7, 16.4 and 17.8  $\mu\text{m}$  bands can be reconstructed by averaging the spatial distributions of the cationic 11.0  $\mu\text{m}$  and neutral 11.2  $\mu\text{m}$  bands. We conclude that the 17.4  $\mu\text{m}$  band is dominated by cations, the 15.8  $\mu\text{m}$  band by neutral species, and the 12.7, 16.4 and 17.8  $\mu\text{m}$  bands by a combination of the two. These results highlight the importance of PAH ionization in spatially differentiating sub-populations by their 15-20  $\mu\text{m}$  emission variability.

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## Theoretical study of deuterated PAHs as carriers for IR emission features in the ISM

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This work proposes deuterated PAH (DPAH<sup>+</sup>) molecules as a potential carrier of the 4.4 and 4.65  $\mu\text{m}$  mid infrared emission bands that have been observationally detected towards the Orion and M17 regions. Density Functional Theory calculations have been carried out on DPAH<sup>+</sup> molecules to see the variations in the spectral behaviour from that of a pure PAH. DPAH<sup>+</sup> molecules show features that arise due to the stretching of the aliphatic C-D bond. Deuterated PAHs have been previously reported as carriers for such features. However, preferred conditions of ionization of PAHs in the interstellar medium (ISM) indicates the possibility of the formation of DPAH<sup>+</sup> molecules. Comparison of band positions of DPAH<sup>+</sup>s

shows reasonable agreement with the observations. We report the effect of size of the DPAH<sup>+</sup> molecules on band positions and intensities. This study also reports a D/H ratio ( $[D/H]_{sc}$ ; the ratio of C – D stretch and C – H stretch bands per  $[D/H]_{num}$ ) that is decreasing with the increasing size of DPAH<sup>+</sup>s. It is noted that large DPAH<sup>+</sup> molecules (no. of C atoms  $\sim 50$ ) match the D/H ratio that has been estimated from observations. This ratio offers prospects to study the deuterium abundance and depletion in the ISM.

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<http://arxiv.org/abs/1508.05311> or

<http://mnras.oxfordjournals.org/cgi/reprint/stv1946?ijkey=O0kpJi3IA8Xkamz&keytype=ref>

## XUV excitation followed by ultrafast non-adiabatic relaxation in PAH molecules as a femto-astrochemistry experiment

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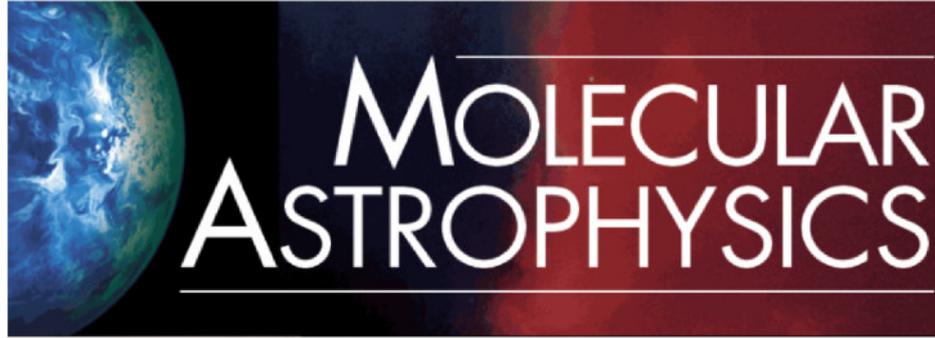
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Recently developed ultrashort extreme ultraviolet (XUV) light sources offer the high excitation energies and ultrafast time-resolution required for probing the dynamics of excited molecular states on femtosecond ( $1 \text{ fs} = 10^{-15} \text{ s}$ ) and even attosecond ( $1 \text{ fs} = 10^{-18} \text{ s}$ ) timescales. Here we use XUV light to ionize neutral PAHs, producing excited cations with an internal energy that can reach several eV. We show that these excited molecules undergo ultrafast relaxation on a few tens of femtoseconds timescales, involving an interplay between the electronic and vibrational degrees of freedom. This ultrafast lifetime of electronically excited PAHs is measured for several PAH molecules. Therefore our work reveals a general property of PAHs that can contribute to elucidate the assignment of diffuse interstellar absorption bands and strengthen models in astrochemistry. It also provides a benchmark for the manner in which coupled electronic and nuclear dynamics determines reaction pathways in large molecules following XUV excitation.

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<http://www.nature.com/ncomms/2015/150813/ncomms8909/full/ncomms8909.html>



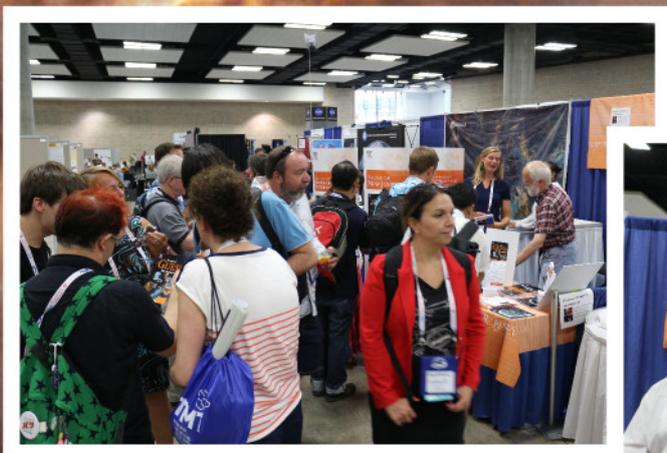
# MOLECULAR ASTROPHYSICS

The official launch of the new journal **Molecular Astrophysics** took place at the IAU XXIX General Assembly in Honolulu, Hawaii, on Wednesday 5 August, 2015.

The **Editor-in-Chief, Xander Tielens**, the **publisher, José Stoop** (Elsevier), and many other scientists celebrated the occasion with champagne and a small speech at the Elsevier booth in the exhibition hall. See some photographs below.

**Molecular Astrophysics** provides a platform for scientists studying the chemical processes that form and dissociate molecules, and control chemical abundances in the universe, particularly in Solar System objects including planets, moons, and comets, in the atmospheres of exoplanets, as well as in regions of star and planet formation in the interstellar medium of galaxies. The themes covered by this journal are planetary and exoplanetary science, astrochemistry, astrobiology, spectroscopy, physical chemistry and chemical physics.

The call for papers is open. Click [here](#) for more information.



Credits: background by Y.-H. Chu (U. Illinois, Urbana-Champaign) and Yâel Nazé (U. Liège, Belgium); photographs by A. Petrigiani

## AstroPAH Newsletter

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Next issue: 20 Oct. 2015  
Submission deadline: 9 Oct. 2015