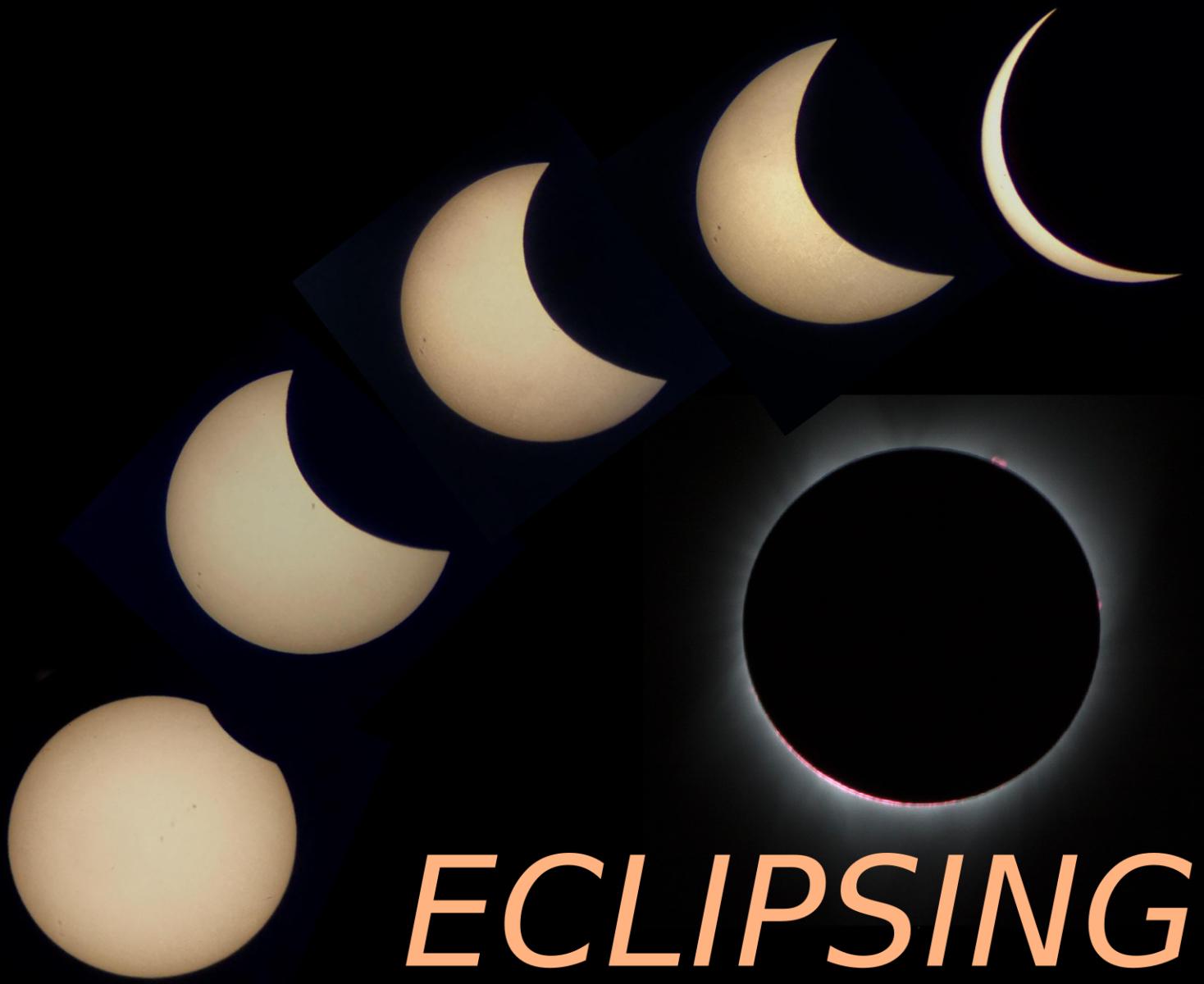


AstroPAH

A Newsletter on Astronomical PAHs

Issue 41 | September 2017



Editorial

Dear Colleagues,

Welcome to the 41st issue of AstroPAH! This month, we show pictures of the latest total solar eclipse on the cover. Eclipses are a fascinating phenomenon, which draw the attention of the community to Astronomy.

This month's In Focus features an interview with Dr. Ji Yeon Seok, an astronomer at the National Astronomical Observatory of China, who tells us more about her career path and her research on interstellar dust and PAHs.

Do not miss any of the interesting papers in our Abstract section, from computational calculations, to observational data analysis, to laboratory studies.

AstroPAH can help you promote your science. Visit our webpage or contact us for more information. You can send us your contributions anytime. For publication in October, see the deadlines below.

We thank you all for your contributions so far!

The Editorial Team

Next issue: 24 October 2017.

Submission deadline: 13 October 2017.

AstroPAH Newsletter

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PAH Picture of the Month

Pictures of the Moon crossing in front of the Sun as seen from Madras (Oregon) on August 21, 2017 during the solar eclipse. The Sun's corona is seen during the total eclipse (white plumes surrounding the dark disk). The red spots also surrounding the disc are called Bailey's beads. They are produced during totality, when the irregular lunar limb topography allows beads of sunlight to shine through in some areas.

Credits: Partial eclipse: Ella Sciamma-O'Brien. Total eclipse: NASA/Carla Thomas



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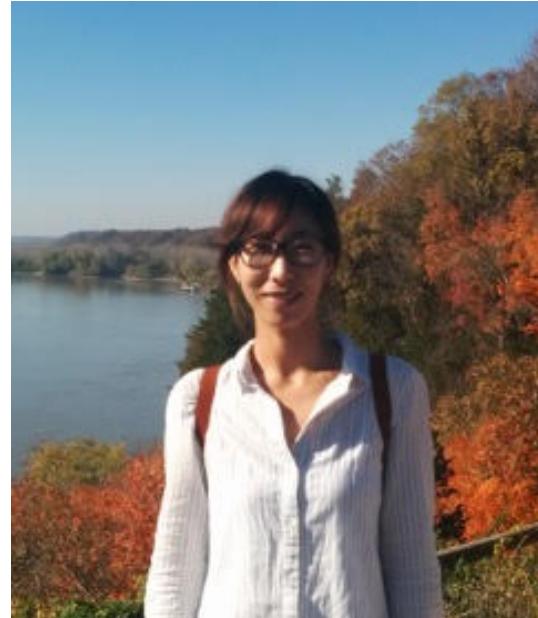
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In FOCUS

Interview with Ji Yeon Seok

Tell us about yourself.

I am currently a LAMOST¹ Fellow at the National Astronomical Observatory of China. I have been working on interstellar dust and polycyclic aromatic hydrocarbons (PAHs) in various physical conditions including protoplanetary disks (PPDs) around pre-main sequence stars, debris disks, H II regions, supernova remnants (SNRs), and even galaxy-evolution timescale both observationally and theoretically. With my research, I would like to understand the formation and destruction of PAHs as well as their impacts on the surrounding environment. I have mainly used two infrared space telescopes (AKARI and Spitzer) with supplementary data from other facilities such as ISO and Herschel. I am also interested in the evolution of massive stars in their final phases such as luminous blue variables, Wolf-Rayet stars, and SNRs and plan to use optical multi-object fiber spectroscopy with LAMOST.



When and why did you start studying PAHs?

I did my bachelor's degree in astronomy at Seoul National University, South Korea and decided in 2006 to continue with my studies in graduate school. I wasn't sure what I wanted to study in astronomy, but I decided to join a group supervised by Prof. Bon-Chul Koo. I liked his lecture very much, and he had a very good reputation among other graduate students. I think it was very fortunate that I entered his group in 2006 because the Japanese infrared satellite, AKARI, had just been launched on 21 February 2006. Prof. Koo and another of his PhD students were heavily involved in several AKARI mission programs, and I had the good fortune

¹ Large Sky Area Multi-Object Fibre Spectroscopic Telescope.

to be able to join them and participate in the AKARI projects. Also, by that time, a number of papers using Spitzer had been published, which allowed me to learn the background about infrared astronomy from literature. One day, I talked with Prof. Koo, and he asked me if I preferred theoretical or observational projects. I chose the latter without any hesitation. Then, he suggested to me to study SNRs in the Large Magellanic Cloud (LMC) using AKARI data. As a first project, I did a systematic study of SNRs using the AKARI LMC survey, which observed about a 10 deg² area of the LMC in five bands (3, 7, 11, 15, and 24 μm). We identified eight SNRs with distinguishable infrared emission among 21 known SNRs included in the LMC survey field. Later, as a follow-up, we picked up several interesting SNRs and carried out spectroscopic observations with AKARI. Even at this time, I did not imagine that I would work on PAHs, but life is just one coincidence after another. We obtained near-infrared (NIR) spectra (\sim 2.5-5 μm) of the SNR N49, one of SNRs interacting with a nearby molecular cloud in the LMC. As N49 shows bright emission in the 3 μm band image, it was an obvious target to examine its NIR emission. Then, my first encounter with PAHs happened unexpectedly when we detected the 3.3 μm aromatic feature in the NIR spectra of N49. This serendipitous detection of PAH emission in N49 is why I started to study PAHs, and I admit that it was the most surprising moment related to PAHs during the course of my research (some more details to be continued!!).

Tell us a little about your latest paper on PAHs.

Our recent paper is about PAHs in protoplanetary disks (PPDs) around pre-main-sequence stars (Seok & Li 2017). We searched for PPDs showing PAH features in the literature, and 69 PPDs, around 14 T Tauri and 55 Herbig Ae/Be stars, were found. To the best of our knowledge, this is the largest sample of PPDs showing PAH features in their IR spectra, which are to be modeled taking precise PAH chemistry into account. We accumulated their IR spectroscopic data from the literature and data archives, composed of 43 NIR and 69 MIR spectra, to analyze the major PAH features at 3.3-11.3 μm. These are important because a simultaneous modeling of as many PAH bands as possible can more accurately constrain their properties. As we aimed to mainly model the PAH emission features, the PAH features are extracted from the original data by subtracting the underlying continuum.

With these continuum-subtracted spectra, we derived the PAH properties adopting the astro-PAH model of Li & Draine (2001) and Draine & Li (2007). There are three key parameters in our model calculations: i) the peak and ii) the width (a_0 and σ) of the lognormal function for the PAH size distribution, and iii) the ionization fraction (ϕ_{ion}) for the charge state. We vary a_0 from 2.0 Å to 5.5 Å with a step of 0.5 Å and σ from 0.2 to 0.9 with a step of 0.1. ϕ_{ion} is the probability of finding a PAH molecule in a nonzero charge state, and it ranges between 0 and 1 with a step of 0.1. For each source, 704 models ($=8 \times 8 \times 11$) are calculated taking into account their stellar parameters (e.g., stellar luminosity and effective temperature), and we searched for the best-fit model that reproduces the observational spectrum most closely. It is worth noting that we also derived the peak of the PAH mass distribution (per logarithmic PAH radius), a_p , from a_0 and σ , which is beneficial to describe and compare the overall PAH size distributions. Then we looked for the correlations of PAH properties with stellar parameters.

We found that a_p shows positive correlation with the stellar effective temperature, T_{eff} , (see Fig. 1), indicating that small PAHs are dominant in disks around cool stars while large PAHs are

dominant in those associated with hot stars. This can naturally be explained by the photodissociation of PAHs induced by energetic photons, which destroy small PAHs more rapidly than large PAHs. Following the photophysics of Li & Lunine (2003, see their Appendix A for details), we derived the destruction timescale depending on T_{eff} , L_* , and the distance of PAHs from the central star (r). Figure 1 (right) clearly shows that in general small PAHs are readily destroyed during the typical lifetime of PPDs. Considering that the lifetime of most of the sources in our sample ranges from 1 to 10 Myr, PAHs smaller than $\approx 4 \text{ \AA}$ are expected to be destroyed by photodissociation. For hotter sources ($T_{eff} > 10,000 \text{ K}$), even PAHs with $\approx 4.5 \text{ \AA}$ are destroyed within $\sim 1 \text{ Myr}$. In addition to T_{eff} , the shift of the peak wavelength of the $7.7 \mu\text{m}$ PAH feature ($\lambda_{7.7}$) shows a moderate correlation with a_p : as PAH molecules become smaller, $\lambda_{7.7}$ tends to shift toward longer wavelengths. This is consistent with the negative correlation between $\lambda_{7.7}$ and T_{eff} that has been previously reported because small PAHs are dominant in disks around cool stars. Unlike a_p , we found that ϕ_{ion} shows no significant correlation with T_{eff} . This lack of correlation is attributed to the diversity of the spatial distribution of PAHs in disks from one to another. Since ϕ_{ion} depends on the starlight intensity, which is a function of distance from the central star, the radial distribution of PAHs should be taken into account to properly interpret ϕ_{ion} .

Have you, as a scientist, had difficulties to balance your career and personal life?

To be honest, it is right now that I am having difficulties to keep a balance between work and my personal life because my son was just born in February and I got back to work in May. My mother came to Beijing to take care of my baby while I work, and I and my husband (who is also a postdoc in the Kavli Institute for Astronomy and Astrophysics at Peking University) adjusted our office hours to minimize the time that only my mom looks after the baby. For example, I work from morning to afternoon and my husband works from noon to early evening. This is an advantage that we have because working hours for a postdoc are usually flexible. Nevertheless, I always feel that I don't spend sufficient time both with my baby and my research. Several professors have advised me that it is very important to spend enough time with my son especially when he is very young. I agree because what he learns from us during this period will have a strong influence on him for the rest of his life. Meanwhile, this is also critical time for my career since it is my third postdoc position (i.e., spent 5 years including the maternity leave), so I should consider a more senior position, which, of course, requires high productivity. Well, anyhow, it's the matter of time, and I try to enjoy being a mother as well as a scientist because both bring me a lot of wonder and delight.

What is the most important advice someone gave to you/ you give to your students?

I am very fortunate in the sense that I have met and worked with a lot of respectable people. They always give me priceless advice and inspiration. One of the most important was "Do the most important task first". I was a postdoc in ASIAA, Taiwan, and we had a regular chat with a director individually. At that time, I had just gotten married, and my husband went to US for his

postdoc. Dr. Paul Ho (the former director of ASIAA) was a director, and I expressed difficulties about the “two-body” problem. He told me “Don’t give up your career and try your best to keep it”. Then, he mentioned that time management would be very crucial. When there are several things to do, prioritize all tasks and do the most important part first. This is important because many people spend lots of time doing less important tasks. I realized that I was also one of these people and worked inefficiently. In particular, when I was involved in several projects at the same time, I sometimes lost my direction. On such occasions, I step back and consider what has the highest priority. This is very helpful for me to keep my pace.

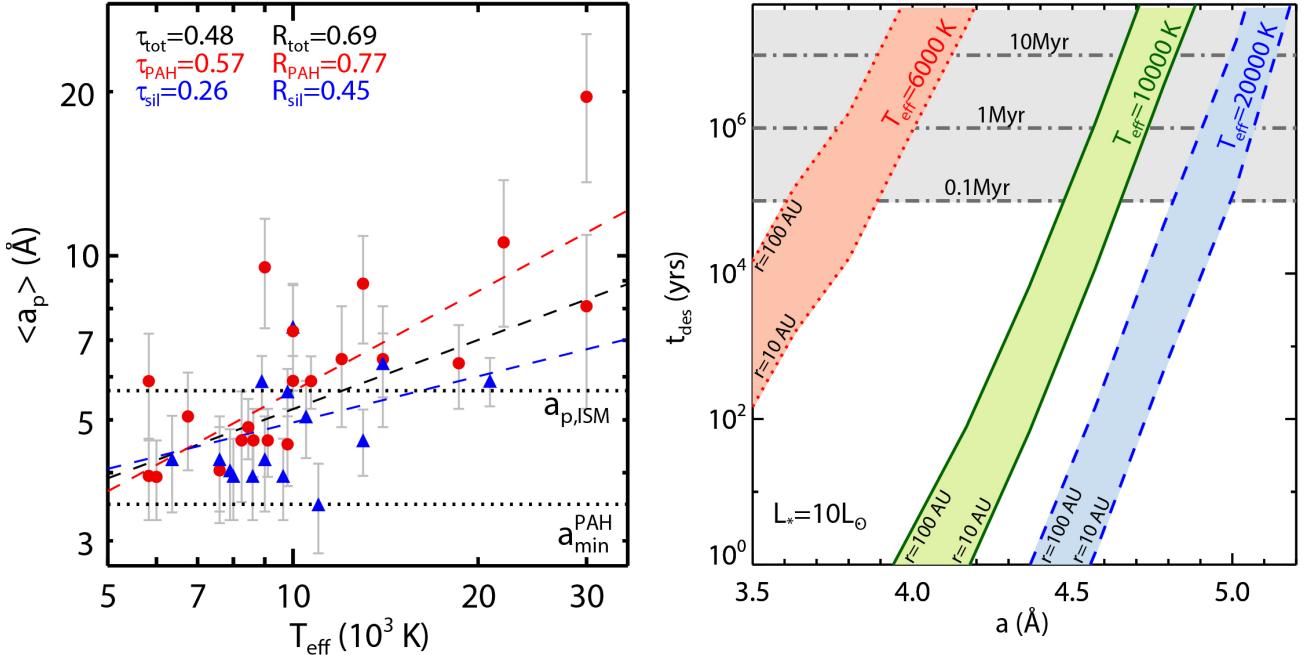


Figure 1: **Left:** Comparison between a_p and the stellar effective temperatures (T_{eff}). $\langle a_p \rangle$ is a median value in the top 70 best-fit models of each source. Circle and triangle symbols denote sources with PAH emission-dominated and silicate emission (or absorption)-dominated spectra, respectively. a_p for the diffuse ISM (i.e., $a_p, \text{ISM} = 5.66 \text{ \AA}$) and the lower cutoff of the PAH size ($= 3.5 \text{ \AA}$), which is the minimum size of PAHs required to survive in the diffuse ISM, are marked by dotted lines as a reference. The correlations between a_p and T_{eff} are fitted with a linear function in logarithmic scale (red, blue, and black dashed lines for the PAH-dominated sources, the silicate-dominated sources, and combined data sets, respectively). Correlation coefficients for the PAH-dominated spectra (R_{PAH}) and those with the silicate emission (or absorption) feature (R_{sil}) are measured separately, and a total correlation coefficient is also given (R_{tot}). **Right:** Photodestruction timescales (τ_{des}) of PAHs as a function of size for $T_{\text{eff}} = 0.6, 1$, and $2 \times 10^4 \text{ K}$ at a given luminosity ($L_* = 10 L_\odot$). For each T_{eff} , τ_{des} at $r=10$ and 100 au are calculated. A typical range of stellar ages of PPDs (i.e., $0.1 - 50 \text{ Myr}$) is designated by the shaded region with representative values of $0.1, 1$, and 10 Myr (dashed-dotted lines). Note that τ_{des} is proportional to r^2 and L_\odot^{-1} (i.e., $\tau_{\text{des}} \propto r^2/L_*$).

Has there been anything that has surprised you about PAHs during the course of your research?

As I mentioned above, the detection of PAH emission in the SNR N49 is one of the most memorable moments about PAHs during my research career. Here is the detailed story... Most of the spectra of N49 were taken in 2008, and I started to examine its NIR spectra in 2009. At a first glance, they looked normal; prominent hydrogen recombination lines such as $\text{Br}\alpha$ and $\text{Br}\beta$ are seen, and several H_2 rotational lines such as H_2 1-0 O(3) and 0-0 S(11) lines are also clearly detected. I measured the intensities of the detected emission lines and compared line ratios of H recombination lines with theoretical predictions in the case of "on-the-spot" approximation (the so-called Case B). Then, measured ratios of $\text{Pf}\delta \lambda 3.297 \mu\text{m}$ to $\text{Br}\alpha$ (~ 0.8 to 2.2 varying within the SNR) turned out to be much higher than that for Case B (~ 0.10 for $n_e \sim 10^2\text{-}10^7 \text{ cm}^{-3}$ and $T_e \sim 5\text{-}30 \times 10^3 \text{ K}$). At the beginning, I was embarrassed as I thought I had made a mistake during data processing, so I double-checked all procedures step-by-step but couldn't find any problems. Then, I began wondering what could cause such high ratios and eventually found that the $3.3 \mu\text{m}$ feature could largely originate from the well-known aromatic C-H stretching transition instead of the $\text{Pf}\delta$ line. In addition to these abnormal ratios, the intensities of the $3.3 \mu\text{m}$ feature do not vary with the $\text{Br}\alpha$ intensities, and the measured line widths of the feature are wider than other ionic/molecular lines. All these aspects support the fact that the $3.3 \mu\text{m}$ feature is indeed due to the PAH emission at $3.3 \mu\text{m}$. After careful inspection of the IRS spectra of N49 from the Spitzer archive, we could also detect other PAH features at 6.2 , 7.7 , and $11.3 \mu\text{m}$.

At that time, only one detection of PAH emission associated SNRs had been reported - the SNR N132D in the LMC with Spitzer (Tappe et al. 2006). In the case of N132D, a $15\text{-}20 \mu\text{m}$ emission hump is mainly detected, which is attributed to C-C-C banding modes of large PAHs (500-4000 carbon atoms). In this sense, the detection of the $3.3 \mu\text{m}$ PAH band feature from N49 was even more surprising because the $3.3 \mu\text{m}$ PAH emission is commonly attributed to small PAHs (<100 carbon atoms), and these can be preferentially destroyed by strong shocks. Other PAH band ratios ($I_{6.2}/I_{7.7}$ and $I_{3.3}/I_{11.3}$) also support the idea that small PAHs are dominant in N49. Thus, we needed an explanation as to how small PAHs can survive in N49. Despite of a lot of literature research, it was not easy to find proper answers about PAH processing in SNRs or shocks, probably due to the rare detection of the PAH emission in SNRs. Then one day, I looked on <https://arxiv.org/archive/astro-ph> and became very excited to find a paper entitled "Polycyclic aromatic hydrocarbon processing in interstellar shocks" by E. Micelotta et al. (yes, she is one of the members of this newsletter's editorial board). Hurrah!!! A few months later, another of their papers came out about polycyclic aromatic hydrocarbon processing in hot gas. Based on the two papers, we explained that PAHs would survive regardless of their size in a dense gas with a moderately low temperature (< 30,000 K) and concluded that for PAHs to exist and radiate in SNRs, both an ambient dense medium and a sufficient heating source around the medium are most likely required (Seok et al. 2012).

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Abstracts

Towards Completing the Cyclopropenylidene Cycle: Rovibrational Analysis of Cyclic N₃⁺, CNN, HCNN⁺, and CNC⁻

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The simple aromatic hydrocarbon, cyclopropenylidene (*c*-C₃H₂), is a known, naturally-occurring molecule. The question remains as to whether its isoelectronic, cyclic, fellow aromatics of *c*-N₃⁺, *c*-CNN, HCNN⁺, and *c*-CNC⁻ are as well. Each of these are exciting objects for observation of Titan, and the rotational constants and vibrational frequencies produced here will allow for remote sensing of Titan's atmosphere or other astrophysical or terrestrial sources. None of these four aromatic species are vibrationally strong absorbers/emitters, but the two ions, HCNN⁺ and *c*-CNC⁻, have dipole moments of greater than 3 D and 1 D, respectively, making them good targets for rotational spectroscopic observation. Each of these molecules is shown here to exhibit its own, unique vibrational properties, but the general trends put the vibrational behavior for corresponding fundamental modes within close ranges of one another, even producing nearly the same heavy atom, symmetric stretching frequencies for HCNN⁺ and *c*-C₃H₂ at 1600 cm⁻¹. The *c*-N₃⁺ cation is confirmed to be fairly unstable and has almost no intensity in its ν₂ fundamental. Hence, it will likely remain difficult to characterize experimentally.

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Physical Chemistry Chemical Physics, 19, 22860-2869 (2017)

<http://pubs.rsc.org/en/Content/ArticleLanding/2017/CP/C7CP04257D>

Low-lying, Rydberg states of polycyclic aromatic hydrocarbons (PAHs) and cyclic alkanes

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TD-DFT calculations of low-lying, Rydberg states of a series of polycyclic hydrocarbons and cyclic alkanes are presented. Systematic variations in binding energies and photoelectron angular distributions for the first members of the s, p and d Rydberg series are predicted for increasing molecular complexity. Calculated binding energies are found to be in very good agreement with literature values where they exist for comparison. Experimental angle-resolved photoelectron spectroscopy results are presented for coronene, again showing very good agreement with theoretical predictions of binding energies and also for photoelectron angular distributions. The Dyson orbitals for the small “hollow” carbon structures, cubane, adamantane and dodecahedrane, are shown to have close similarities to atomic s, p and d orbitals, similar to the superatom molecular orbitals (SAMOs) reported for fullerenes, indicating that these low-lying, diffuse states are not restricted to π -conjugated molecules.

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<http://pubs.rsc.org/en/Content/ArticleLanding/2017/CP/C7CP03913A#!divAbstract>

The 15273 Å diffuse interstellar band in the dark cloud Barnard 68

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High obscuration of background stars behind dark clouds precludes the detection of optical diffuse interstellar bands (DIBs) and hence our knowledge of DIB carriers in these environments. Taking advantage of the reduced obscuration of star-light in the near-infrared (NIR) we used one of the strongest NIR DIBs at 15273 Å to probe the presence and properties of its carrier throughout the nearby interstellar dark cloud Barnard 68. Equivalent widths (EW) have been measured for different ranges of visual extinction AV, using VLT-KMOS H-band (1.46-1.85 micron) moderate-resolution ($R = 4000$) spectra of 43 stars situated behind the cloud. To do so we fitted the data using synthetic stellar spectra from the APOGEE project and TAPAS synthetic telluric transmissions appropriate for the observing site and time period. The results show an increase of DIB EW with increasing AV. However, the rate of increase is much flatter than expected from the EW-AV quasi-proportionality established for this DIB in the Galactic diffuse interstellar medium. Based on a simplified inversion assuming sphericity, it is found that the volume density of the DIB carrier is 2.7 and 7.9 times lower than this expected average value in the external and central regions of the cloud which have $n(H) = 0.4$ and $3.5 \times 10^5 \text{ cm}^{-3}$, respectively. Further measurements with multiplex NIR spectrographs should allow detailed modeling of such an edge effect of this DIB and other bands and help to clarify its actual origin.

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<http://arxiv.org/abs/1709.00963>

Polyaromatic disordered carbon grains as carriers of the UV bump: Far-UV to mid-IR spectroscopy of laboratory analogs

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Context. A multiwavelength study of laboratory carbons with varying degrees of hydrogenation and sp² hybridization is required to characterize the structure of the carbonaceous carriers of interstellar and circumstellar extinction.

Aims. We study the spectral properties of carbonaceous dust analogs from the far-ultraviolet to the mid-infrared and correlate features in both spectral ranges to the aromatic/aliphatic degree.

Methods. Analogs to carbonaceous interstellar dust encountered in various phases of the interstellar medium have been prepared in the laboratory. These are amorphous hydrogenated carbons (a-C:H), analogs to the diffuse interstellar medium component, and soot particles, analogs to the polyaromatic component. Thin films ($d < 100$ nm) have been measured in transmission in the vacuum-ultraviolet (VUV; 120–210 nm) within the atmospheric pressure experiment (APEX) chamber of the DISCO beam line at the SOLEIL synchrotron radiation facility. Spectra of these films were further measured through the UV-Vis (210 nm–1 μm) and in the mid-infrared (3–15 μm).

Results. Tauc optical gaps, E_g , are derived from the visible spectra. The major spectral features are fitted through the VUV to the mid-infrared to obtain positions, full-widths at half maximum (FWHM), and integrated intensities. These are plotted against the position of the $\pi - \pi^*$ electronic transitions peak. Unidentified or overlapping features in the UV are identified by correlations with complementary infrared data. A correlation between the optical gap and position of the $\pi - \pi^*$ electronic transitions peak is found. The latter is also correlated to the position of the sp³ carbon defect band at ~8 μm, the aromatic C=C stretching mode position at ~6 μm, and the H/C ratio.

Conclusions. Ultraviolet and infrared spectroscopy of structurally diverse carbon samples are used to constrain the nanostructural properties of carbon carriers of both circumstellar and interstellar extinction, such as the associated coherent lengths and the size of polyaromatic units. Our study suggests that carriers of the interstellar UV bump should exhibit infrared bands akin to the A/B classes of the aromatic infrared bands, while the circumstellar bump carriers should exhibit bands corresponding to the B/C classes.

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On dust irradiation in planetary nebulae in the context of survivability of ices

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A large number of molecules are observed in planetary nebulae, including simple and, - the most common (H_2 , CO and OH), more complex (H_2O , SiO, HCN, HNC, HCO^+), and even the polycyclic aromatic hydrocarbons and fullerenes containing a few dozen and more atoms. Water molecules are observed, as a rule, in the young objects, in the gas phase (water "fountains" and related water masers) and solid phase (emission of crystalline ice particles). On the other hand, the results of calculations by the Cloudy computer program, given in this paper, show that the abundance of water ice in planetary nebulae, other conditions being equal, depends on the ionization rate of hydrogen, which depends in turn on the flux of energetic particles (protons and alpha particles) in the range of MeV energies and higher. Calculated water ice column densities reach values of up to 10^{19} - 10^{20} cm^{-2} at the usual average ISM H_2 ionisation rate of 10^{-16} s^{-1} and sharply decrease at rates that are a thousand times larger. The possibility of an increased flux of energetic particles in planetary nebulae under conditions of the standard interacting stellar winds scenario is discussed, and it is concluded that the flux may locally exceed by 1-3 orders of magnitude that of galactic cosmic rays. This may have important implications for the chemistry of complex compounds under conditions of planetary nebulae, in particular, for models of the origin of fullerenes.

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<http://www.sciencedirect.com/science/article/pii/S2405675816300549>

Size Effect in the Ionization Energy of PAH Clusters

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We report the first experimental measurement of the near-threshold photo-ionization spectra of polycyclic aromatic hydrocarbon clusters made of pyrene $C_{16}H_{10}$ and coronene $C_{24}H_{12}$, obtained using imaging photoelectron photoion coincidence spectrometry with a VUV synchrotron beamline. The experimental results of the ionization energy are confronted to calculated ones obtained from simulations using dedicated electronic structure treatment for large ionized molecular clusters. Experiment and theory consistently find a decrease of the ionization

energy with cluster size. The inclusion of temperature effects in the simulations leads to a lowering of this energy and to a quantitative agreement with the experiment. In the case of pyrene, both theory and experiment show a discontinuity in the IE trend for the hexamer. This work demonstrates the ability of the models to describe the electronic structure of PAH clusters and suggests that these species are ionized in astronomical environments where they are thought to be present.

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