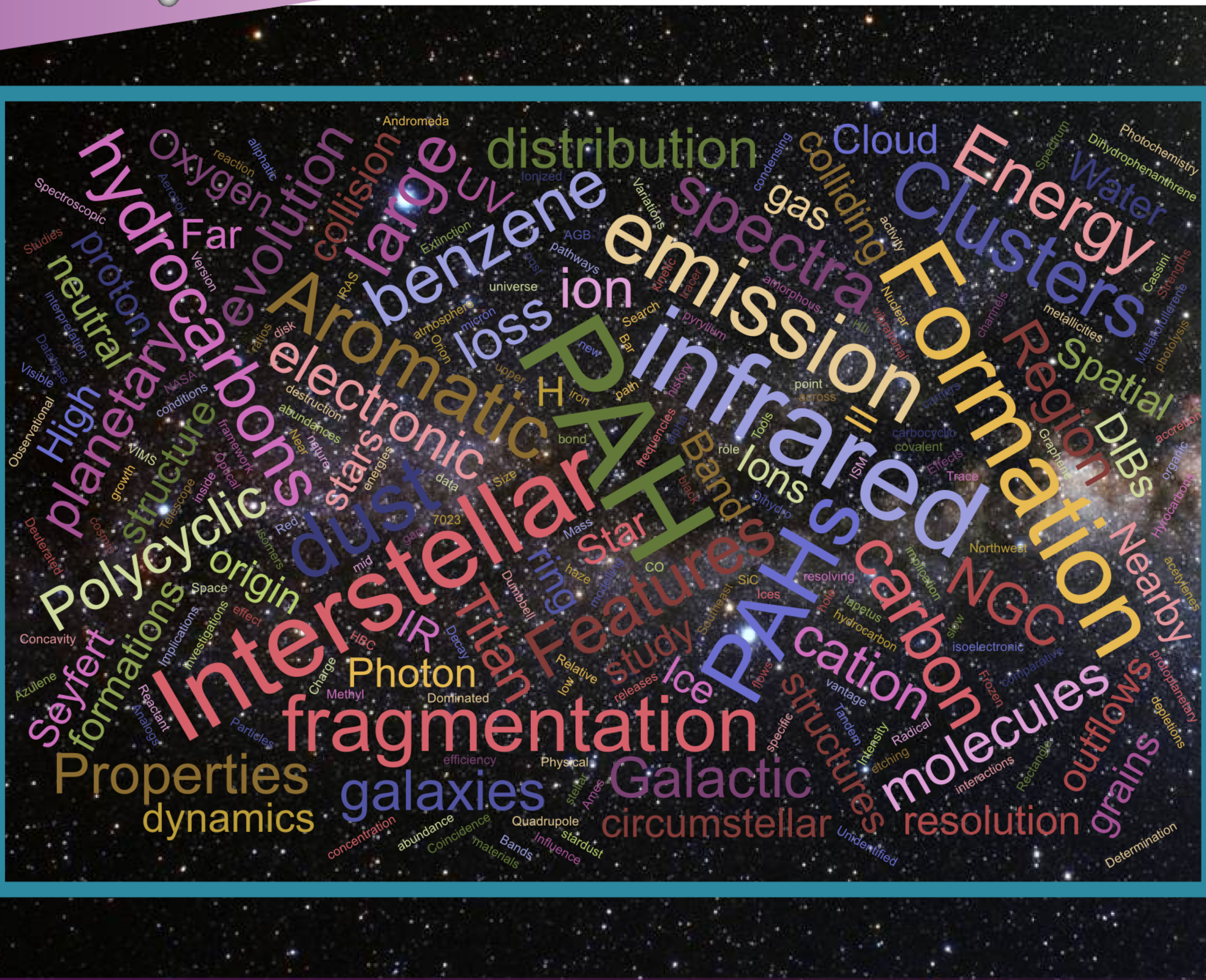
AstroPAH

A Newsletter on Astronomical PAHs

Issue 48 | May 2018



Editorial

Dear Colleagues,

May is the perfect month for spring cleaning. To start, a word cloud of previous AstroPAH newsletters is featured on the cover. Not surprisingly, PAH seems to be the most frequently used word, closely followed by Infrared and Interstellar. Also in light of this spring cleaning, we would like to take the opportunity to make an inventory and analyse the impact of our AstroPAH newsletter, in preparation for our upcoming 5th anniversary later this year.

In Focus this month is a survey to collect your input. Please take a look at the In Focus and give us your feedback via the Google form we have created. We promise you, we made an effort to keep the questions short and simple. It should thus only take you a few minutes. Thank you in advance, we greatly appreciate it.

The abstracts this month cover a variety of topics: news about benzene ice on Titan, nanodiamonds on a meteorite, the charge state of PAHs across different nebula types, silicate dust in stellar outflows, and a novel UV/visible spectrometer. Take a look to find out about the details.

Do you want to highlight your research, a facility or another topic, please contact us for a possible In Focus. Of course, do not forget to send us your abstracts! We also encourage you to send in your vacancies, conference announcements and more. For publication in the next AstroPAH, see the deadlines below.

The Editorial Team

Next issue: 21 June 2018.
Submission deadline: 8 June 2018.

Contact us:

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

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PAH Picture of the Month

AstroPAH word cloud.

Credits: Background Image - A. Fujii. Composition - A. Candian.

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

In Focus

AstroPAH Needs Your Feedback!

Please fill out the survey to let us know how we can improve the AstroPAH newsletter.

Dear subscribers,

Do you know that AstroPAH will turn 5 in October this year?

The main goal of AstroPAH is to bridge the gap in communication between scientists working on different aspects of the PAH model (experimental, theorerical, astronomical observation) and promote further development in the field.

In preparation for our 5^{th} anniversary celebration, we would like to get some feedback from you, our readers and contributors.

Please take a moment to answer a few questions to let us know what you would like to see in future volumes of the newsletter and what you think could be improved. Your feedback will help us improve the different sections of the AstroPAH newsletter and how it serves our community.

We have created a Google form to make it simple and fast. If you could please take this survey before June 25 that would be great! Follow the link below:

Click here to answer the survey.

Thank you!

Isabel, Alessandra, Elisabetta, Annemieke, Ella, Amanda, and Xander

Here are the questions you will find in the survey:

- Ten AstroPAH newsletters are published every year. How many of them do you typically read?

- How useful is AstroPAH for your work?

- How has AstroPAH helped you so far?

- On a scale of 1 to 5 (5 being the highest grade), how much do you like the different sections of AstroPAH?

- Out of these five AstroPAH sections, which do you think could use some improvement, and in what form?

- Are you aware that you can send contributions to any of the AstroPAH sections (Abstracts, Picture of the Month, In Focus, Announcements, Meetings)?

- Please rate the contribution submission methods made available on the AstroPAH website (http://astropah-news.strw.leidenuniv.nl/submit.html)

- Do you have any suggestions for improving the contribution submission methods?

- Which type of In Focus are you most interested in?

- Do you have any suggestions for the In Focus section (research topics we have not yet presented, new types of in Focus,...)?

- What is your current occupation?

- What is(are) your main research topic(s)?

- What methods do you use?

- Do you have any other suggestions, criticisms, comments?

Abstracts

Study of Titan's fall southern stratospheric polar cloud composition with Cassini/CIRS: detection of benzene ice

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We report the detection of a spectral signature observed at 682 cm^{-1} by the Cassini Composite Infrared Spectrometer (CIRS) in nadir and limb geometry observations of Titan's southern stratospheric polar region in the middle of southern fall, while stratospheric temperatures are the coldest since the beginning of the Cassini mission. In the same period, many gases observed in CIRS spectra (C_2H_2, HCN, C_4H_2, C_3H_4, HC_3N and C_6H_6) are highly enriched in the stratosphere at high southern latitude due to the air subsidence of the global atmospheric circulation and some of these molecules condense at much higher altitude than usually observed for other latitudes. The 682 cm^{-1} signature, which is only observed below an altitude of 300-km, is at least partly attributed to the benzene (C_6H_6) ice ν_4 C-H bending mode. While we first observed it in CIRS nadir spectra of the southern polar region in early 2013, we focus here on the study of nadir data acquired in May 2013, which have a more favorable observation geometry. We derived the C_6H_6 ice mass mixing ratio in 5° latitude bins from the south pole to 65°S and infer the C_6H_6 cloud top altitude to be located deeper with increasing distance from the pole. We additionally analyzed limb data acquired in March 2015, which were the first limb dataset available after the May 2013 nadir observation, in order to infer a vertical profile of its mass mixing ratio in the 0.1 – 1 mbar region (250 – 170 km). We derive an upper limit of $\sim$1.5 µm for the equivalent radius of pure C_6H_6 ice particles from the shape of the observed emission band, which is consistent with our estimation of the ice particle size from condensation growth and sedimentation timescales. We compared the ice mass mixing ratio with the haze mass mixing

ratio inferred in the same region from the continuum emission of CIRS spectra, and derived that the haze mass mixing ratios are $\sim$30 times larger than the C_6H_6 ice mass mixing ratios for all observations. Several other unidentified signatures are observed near 687 and 702 cm^{-1} and possibly 695 cm^{-1}, which could also be due to ice spectral signatures as they are observed in the deep stratosphere at pressure levels similar to the C_6H_6 ice ones. We could not reproduce these signatures with pure nitrile ices (HCN, HC_3N,CH_3CN, C_2H_5CN and C_2N_2) spectra available in the literature except the 695 cm^{-1} feature that could possibly be due to C_2H_3CN ice. From this tentative detection, we derive the corresponding C_2H_3CN ice mass mixing ratio profile and also inferred an upper limit of its gas volume mixing ratio of 2×10^{-7} at 0.01 mbar at 79°S in March 2015.

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https://arxiv.org/abs/1805.01414

Infrared Spectroscopy of Carbonaceous-chondrite Inclusions in the Kapoeta Meteorite: Discovery of Nanodiamonds with New Spectral Features and Astrophysical Implications

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We report the finding of nanodiamonds, coexisting with amorphous carbon, in carbonaceous-chondrite (CC) material from the Kapoeta achondritic meteorite by Fourier-transform infrared (FTIR) spectroscopy and micro-Raman spectroscopy. In the CH stretching region (3100-2600 cm^{-1}), the FTIR spectrum of the Kapoeta CC material (KBr pellet) shows bands attributable to aliphatic CH_2 and CH_3 groups, and is very similar to IR spectra of organic matter in carbonaceous chondrites and the diffuse interstellar medium. Nanodiamonds, as evidenced by micro-Raman spectroscopy, were found in a dark region ($\sim$400 µm in size) in the KBr pellet. Micro-FTIR spectra collected from this region are dramatically different from the KBr-pellet spectrum, and their C-H stretching region is dominated by a strong and broad absorption band centered at $\sim$2886 cm^{-1} (3.47 µm), very similar to that observed in IR absorption spectra of hydrocarbon dust in dense interstellar clouds. Micro-FTIR spectroscopy also indicates the presence of an aldehyde and a nitrile, and both of the molecules are ubiquitous in dense interstellar clouds. In addition, IR peaks in the 1500-800 cm^{-1} region are also observed, which may be attributed to different levels of nitrogen aggregation in diamonds. This is the first evidence for the presence of the 3.47 µm interstellar IR band in meteorites. Our results further support the assignment of this band to tertiary CH groups on the surfaces of nanodiamonds. The presence of the above interstellar bands and the absence of shock features in the Kapoeta nanodiamonds, as indi-

cated by Raman spectroscopy, suggest formation by a nebular-condensation process similar to chemical-vapor deposition.

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A fibre-coupled UHV-compatible variable angle reflection-absorption UV/visible spectrometer

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We present a novel UV/visible reflection-absorption spectrometer for determining the refractive index, n, and thicknesses, d, of ice films. Knowledge of the refractive index of these films is of particular relevance to the astrochemical community, where they can be used to model radiative transfer and spectra of various regions of space. In order to make these models more accurate, values of n need to be recorded under astronomically relevant conditions, that is, under ultra-high vacuum (UHV) and cryogenic cooling. Several design considerations were taken into account to allow UHV compatibility combined with the ease of use. The key design feature is a stainless steel rhombus coupled to an external linear drive (z-shift) allowing a variable reflection geometry to be achieved, which is necessary for our analysis. Test data for amorphous benzene ice are presented as a proof of concept, the film thickness, d, was found to vary linearly with surface exposure, and a value for n of 1.43 $\pm$ 0.07 was determined.

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The Charge State of Polycyclic Aromatic Hydrocarbons across a Reflection Nebula, an H II Region, and a Planetary Nebula

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Low-resolution Spitzer-IRS spectral map data of a reflection nebula (NGC 7023), H II region (M17), and planetary nebula (NGC 40), totaling 1417 spectra, are analyzed using the data and tools available through the NASA Ames PAH IR Spectroscopic Database. The polycyclic aromatic hydrocarbon (PAH) emission is broken down into PAH charge and size subclass contributions using a database-fitting approach. The resulting charge breakdown results are combined

with those derived using the traditional PAH band strength ratio approach, which interprets particular PAH band strength ratios as proxies for PAH charge. Here the 6.2/11.2 µm PAH band strength ratio is successfully calibrated against its database equivalent: the $n_{\mathrm{PAH}^+}/n_{\mathrm{PAH}^0}$ ratio. In turn, this ratio is converted into the PAH ionization parameter, which relates it to the strength of the radiation field, gas temperature, and electron density. Population diagrams are used to derive the H_2 density and temperature. The bifurcated plot of the 8.6 versus 11.2 µm PAH band strength for the northwest photo dissociation region in NGC 7023 is shown to be a robust diagnostic template for the $n_{\mathrm{PAH}^+}/n_{\mathrm{PAH}^0}$ ratio in all three objects. Template spectra for the PAH charge and size subclasses are determined for each object and shown to favorably compare. Using the determined template spectra from NGC 7023 to fit the emission in all three objects yields, upon inspection of the Structure SIMilarity maps, satisfactory results. The choice of extinction curve proves to be critical. Concluding, the distinctly different astronomical environments of a reflection nebula, H II region, and planetary nebula are reflected in their PAH emission spectra.

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http://iopscience.iop.org/article/10.3847/1538-4357/aabcbe

The formation of astrophysical Mg-rich silicate dust

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We present new results for ground-state candidate energies of Mg-rich olivine (MRO) clusters and use the binding energies of these clusters to determine their nucleation rates in stellar outflows, with particular interest in the environments of core-collapse supernovae (CCSNe). Low-lying structures of clusters $(Mg_2SiO_4)_n$ $2 \leq n \leq 13$ are determined from a modified minima hopping algorithm using an empirical silicate potential in the Buckingham form. These configurations are further refined and optimized using the density functional theory code Quantum Espresso. Utilizing atomistic nucleation theory, we determine the critical size and nucleation rates of these clusters. We find that configurations and binding energies in this regime are very dissimilar from those of the bulk lattice. Clusters grow with SiO_4-MgO layering and exhibit only global, rather than local, symmetries. When compared to classical nucleation theory we find suppressed nucleation rates at most temperatures and pressures, with enhanced nucleation rates at very large pressures. This implies a slower progression of silicate dust formation in stellar environments than previously assumed.

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https://www.sciencedirect.com/science/article/pii/S2405675817300283#

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