AstroPAH

A Newsletter on Astronomical PAHs

Issue 67 • April 2020

Hubble's 30th Anniversary

Editorial

Dear Colleagues,

This is the 67th volume of the AstroPAH newsletter.

In addition to the Abstract and the EAS Virtual Meeting announcement in this newsletter, we also suggest our readers to check the Spitzer Retrospective prepared by Nature Astronomy. You can find it clicking here.

Due to the COVID-19 pandemic, we are not publishing the In Focus section.

Stay safe!

The Editorial Team

Next issue (aprox.): 21 May 2020.
Submission deadline: 8 May 2020.

Contact us:

astropah@strw.leidenuniv.nl

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

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PAH Picture of the Month

This image was taken with the NASA/ESA Hubble Space Telescope to celebrate its 30-year anniversary. The image features the nebulae NGC 2014 and NGC 2020, part of a star-forming region in the Large Magellanic Cloud. Happy birthday, Hubble!

Credits: NASA, ESA, and STScI

Abstracts

Hydrogenation and dehydrogenation reactions of the phenalenyl radical/1H-phenalene system at low temperatures

Anita Scheneiker[1], **István Pál Csonka**[1], **György Tarczay**[1]

[1]MTA-ELTE Lendület Laborytory Astrochemistry Research Group, Eötvös University, Budapest, Hungary

Phenalenyl radical was generated in situ in inert matrices by laser UV photolysis of 1H-phenalene, and was identified by recording laser induced fluorescence and IR spectra. Theoretical computations predict that the H atom addition to phenalenyl radical is barrierless, while the H atom abstraction from 1H-phenalene has only a small barrier. Upon annealing the Xe matrix after the photolysis, the radical and the H atom recombine, while H atom abstraction from 1H-phenalene is a possible explanation for additional spectral changes. These results show that the phenalenyl radical/1H-phenalene system can be a very effective catalyst in the formation of interstellar H2.

E-mail: tarczay@caesar.elte.hu

Chemical Physics Letters
https://www.sciencedirect.com/science/article/pii/S0009261420300981

Do defects in PAHs promote catalytic activity in space? Stone–Wales pyrene as a test case

Dario Campisi[1] **and Alessandra Candian**[1,2]

[1] Leiden Observatory, Leiden University, Niels Bohrweg 2, 2333 CA Leiden, The Netherlands

[2] van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands

Using density functional theory (DFT), we studied the formation of Stone–Wales defects in pyrene, as a prototype PAH molecule. In addition, we studied the reactivity of the defective and pristine pyrenes toward hydrogenation, a process that can occur in some regions of the interstellar medium. We found that the formation of the defect requires overcoming energies of the order of 8.4 eV, but the defective structure is stable due to the high reverse reaction barrier (approx. 6 eV). We also found that the presence of the defect decreases the sticking barrier for the first hydrogenation and promotes more stable singly and doubly hydrogenated intermediates with respect to that of the pristine pyrene. Finally, our results show that both Stone–Wales pyrene and pristine pyrenes can lead to the formation of H2 through an extraction mechanism involving H atoms attached on distal carbon atoms with energy barriers below 2 eV.

E-mails: campisi@strw.leidenuniv.nl, a.candian@uva.nl

Physical Chemistry Chemical Physics (PCCP)
https://pubs.rsc.org/en/content/articlelanding/2020/cp/c9cp06523g#!divAbstract
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Spitzer's perspective of polycyclic aromatic hydrocarbons in galaxies

Aigen Li[1]

[1] Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211, USA

Polycyclic aromatic hydrocarbon (PAH) molecules, as revealed by the distinctive set of emission bands at 3.3, 6.2, 7.7, 8.6, 11.3 and 12.7 μm characteristic of their vibrational modes, are abundant and widespread throughout the Universe. They are ubiquitously seen in a wide variety of astrophysical regions, ranging from planet-forming disks around young stars to the interstellar medium (ISM) of the Milky Way and external galaxies out to high redshifts at $z \gtrsim 4$. PAHs profoundly influence the thermal budget and chemistry of the ISM by dominating the photoelectric heating of the gas and controlling the ionization balance. Here, I review the current state of knowledge of the astrophysics of PAHs, focusing on their observational characteristics obtained from the *Spitzer Space Telescope* and their diagnostic power for probing the local physical and chemical conditions and processes. Special attention is paid to the spectral properties of PAHs and their variations revealed by the *Infrared Spectrograph* (IRS) on board *Spitzer* across a much broader range of extragalactic environments (e.g., distant galaxies, early-type galaxies, galactic halos, active galactic nuclei, and low-metallicity galaxies) than was previously possible with the *Infrared Space Observatory* (ISO) or any other telescope facilities. Also highlighted is the relation between the PAH abundance and the galaxy metallicity established for the first time by *Spitzer*.

E-mail: lia@missouri.edu

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http://www.nature.com/articles/s41550-020-1051-1
http://arxiv.org/abs/2003.10489

DFT study on interstellar PAH molecules with aliphatic side groups

Mridusmita Buragohain[1], Amit Pathak[2] and Itsuki Sakon[1], Takashi Onaka[3,1]

[1] Department of Astronomy, Graduate School of Science, The University of Tokyo, Tokyo 113-0033, Japan

[2] Department of Physics, Banaras Hindu University, Varanasi 221 005, India

[3] Department of Physics, Faculty of Science and Engineering, Meisei University, Tokyo 191-8506, Japan

Polycyclic Aromatic Hydrocarbon (PAH) molecules have been long adjudged to contribute to the frequently detected distinct emission features at 3.3, 6.2, 7.7, 8.6, 11.2 and 12.7 μm with weaker and blended features distributed in the 3−20 μm region. The comparatively weaker 3.4 μm emission feature has been attributed to have an aliphatic origin as carrier. PAH with aliphatic functional group attached to it is one of the proposed potential candidate carriers for the 3.4 μm emission band, however, the assignment of carrier is still enigmatic. In this work, we employ Density Functional Theory (DFT) calculation on a symmetric and compact PAH molecule; coronene ($C_{24}H_{12}$) with aliphatic side group to investigate any spectral similarities with observed features at 3−4 μm. The side groups considered in this study are −H (hydrogenated), $-CH_3$ (methyl), $-CH_2-CH_3$ (ethyl) and $-CH{=}CH_2$ (vinyl) functional groups. Considering the possible presence of deuterium (D) in PAHs, we also include D in the aliphatic side group to study the spectral behavior. We present a detailed analysis of the IR spectra of these molecules and discuss possible astrophysical implications.

E-mail: mridusmita@astron.s.u-tokyo.ac.jp, amitpah@gmail.com

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C_{60}^+ as a diffuse interstellar band carrier; a spectroscopic story in 6 acts

H. Linnartz[1], J.Cami[2,3,4], M.Cordiner[5,6], N.L.J.Cox[7], P.Ehrenfreund[8,9], B.Foing[10], M.Gatchell[11,12], P.Scheier[11]

[1]Laboratory for Astrophysics, Leiden Observatory, Leiden University, PO Box 9513, NL2300 RA Leiden, the Netherlands

[2]Department of Physics and Astronomy and Centre for Planetary Science and Exploration (CPSX), The University of Western Ontario, London, ON N6A 3K7, Canada

[3]Institute for Earth and Space Exploration, The University of Western Ontario, London, ON N6A 3K7, Canada

[4]SETI Institute, 189 Bernardo Avenue, Suite 100, Mountain View, CA 94043, USA

[5]NASA Goddard Space Flight Center, 8800 Greenbelt Road, Greenbelt, MD 20771, USA

[6]Department of Physics, Catholic University of America, Washington, DC 20064, USA

[7]ACRI-ST, 260 route du Mon Pintard, Sophia Antipolis, France

[8]Leiden Observatory, Leiden University, PO Box 9513, NL2300 RA Leiden, the Netherlands

[9]George Washington University, Washington, DC, USA

[1]0ESA ESTEC SCI-S, Noordwijk, the Netherlands

[1]1Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Technikerstrasse 25, Innsbruck A-6020, Austria

[1]2Department of Physics, Stockholm University, 106 91 Stockholm, Sweden

In 2019 it was exactly 100 years ago that the first two DIBs, diffuse interstellar bands, were discovered by Mary Lea Heger. Today some 500 + DIBs are known. In numerous observational, modelling and laboratory studies, efforts have been made to identify the carriers of these absorption features that are observed in the light of reddened stars crossing diffuse and translucent clouds. Despite several claims over the years that specific DIBs could be assigned to specific species, not one of these withstood dedicated follow-up studies. An exception is C_{60}^+. In 2015, Campbell et al. showed that two strong bands, recorded in the laboratory around 960 nm, coincided precisely with known DIBs and in follow-up studies three more matches between transitions and new observational DIB studies were claimed. Over the last four years the evidence for C_{60}^+ as the first identified DIB carrier – including new laboratory data and Hubble Space Telescope observations – has been accumulating, but not all open issues have been solved yet. This article summarizes 6 spectroscopic achievements that sequentially contributed to what seems to become the first DIB story with a happy end.

E-mail: linnartz@strw.leidenuniv.nl

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EAS 2020 VIRTUAL Meeting: Abstract Submission Reopened

Leiden, The Netherlands
29 June -3 July 2020

Due to the COVID-19 pandemic, the European Astronomical Society (EAS) 2020 meeting will move to a virtual meeting with attendance fees of **80 EUR** (**50 EUR** for one-day attendance).

The Abstract Portal has been re-opened to collect new submissions both for Virtual Talk Contribution and e-posters, with deadline **May 3rd** and notification of acceptance by **Mid May.**

With this, we would like to invite submissions for our Special Session 11 **"The Molecular Journey: from stars to disks"**

AIM & SCOPE
In this special session we will focus on the study of molecules and their isotopologues and what they can teach us about the journey of molecules in our Galaxy. The scope is to bring the community together to showcase molecular insights in the evolution of matter from old stars to the ISM and into newly formed planets, to highlight recent advances in molecular astrophysics, to design strategies to best exploit the new astronomical facilities, and to provide fertile ground for future, interdisciplinary collaborations.

TOPICS
Molecules & Stellar Ejecta
The molecular ISM & Star Formation
Molecules & Protoplanetary Disks (and exoplanets)

Limited financial support may be available for early career researchers (PhD students and postdocs). For information and/or question: a.candian@uva.nl

On behalf of the SOC
Alessandra Candian (UvA)
Annemieke Petrignani (UvA)
Marie Van de Sande (KULeuven)
Serena Viti (UCL/Leiden)
Tom Millar (QUB)
Francesco Fontani (INAF)

E-mail for contact: a.candian@uva.nl

Webpage: https://eas.unige.ch/EAS2020/session.jsp?id=SS11

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