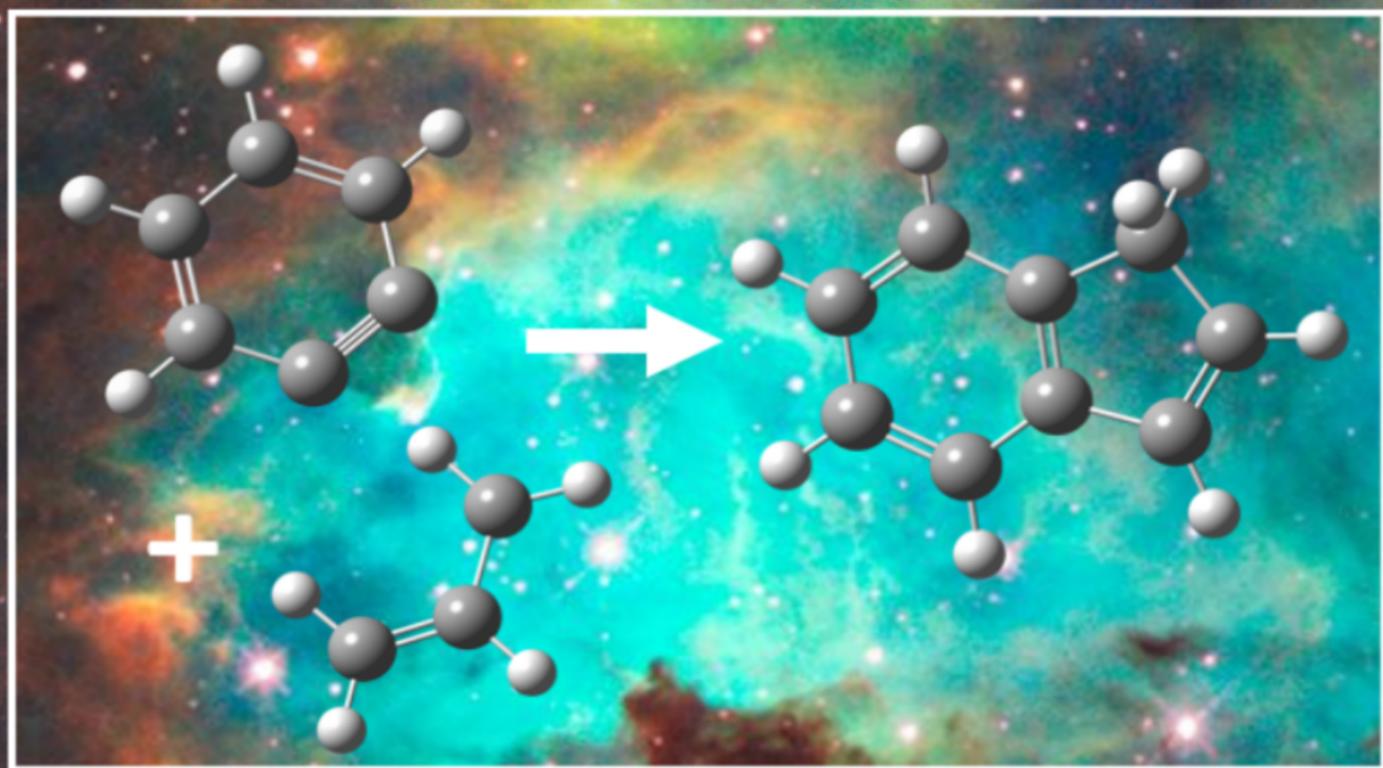


AstropAH

A Newsletter on Astronomical PAHs

Issue 69 • June 2020



**Indene formation from
o-benzyne and allyl**



Editorial

Dear Colleagues,

Welcome to the 69th AstroPAH volume. We hope you are all doing well and staying healthy.

This month, we share with you five Astro-PAH-related recent publications covering studies from the rotational spectroscopy of acenaphthene, to atomic and diatomic carbon-based gas/solid phase chemistry, to the interaction of amorphous solid water with PAHs.

We would also like to draw your attention to a postdoctoral opening on the study of PAHs, fullerenes and soot spectroscopy in Thomas Pino's ISMO group at the University of Paris-Saclay, France. The expected start date is this coming September, and more information is provided in our Announcements section.

We hope you enjoy reading our newsletter, and we thank you for your dedication and interest in AstroPAH! In the meantime, please continue sending us your contributions, and if you wish to contact us, feel free to use our [email](#).

Please be safe and stay healthy.

Enjoy reading our newsletter!

The Editorial Team

**Next issue: 23 July 2020.
Submission deadline: 10 July 2020.**

AstroPAH Newsletter

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PAH Picture of the Month

McCabe et al. (2020) report on a combined experimental and theoretical study of the reaction allyl + *o*-benzyne forming indene. See more about the work in the Abstract section.

Credits: McCabe et al. (2020). Background image by NASA, ESA and M. Livio (STScI).



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Abstracts

Reconnaissance of the uncharted low energy vibrational motions of acenaphthene

^{1,2,3}Sébastien Gruet, ^{1,2,3}Amanda L. Steber, ^{1,2}Melanie Schnell

¹Deutsches Elektronen Synchrotron, Notkestraße 85, D-22607 Hamburg, Germany

²Institut für Physikalische Chemie, Christian-Albrechts-Universität zu Kiel, Max-Eyth-Straße 1, D-24118 Kiel, Germany

³The Hamburg Centre for Ultrafast Imaging at the Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg, Germany

The room-temperature, millimeter-wave rotational spectrum of the small polycyclic aromatic hydrocarbon acenaphthene has been measured between 75 - 110 GHz. Accurate rotational and distortion parameters are presented due to the over 1400 transitions that have been included into a global fit. Besides observing transitions of the ground vibrational state, six vibrationally excited states have been identified: four fundamental modes (ν_{30} , ν_{41} , ν_{40} , ν_{29}), one overtone ($2\nu_{30}$), and one combination band ($\nu_{41}+\nu_{30}$). This is the first report of four of these excited states observed in the gas phase as two of the fundamental modes are IR inactive and the intensities of the overtone and combination bands are generally too weak to be observed. These excited states reside less than 300 cm^{-1} above the ground state, and an experimental approximation of their band centers is presented. The rotational constants and line lists can be used to facilitate the search for this polycyclic aromatic hydrocarbon in the interstellar medium.

E-mail: amanda.steber@desy.de and melanie.schnell@desy.de

Journal of Molecular Spectroscopy 371, 111296 (2020)

<https://www.sciencedirect.com/science/article/abs/pii/S0022285220300643>

<https://doi.org/10.1016/j.jms.2020.111296>

Selective identification of cyclopentaring-fused PAHs and side-substituted PAHs in a low pressure premixed sooting flame by photoelectron photoion coincidence spectroscopy

¹X. Mercier, ¹A. Faccinetto, ¹S. Batut, ¹G. Vanhove, ^{2,3}D. K. Bozanic, ^{2,4}H. R. Hróðmarsson, ²G. A. Garcia, ²L. Nahon

¹Université Lille, CNRS, UMR 8522 - PC2A - Physicochimie des Processus de Combustion et de l'Atmosphère, F-59000 Lille, France

²Synchrotron SOLEIL, L'Orme des Merisiers, St. Aubin, BP 48, 91192 Gif sur Yvette, France

³Current institutional address: Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

⁴Current institutional address: Laboratory for Astrophysics, Leiden Observatory, Leiden University, PO Box 9513, NL-2300 RA Leiden, The Netherlands

This work reports on the selective on line identification of polycyclic aromatic hydrocarbons (PAHs) formed in a low-pressure methane sooting flame, carried out using the double imaging Photoelectron Photoion Coincidence Spectroscopy method (*i*²PEPICO) on the DESIRS VUV beamline at the synchrotron SOLEIL. Generally, this work demonstrates the capabilities of the *i*²PEPICO method to identify PAHs in sooting flames, and in particular to distinguish cyclopentaring fused PAHs (CP-PAHs) and side-substituted PAHs from their benzenoid isomers. Experimental threshold photoelectron spectra of four CP-PAHs: acenaphthylene (C₁₂H₈, 152 *m/z*), acenaphthene (C₁₂H₁₀, 154 *m/z*), fluoranthene (C₁₆H₁₀, 202 *m/z*) and benzo(ghi)fluoranthene (C₁₈H₁₀, 226 *m/z*) are also reported for the first time.

E-mail: hrodmarsson@strw-leidenuniv.nl

Accepted in Physical Chemistry Chemical Physics

The chemistry of cosmic dust analogues from C, C₂ and C₂H₂ in C-rich circumstellar envelopes

Gonzalo Santoro¹, Lidia Martínez¹, Koen Lauwaet², Mario Accolla¹, Guillermo Tajuelo-Castilla¹, Pablo Merino^{1,3}, Jesús M. Sobrado⁴, Ramón J. Peláez⁵, Víctor J. Herrero⁵, Isabel Tanarro⁵, Álvaro Mayoral⁶, Marcelino Agúndez³, Hassan Sabbah⁷, Christine Joblin⁷, José Cernicharo³ and José Ángel Martín-Gago¹

¹ Instituto de Ciencia de Materiales de Madrid (ICMM. CSIC). Materials Science Factory. Structure of Nanoscopic Systems Group. c/ Sor Juana Inés de la Cruz 3, 28049 Cantoblanco, Madrid, Spain.

² IMDEA Nanociencia. Ciudad Universitaria de Cantoblanco, 28049 Cantoblanco, Madrid, Spain.

³ Instituto de Física Fundamental (IFF. CSIC). Group of Molecular Astrophysics. c/ Serrano 123, 28006 Madrid, Spain.

⁴ Centro de Astrobiología (CAB. INTA-CSIC). Crta- de Torrejón a Ajalvir km4, 28850, Torrejón de Ardoz, Madrid, Spain.

⁵ Instituto de Estructura de la Materia (IEM.CSIC). Molecular Physics Department. c/ Serrano 123, 28006 Madrid, Spain.

⁶ School of Physical Science and Technology, ShanghaiTech University, 393 Middle Huaxia Road, Pudong, Shanghai, 201210, People's Republic of China.

⁷ IRAP, Université de Toulouse, CNRS, CNES. 9 Av. du Colonel Roche, 31028 Toulouse Cedex 4, France.

Interstellar carbonaceous dust is mainly formed in the innermost regions of circumstellar envelopes around carbon-rich asymptotic giant branch stars (AGBs). In these highly chemically stratified regions, atomic and diatomic carbon, along with acetylene, are the most abundant species after H₂ and CO. In a previous study, we addressed the chemistry of carbon (C and C₂) with H₂ showing that acetylene and aliphatic species form efficiently in the dust formation region of carbon-rich AGBs whereas aromatics do not. Still, acetylene is known to be a key ingredient in the formation of linear polyacetylenic chains, benzene, and polycyclic aromatic hydrocarbons (PAHs), as shown by previous experiments. However, these experiments have not considered the chemistry of carbon (C and C₂) with C₂H₂. In this work, by employing a sufficient amount of acetylene, we investigate its gas-phase interaction with atomic and diatomic carbon. We show that the chemistry involved produces linear polyacetylenic chains, benzene, and other PAHs, which are observed with high abundances in the early evolutionary phase of planetary nebulae. More importantly, we have found a non negligible amount of pure and hydrogenated carbon clusters as well as aromatics with aliphatic substitutions, both being a direct consequence of the addition of atomic carbon. The incorporation of alkyl substituents into aromatics can be rationalized by a mechanism involving hydrogen abstraction followed by methyl addition. All the species detected in the gas phase are incorporated into nanometric-sized dust analogs, which consist of a complex mixture of sp, sp², and sp³ hydrocarbons with amorphous morphology.

E-mail: gonzalo.santoro@icmm.csic.es; gago@icmm.csic.es

The Astrophysical Journal 895, 97 (2020)

<https://doi.org/10.3847/1538-4357/ab9086>

Off the beaten path: Almost clean formation of indene from the *ortho*-benzyne + allyl reaction

Morgan N. McCabe¹, Patrick Hemberger², Engelbert Reusch³, Andras Bodi², and Jordy Bouwman¹

¹ Laboratory for Astrophysics, Leiden Observatory, Leiden University, PO Box 9513, 2300 RA Leiden, The Netherlands

² Laboratory for Synchrotron Radiation and Femtochemistry, Paul Scherrer Institute, 5232 Villigen, Switzerland

³ Institute of Physical and Theoretical Chemistry, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany

Polycyclic aromatic hydrocarbons (PAHs) play an important role in chemistry both in the terrestrial setting and in the interstellar medium. Various, albeit often inefficient, chemical mechanisms have been proposed to explain PAH formation, but few yield polycyclic hydrocarbons cleanly. Alternative and quite promising pathways have been suggested to address these shortcomings with key starting reactants including resonance stabilized radicals (RSRs) and *o*-benzyne, a biradical. Here we report on a combined experimental and theoretical study of the reaction allyl + *o*-benzyne. Indene was found to be the primary product and statistical modeling predicts only 0.1% phenylallene and 0.1% 3-phenyl-1-propyne as side products. The quantitative and likely barrierless formation of indene yields important insights into the role resonance stabilized radicals play in the formation of polycyclic hydrocarbons.

E-mail: bouwman@strw.leidenuniv.nl

J. Phys. Chem. Lett. 11, 2859 (2020)

<https://pubs.acs.org/doi/abs/10.1021/acs.jpcllett.0c00374>

Perturbation of the surface of Amorphous Solid Water by the adsorption of Polycyclic Aromatic Hydrocarbons

Eric Michoulier^{1,2}, Céline Toubin¹, Aude Simon², Joëlle Mascetti³, Christian Aupetit³, and Jennifer A. Noble⁴

¹ Laboratoire de Physique des Lasers, Atomes et Molécules, Université de Lille, Cité Scientifique, Villeneuve d'Ascq, France

² Laboratoire de Chimie et Physique Quantiques, Université Paul Sabatier, Toulouse, France

³ Institut des Sciences Moléculaires, Université de Bordeaux, Talence, France

⁴ Aix-Marseille Université, PIIM, Centre St-Jérôme, Marseille, France

This joint theoretical and experimental study establishes that the adsorption of polycyclic aromatic hydrocarbons (PAHs) onto the amorphous ice surface provokes a broadening and redshift of the "dangling"OH (dOH) ice spectral feature, the redshift increasing with PAH size up to 85 cm^{-1} . It also reveals that, in certain interaction configurations, adsorption induces substantial reorganisation of the hydrogen-bonding network at the ice surface. Comparison with experiments validates the novel theoretical methodology relying on the density functional based tight binding approach, which offers a compromise between system size and accuracy enabling a wide sampling of surface structures. Applied in an astrophysical context, this study suggests that widening of the dOH feature by adsorption of aromatic molecules could explain its absence heretofore in observational ice spectra, offering hope that future missions with higher sensitivity will verify its presence or absence in dense regions.

E-mail: jennifer.noble@univ-amu.fr

Journal of Physical Chemistry C 2020, 124, pp. 2994-3001.

<https://pubs.acs.org/10.1021/acs.jpcc.9b09499> <https://hal.archives-ouvertes.fr/hal-02447448>



Announcements

Postdoctoral position on the study of PAHs, fullerenes and soot nuclei spectroscopy, astrophysical applications (H/F)

**Communicated by Thomas Pino
(Université Paris-Saclay)**

Dear all,

A post-doctoral position for the study of spectroscopy of PAHs, fullerenes and soot nuclei and astrophysical applications is open for recruitment with Thomas Pino in the SYSTEMAE research team at ISMO. To access information and apply, please follow the link:

<https://bit.ly/2Yq1ZDe> (French and English)

Best regards,
Thomas Pino.

AstroPAH Newsletter

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

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