




AstropAH

A Newsletter on Astronomical PAHs

Issue 97 • April 2023



The Hubble 12 Planetary Nebula



Editorial

Dear Colleagues,

Welcome to our new AstroPAH volume no. 96! We hope all of you are healthy and doing well! We thank you all for your contributions to AstroPAH, in particular the abstracts covering C₆₀ spectroscopy, C₄₀ synthesis, and dissociation chemistry of pyridine and benzonitrile.

The amazingly symmetric planetary nebula Hubble 12 illustrates our cover this month. Such kind of objects contributes significantly to the galactic carbon budget.

Our In Focus entitled *Highlighting AstroPAH research at DESIREE* was kindly prepared by Mark Stockett, Michael Gatchell, and Henning Zettergen and covers the Double ElectroStatic Ion Ring ExpERiment facility at Stockholm University.

We draw your attention to two important announcements. First, the Astrochemistry Subdivision of the American Chemical Society (ACS) will have a symposium at the ACS Fall 2023 meeting which will be held in San Francisco, August 13–17. Second, Prof. Otto Dopfer is proposing a Postdoc position and a PhD position in Molecular Physics/Laboratory Astrophysics at the Berlin Institute of Technology in Germany. Deadline for application is May 1st.

If you are on Instagram, be sure to check out our next [PAH of the Month!](#)

We hope you enjoy reading our newsletter, and we thank you for your dedication and interest in AstroPAH! Please continue sending us your contributions, and if you wish to contact us for a future In Focus or other ideas, feel free to use our [email](#).

The Editorial Team

**Next issue: 18 April 2023.
Submission deadline: 5 April 2023.**

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PAH Picture of the Month

The hour glass shaped object in our cover is the planetary nebula Hubble 12. This object lies in the constellation of Cassiopeia and it was formed as a Sun-like star approached the end of its life. The image was taken with the NASA/ESA Hubble Space Telescope. The infrared spectrum of this object shows bands produced by carbon and crystalline silicate species ([Ohsawa et al. 2016](#), [Hsia et al. 2021](#)).

Credits: NASA, ESA. Acknowledgement: Josh Barrington

Highlighting AstroPAH research at DESIREE

by Mark H Stockett, Michael Gatchell, and Henning Zettergren

The DESIREE Infrastructure

The DESIREE (Double ElectroStatic Ion Ring ExpERiment) facility is a Swedish national research infrastructure located at Stockholm University. The heart of the facility is a pair of electrostatic storage rings for keV ion beams, which are cooled to cryogenic temperatures around 13 K. The low temperature and extreme high vacuum in the storage rings provide ‘molecular cloud in a box’ conditions ideal for experimental studies of ultra-slow unimolecular processes like vibrational de-excitation, isomerisation, and statistical fragmentation. The dual-ring construction enables world-unique possibilities for investigations of interactions between ions of opposing charges such as mutual neutralisation (ion-ion recombination). Here we highlight some recent AstroPAH-related results from DESIREE.

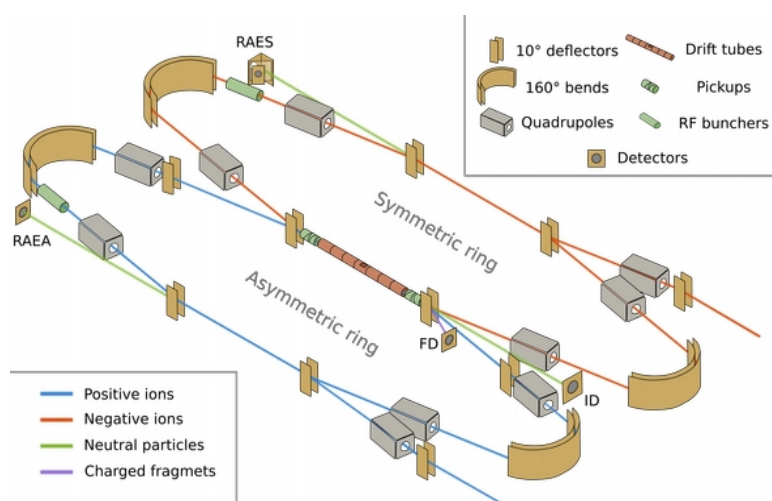


Figure 1 – The DESIREE storage rings.

Dissociation and radiative stabilisation

Experiments using electrostatic ion beam storage devices have revealed the importance of radiative stabilisation of PAH radical cations by Recurrent Fluorescence (RF), *i.e.* the emission of optical photon from thermally excited electronic states. In a typical experiment (Stockett et al., 2020; Zhu et al., 2022; Bernard et al., 2023), the RF rate coefficient is determined indirectly by comparing measurements of the time-dependent dissociation rate of stored beams of vibrationally excited ions with master equation simulations of the relevant

processes (Fig. 2). Using the state-of-the-art neutral product imaging detector at DESIREE, this technique has been extended to enable direct determination of dissociation rate coefficients and radiative cooling rates from the Kinetic Energy Release (KER) distributions of source-heated and laser-excited PAH cations. For example, recent DESIREE results from DESIREE have shown that RF efficiently stabilizes 1-cyanonaphthalene (1-CNN) cations, helping to rationalise the unexplained high observed abundance of neutral 1-CNN in the cold cloud TMC-1 [Stockett et al. \(2023\)](#).

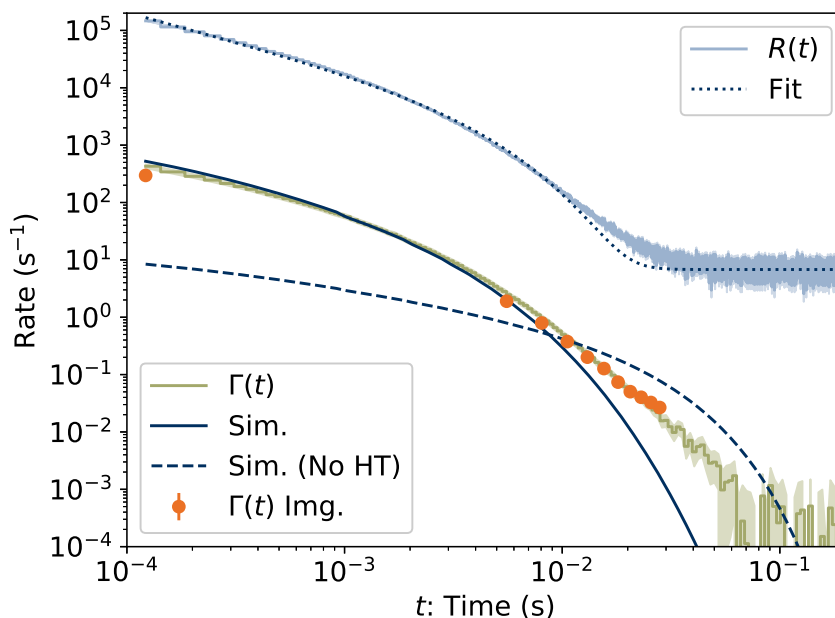


Figure 2 – Dissociation rate of 1-cyanonaphthalene cations.

Stability of shock-processed defect PAHs

Collisions with H, He, and C atoms at velocities around 100 km s^{-1} in supernova shocks or stellar winds are thought to be an important destruction pathway for PAHs in space. Such collisions may induce non-statistical ‘knockout’ fragmentation ([Gatchell and Zettergren, 2016](#)), the products of which have been detected in laboratory experiments ([Stockett et al., 2015](#)). These so-called defect PAHs have dangling bonds and could serve as reactive sites for astrochemistry provided they survive on long enough timescales. Experiments at DESIREE showed that this is indeed the case ([Gatchell et al., 2021](#)). Coronene cations $\text{C}_{24}\text{H}_{12}^+$ were first collided with He atoms at a velocity of 72 km s^{-1} . The defective $\text{C}_{23}\text{H}_{12-x}^+$ products were then selected and stored in DESIREE. Using a sensitive ion counting technique, it was shown that only a small fraction of the products decay further through dissociation on timescales up to about 10 ms. After this, the

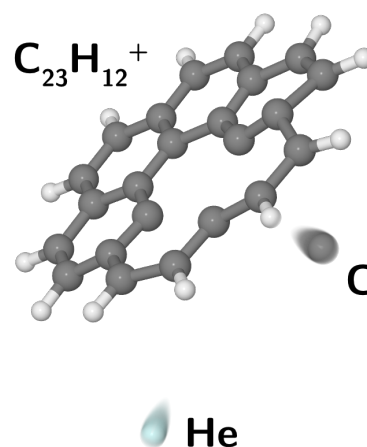


Figure 3 – A carbon atom being knocked out from a coronene cation by a helium atom.

remaining defect coronene cations stored in the ring, which made up 80 percent of the initial population, remained stored for the duration of the experiment, up to 1 s after formation. These results proved that PAH fragments that have lost a single carbon atom through knock-out can indeed be stable on astronomical timescales.

Action spectroscopy and IR radiative cooling

Vibrational de-excitation of photo-excited PAHs is thought to give rise to the Aromatic Infrared Bands observed in emission throughout the Interstellar Medium. Experimental studies of this ultra-slow process are challenging because they require that the excited PAHs be isolated in a collision-free environment for hundreds of milliseconds to tens of seconds. Due to the excellent vacuum conditions, the DESIREE storage rings boast collision-limited lifetimes of several hundred seconds. At DESIREE, methods have been developed to indirectly probe the IR emission rate by monitoring the evolution of the visible absorption spectrum of initially hot ensembles of ions. The photodissociation or photodetachment (for anions) action spectrum is used as a proxy for absorption, with the long sampling time of the storage ring eliminating the possibility of kinetic shifts skewing the result. The rate at which hot-band contributions to the action spectrum fade with storage time in the ring can be compared to master equation simulations of the vibrational de-excitation process. This method has been applied to coronene cations (Stockett et al., 2019a,b), and *para*-benzoquinone anions (Zhu et al., 2022), a prototype for functionalised PAHs thought to form in interstellar ices. These results have typically shown good agreement with a Simple Harmonic Cascade model of de-excitation, but discrepancies attributed to neglect of anharmonic effects have been noted.

Mutual Neutralisation

Mutual Neutralisation (MN) reactions, $A^+ + B^- \rightarrow A+B$, are believed to be important in e.g. molecular clouds where molecules such as PAHs or fullerenes may be the main carriers of negative charges. However, to the best of our knowledge, there are no such experimental studies reported in the literature involving these important classes of molecules under conditions mimicking those in space. MN reactions for a range of atomic collisions systems have recently been studied at DESIREE (see <https://www.desiree-infrastructure.com/publications>) and the first experiments with PAHs and fullerenes have been successfully carried out. These are key to benchmark theory and models with the aim to advance the fundamental understanding of MN processes and their significance in astrophysical environments.

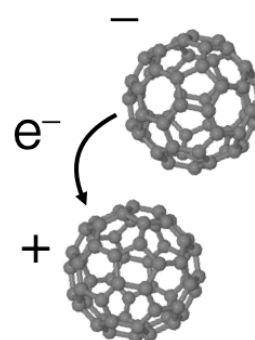


Figure 4 – MN reaction involving oppositely charged fullerenes

Apply for beamtime!

DESIREE is an open-access user facility providing up to 30 weeks of user beam time per year. The proposal submission deadlines are April 30 and October 31 for experiments to be carried out September-December and January-June, respectively. The proposals are evaluated by a panel of external reviewers. If you are interested in performing your AstroPAH research at DESIREE, contact one of the authors or visit the website:

<https://www.desiree-infrastructure.com/>

This DESIREE Infrastructure receives funding from the Swedish Research Council (Contract Nos. 2017-00621 and 2021-00155).



Dr Mark H. Stockett earned his Ph.D. in physics from the University of Wisconsin in 2011. He was a postdoctoral researcher at Stockholm University (SU) and Aarhus University (AU) and is now Docent in Physics at SU. His research uses action spectroscopy to probe the photophysics of molecular ions in the gas phase and their interaction at interfaces.

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Prof. Henning Zettergren has a PhD in physics from SU (2005), and has been a postdoctoral researcher at the Universidad Autonoma de Madrid and AU. He is now the deputy director for the DESIREE infrastructure (SU) and the chair of the MD-GAS COST Action CA-18212 (www.mdgas.eu). His research focuses on the interaction dynamics of carbon containing molecules and their clusters in the gas phase through combined experimental and theoretical studies at DESIREE.

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Dr. Michael Gatchell obtained a PhD in physics from SU in 2016. He was then a postdoctoral researcher at the University of Innsbruck before returning to SU in 2020, where he is now a senior researcher. His current research mainly focuses on studying chemical reactions in cold atomic and molecular clusters grown in helium nanodroplets.

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References

- Mark H. Stockett, James N. Bull, Jack T. Buntine, Eduardo Carrascosa, MingChao Ji, Naoko Kono, Henning T. Schmidt, and Henning Zettergren. *Unimolecular fragmentation and radiative cooling of isolated PAH ions: A quantitative study*. *J. Chem. Phys.*, 153(15):154303, 2020. doi: 10.1063/5.0027773. URL <https://aip.scitation.org/doi/abs/10.1063/5.0027773>.
- Boxing Zhu, James N. Bull, MingChao Ji, Henning Zettergren, and Mark H. Stockett. *Radiative cooling rates of substituted PAH ions*. *J. Chem. Phys.*, 157(4):044303, 2022. doi: 10.1063/5.0089687. URL <https://doi.org/10.1063/5.0089687>.
- Jérôme Bernard, MingChao Ji, Suvasthika Indrajith, Mark H. Stockett, José E. Navarro Navarrete, Naoko Kono, Henrik Cederquist, Serge Martin, Henning T. Schmidt, and Henning Zettergren. *Efficient radiative cooling of tetracene cations c18h12+: absolute recurrent fluorescence rates as a function of internal energy*. *Phys. Chem. Chem. Phys.*, pages –, 2023. doi: 10.1039/D3CP00424D. URL <http://dx.doi.org/10.1039/D3CP00424D>.
- Mark H. Stockett, James N. Bull, Henrik Cederquist, Suvasthika Indrajith, MingChao Ji, José E. Navarro Navarrete, Henning T. Schmidt, Henning Zettergren, and Boxing Zhu. *Efficient stabilization of cyanonaphthalene by fast radiative cooling and implications for the resilience of small pahas in interstellar clouds*. *Nature Communications*, 14(1):395, 2023. ISSN 2041-1723. doi: 10.1038/s41467-023-36092-0. URL <https://doi.org/10.1038/s41467-023-36092-0>.
- Michael Gatchell and Henning Zettergren. *Knockout driven reactions in complex molecules and their clusters*. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 49(16): 162001, aug 2016. doi: 10.1088/0953-4075/49/16/162001. URL <https://dx.doi.org/10.1088/0953-4075/49/16/162001>.
- M H Stockett, M Gatchell, T Chen, N de Ruelle, L Giacomozzi, M Wolf, H T Schmidt, H Zettergren, and H Cederquist. *Threshold energies for single-carbon knockout from polycyclic aromatic hydrocarbons*. *J. Phys. Chem. Lett.*, 6(22):4504–4509, 2015. URL <http://dx.doi.org/10.1021/acs.jpcllett.5b02080>.
- Michael Gatchell, João Ameixa, MingChao Ji, Mark H. Stockett, Ansgar Simonsson, Stephan Denifl, Henrik Cederquist, Henning T. Schmidt, and Henning Zettergren. *Survival of polycyclic aromatic hydrocarbon knockout fragments in the interstellar medium*. *Nature Communications*, 12:6646, 2021. URL <https://www.nature.com/articles/s41467-021-26899-0>.
- Mark H Stockett, Mikael Björkhage, Henrik Cederquist, Henning Schmidt, and Henning Zettergren. *Storage time dependent photodissociation action spectroscopy of polycyclic aromatic hydrocarbon cations in the cryogenic electrostatic storage ring DESIREE*. *Faraday Discuss.*, 217:126–137, 2019a. doi: 10.1039/C8FD00161H. URL <http://dx.doi.org/10.1039/C8FD00161H>.
- Mark H. Stockett, Mikael Björkhage, Henrik Cederquist, Henning T. Schmidt, and Zettergren Henning. *Intrinsic absorption profile and radiative cooling rate of a PAH cation revealed by action spectroscopy in the cryogenic electrostatic storage ring DESIREE*. *Proc. Int. Astron. Union*, 15(S350):127–131, 2019b. doi: 10.1017/S1743921319007130. URL <http://dx.doi.org/10.1017/S1743921319007130>.



Abstracts

Gas Phase Synthesis of the C₄₀ Nano Bowl C₄₀H₁₀

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Nanobowls represent vital molecular building blocks of end-capped nanotubes and fullerenes detected in combustion systems and in deep space such as toward the planetary nebula TC-1, but their fundamental formation mechanisms have remained elusive. By merging molecular beam experiments with electronic structure calculations, we reveal a complex chain of reactions initiated through the gas-phase preparation of benzocorannulene (C₂₄H₁₂) via ring annulation of the corannulenyl radical (C₂₀H₉[•]) by vinylacetylene (C₄H₄) as identified isomer-selectively in situ via photoionization efficiency curves and photoion mass-selected threshold photoelectron spectra. In silico studies provided compelling evidence that the benzannulation mechanism can be expanded to pentabenzocorannulene (C₄₀H₂₀) followed by successive cyclodehydrogenation to the C₄₀ nanobowl (C₄₀H₁₀) – a fundamental building block of buckminsterfullerene (C₆₀). This high-temperature pathway opens up isomer-selective routes to nanobowls via resonantly stabilized free-radical intermediates and ring annulation in circumstellar envelopes of carbon stars and planetary nebulae as their descendants eventually altering our insights of the complex chemistry of carbon in our Galaxy.

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Nat. Commun., **14**:1527 (2023)

<https://doi.org/10.1038/s41467-023-37058-y>

<https://www.nature.com/articles/s41467-023-37058-y>

Probing radical versus proton migration in the aniline cation with IRMPD spectroscopy

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Intramolecular radical and proton migration in the gas phase are important processes driving the dissociation reactions underlying common tandem mass spectrometry processes, such as collision-induced and electron-induced dissociation reactions (CID and ExD). Mechanistic insights in these processes requires experiments that probe the molecular structures of ions along the reaction pathways, usually combined with quantum-chemical calculations. The combination of ion trap mass spectrometry with IR laser spectroscopy, pioneered among others by Dieter Gerlich, provides a particularly effective method to explore details of the ion structures. In this work, we employ infrared multiple-photon dissociation (IRMPD) spectroscopy and density functional theory (DFT) calculations to probe the reactant and product ion structures of a homolytic bond cleavage reaction. First, we employ IRMPD spectroscopy to establish that protonation of the 4-bromoaniline precursor occurs on the amine moiety and then that C-Br homolytic cleavage produces the π -radical cation of aniline. Transition-state calculations are performed to compare the various pathways that connect reactant and product ions, including both proton and radical transfer mechanisms.

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Molecular Physics, e2192307 (2023)

<https://doi.org/10.1080/00268976.2023.2192307>

Fingerprinting fragments of fragile interstellar molecules: dissociation chemistry of pyridine and benzonitrile revealed by infrared spectroscopy and theory

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The cationic fragmentation products in the dissociative ionization of pyridine and benzonitrile have been studied by infrared action spectroscopy in a cryogenic ion trap instrument at the Free-Electron Lasers for Infrared eXperiments (FELIX) Laboratory. A comparison of the experimental vibrational fingerprints of the dominant cationic fragments with those from quantum chemical calculations revealed a diversity of molecular fragment structures. The loss of HCN/HNC is shown to be the major fragmentation channel for both pyridine and benzonitrile. Using the determined structures of the cationic fragments, potential energy surfaces have been calculated to elucidate the nature of the neutral fragment partner. In the fragmentation chemistry of pyridine, multiple non-cyclic structures are formed, whereas the fragmentation of benzonitrile dominantly leads to the formation of cyclic structures. Among the fragments are linear cyano-(di)acetylene⁺, methylene-cyclopropene⁺ and o- and m-benzyne⁺ structures, the latter possible building blocks in interstellar polycyclic aromatic hydrocarbon (PAH) formation chemistry. Molecular dynamics simulations using density functional based tight binding (MD/DFTB) were performed and used to benchmark and elucidate the different fragmentation pathways based on the experimentally determined structures. The implications of the difference in fragments observed for pyridine and benzonitrile are discussed in an astrochemical context.

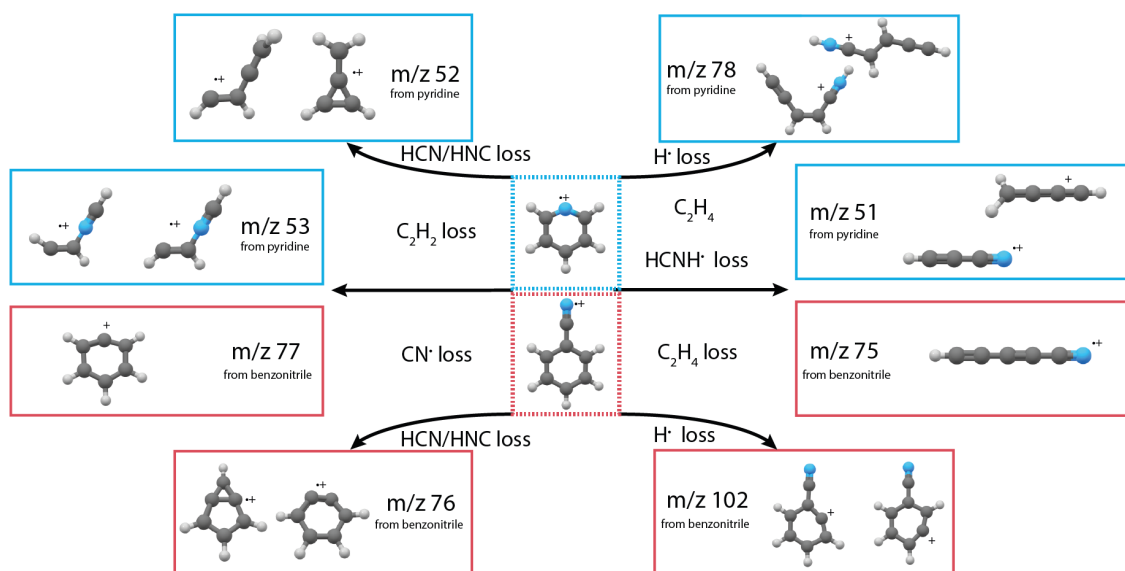


Figure 5 – Fragmentation pathways of benzonitrile and pyridine are elucidated using cryogenic infrared ion spectroscopy, quantum-chemical calculations and molecular dynamics simulations.

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Faraday Discuss., Accepted Manuscript (2023)

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Infrared spectra of protonated and deuterated C_{60} in interstellar environments

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With the credible detection of C_{60} , C_{70} and C_{70}^+ in the interstellar medium (ISM), new prospects have opened up for the search of other fullerenes and their derivatives. Since fullerenes show high proton affinities, their protonated forms should predominate in the ISM, which can easily go through deuterium enrichment. Here, we present the infrared (IR) spectra and standard enthalpy of formation of $C_{60}H^+$, $C_{60}D^+$, $C_{60}H_{18}^+$ and $C_{60}D_{18}^+$ using Density Functional Theory (DFT) in singly ionized forms. The obtained computed IR spectra are compared with the observations. The results show that the four mid-infrared bands of neutral C_{60} are still visible in $C_{60}H^+$ and $C_{60}D^+$, but their strength diminishes in $C_{60}H_{18}^+$ and $C_{60}D_{18}^+$. As a conclusion, it is possible that the IR bands ascribed to C_{60} are a mixture of pure and slightly protonated and deuterated fullerenes. In this way, the observed scattering of the C_{60} band ratios could be explained.

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Photoabsorption of microhydrated naphthalene and its cyano-substituted derivatives: Probing prereactive models for photodissociation in molecular clouds

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We investigate the photoionization pathways of naphthalene, 1-, and 2-cyanonaphthalene upon complexation with the water dimer, aiming to understand the photodissociation process under conditions of the interstellar medium (ISM). We analyze the intermolecular bonding pattern, equilibrium rotational properties, energy complexation, far-IR spectra, and ionic trends of the possible photoproducts using dispersion-corrected density functional theory (DFT-D) and time-dependent DFT (TD-DFT). For the different configurations, we evaluate the possible charge-transfer (CT) excitations near the photoionization limit. Our results indicate that, in high radiation regions of the ISM (> 8.0 eV), CT excitations occur from localized occupied molecular orbitals (MOs) in the aromatic molecules to mixed unoccupied MOs in the complexes, favoring cationic aromatic species in these conditions. We notice that the photoabsorption spectra depend on the type of intermolecular interactions (H-bonds or O-H \cdots p bonds) in the complexes, as well as the presence and position (1 or 2) of the cyano-functional group in naphthalene. For hydrated naphthalene, the O-H \cdots p complexes assume a more relevant role for photodissociation. In the case of the cyano-substituted derivatives, the H-bonded structures are more favorable to be considered as prereactive models. However, the cyano group at position 2 indicates that CT excitations toward the water dimer are more likely to occur.

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J. Phys. Chem. A (2023)

<https://doi.org/10.1021/acs.jpca.3c00487>

Gas-phase electronic action absorption spectra of protonated oxygen-functionalized polycyclic aromatic hydrocarbons (OPAHs)

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Context. Extended red emission (ERE) denotes a broad unassigned feature extending from 540 to 800 nm observed in many regions of the interstellar medium (ISM), and is thought to originate from photoluminescence of cosmic dust. However, definitive assignment of specific carriers remains to be achieved.

Aims. Our aim is to investigate the photoabsorption spectra of astrophysically relevant protonated oxygen-functionalized polycyclic aromatic hydrocarbons (OPAHs) to probe their ability to absorb photons in the near-ultraviolet (UV) and visible (vis) spectral region and to search for any low-lying electronic states that may account for the ERE.

Methods. Gas-phase electronic action absorption spectra of the protonated OPAHs were recorded in the spectral range of 200 – 700 nm using the ELISA ion-storage ring. Additional time-dependent density functional theory (TD-DFT) calculations were performed to compute excited state transitions that complement the experimental spectra.

Results. A set of five protonated (O)PAHs was considered, namely pentacene and the four oxygen-functionalized PAHs, pentacenequinone, pentacenetetrone, anthraquinone, and phenanthrenequinone. All pentacene-related species show a main absorption band between 400 and 500 nm, while the smaller OPAHs, anthraquinone and phenanthrenequinone, generally absorb further to the blue compared to the pentacenes. Interestingly, pentacenequinone and phenanthrenequinone exhibit wide absorption plateaus towards the red side of their main absorption band(s), which places them among the potential candidates to contribute to ERE. Additional photodissociation mass spectra reveal the formation of smaller functionalized PAHs and small oxygen-bearing species.

Conclusions. Our results demonstrate the ability of OPAHs to absorb in the UV/vis spectral region. Among the four studied OPAHs, two revealed very broad absorption characteristics at wavelengths up to 700 nm, which makes them suitable candidates to contribute to a part of the ERE spectrum. Moreover, these two OPAHs, pentacenequinone and phenanthrenequinone, could dissociate efficiently into oxygen-bearing molecules and smaller functionalized PAHs in photon-dominated regions (PDRs) of the ISM.

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Astron. Astrophys., Forthcoming article (2023)

<https://doi.org/10.1051/0004-6361/202346003>



Meetings

The Astrochemistry Subdivision: A Decade of Progress and Prospects for the Next Decade American Chemical Society Fall 2023 National Meeting

San Francisco, USA, and online
13–17 August, 2023

<http://astro.phys-acs.org/symposia/Fall2023.html>

The Astrochemistry Subdivision convened its first symposium 10 years ago, at the Fall 2013 National Meeting. It has been a decade of immense progress for the field of astrochemistry, and many members of the Subdivision have made seminal contributions to the field. The astronomical detection of new molecules has exploded in recent years with the Atacama Large Millimeter Array (ALMA) and large single-dish observatories (e.g., GBT, IRAM 30m) leading the way. 2021 alone saw announcements for the detection of over 30 new molecules, far more than the annual averages from the previous years. The James Webb Space Telescope has recently been deployed and has already sent back stunning imagery of the cosmos. All observations are founded upon critical experimental and theoretical chemistry contributions, which provide a steady stream of data and predictions. Observation, experiment, and theory all complement each other enormously. As a symposium that looks both back over the accomplishments of the last decade and forward toward the prospects of the next decade, we will encourage our speakers to share their dreams and ambitions for what might be learned in the years to come.

Organizers

Prof. David E. Woon (University of Illinois at Urbana-Champaign)

Dr. Olivia H. Wilkins (NASA Goddard Space Flight Center)

Meeting Social Media Hashtags: [#ACSastrochem10](#) [#ACSFall2023](#)

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Announcements

Postdoc and PhD positions in Molecular Physics/Physical Chemistry/ Laboratory Astrophysics

Advertised by Prof. Dr. Otto Dopfer

Deadline for application: May 1, 2023

https://www.ioap.tu-berlin.de/menue/arbeitsgruppen/ag_dopfer/

A (senior) postdoctoral position for up to five years and a PhD position (3 years) is available in the laser molecular spectroscopy and environmental physics group of Otto Dopfer at the Berlin Institute of Technology (TU Berlin), Germany.

The predominantly experimental research of our group involves the laser spectroscopic, mass spectrometric, and quantum chemical investigation of molecules, radicals, ions, clusters, and nanostructures in the gas phase, with strong relevance to a broad range of interdisciplinary topics ranging from materials science to biophysics, catalysis, astrochemistry, environmental chemistry, and plasma physics. Available equipment includes a variety of pulsed and tuneable IR and UV lasers, several ion sources and cryogenic rf-traps, as well as several types of tandem mass spectrometers. The group is also strongly involved in international collaborations with groups in Japan, France, Italy, UK, Netherlands, and has been a regular user of the IR free electron laser facilities CLIO (France), FELIX (Netherlands), and more recently the FHI-FEL (Berlin).

Qualified candidates for the postdoc position hold a PhD in Physics, Physical Chemistry, or related fields with a strong publication record and ideally already some initial postdoctoral experience (all in experimental science) which is not substantially longer than 5 years. Qualified candidates for the PhD position hold a MSc in Physics, Physical Chemistry, or related fields.

The successful postdoc candidate will be involved in supervising PhD and undergraduate students, will take high responsibility for several existing research projects, and will be strongly involved in developing new research directions (i.e. writing proposals). The position is ideal for candidates who are pursuing an academic career (with possibility for Habilitation) by developing also their own research interests. The position is funded by TU Berlin and involves also teaching duties in the area of Experimental (mostly Molecular) Physics (either in German or in English).

Experience in several of the following fields is mandatory for the postdoc position and highly

advantageous for the PhD position: (1) laser spectroscopy, mass spectrometry, ion sources and traps, cluster science (2) vacuum, optics, data acquisition, construction of apparatus (3) writing of publications, reports, and proposals (4) strong communication and presentation skills.

Interested and highly qualified candidates are encouraged to send their application (in a single pdf file) to Prof. Otto Dopfer (dopfer@physik.tu-berlin.de), including a cover letter, a CV (including a list of publications), a statement of qualifications relevant for the position (max. 1 page), a statement of research interests (max. 1 page) as well as names and complete addresses of two referees. Evaluation of the applications will begin at May 1 (2023) and will continue until the position is filled. The desired starting date is as soon as possible but this is negotiable to some extent.

Berlin is an international city and offers an exciting scientific and cultural environment.

E-mail for contact: dopfer@physik.tu-berlin.de

AstroPAH Newsletter

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

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Submission deadline: 5 April 2023