AstroPAH

A Newsletter on Astronomical PAHs

Issue 70 • July 2020

Omega Nebula

Editorial

Dear Colleagues,

Welcome to our 70^{th} AstroPAH volume. We hope all of you are healthy and doing well.

We are pleased to showcase the Omega nebula as our Picture of the Month taken by astrophotographer Trevor Jones from Astrobackyard. Be sure to check out his website for his photo gallery and more information on how to become an astrophotographer, equipment, and image processing techniques.

Many new exciting publications are featured in this issue, covering new studies from PAH cations to electronic spectroscopy and the effect of helium in fullerene cages. We also share updates from the Astrochemistry Discussions group. More information including how to sign up for the mailing list and access to the archive of talks is provided in the Announcements section. The online lectures part of the Astrochemistry Webinar Series organized by the Student Chapter of the American Vacuum Society at the University of Central Florida are now available to watch on Youtube. Be sure to check those out as well!

The first IAU Laboratory Astrophysics Symposium, IAU S350, took place at the University of Cambridge in 2019, and we are happy to share that the proceedings of that meeting will be made public soon. The upcoming proceedings, edited by Dr. Farid Salama, co-edited by Dr. Harold Linnartz, will be published in August/September.

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: 17 September 2020.
Submission deadline: 4 September 2020.

Contact us:

astropah@strw.leidenuniv.nl
http://astropah-news.strw.leidenuniv.nl
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PAH Picture of the Month

The Omega nebula (Messier 17 - M17) is an emission nebula approximately 5500 light-years from Earth. It includes an H II region where star formation has recently taken place and is considered to be one of the brightest and most massive star-forming regions in our galaxy.

Credits: The image was taken by Astrobackyard (Trevor Jones) who has been an astrophotographer since 2010. His latest work and information (including how to become an astrophotographer) can be found on his **website** and his **Instagram**, **Twitter**, **YouTube**, and **Facebook** links. Further information about the image itself (e.g. equipment used, exposure time, image processing, etc.), can be found **here**.

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Overcoming the Out-of-plane Bending Issue in an Aromatic Hydrocarbon: The Anharmonic Vibrational Frequencies of c-(CH)$C_3H_2^+$

Brent R. Westbrook[1], **Weston A. Del Rio**[1], **Timothy J. Lee**[2], **and Ryan C. Fortenberry**[1]

[1] Department of Chemistry & Biochemistry, University of Mississippi, University, MS 38677-1848, USA

[2] MS 245-3, NASA Ames Research Center, Moffett Field, CA 94035, USA

The challenges associated with the out-of-plane bending problem in multiply-bonded hydrocarbon molecules can be mitigated in quartic force field analyses by varying the step size in the out-of-plane coordinates. Carbon is a highly prevalent element in astronomical and terrestrial environments, but this major piece of its spectra has eluded theoretical examinations for decades. Earlier explanations for this problem focused on method and basis set issues, while this work seeks to corroborate the recent diagnosis as a numerical instability problem related to the generation of the potential energy surface. Explicit anharmonic frequencies for c-(CH)$C_3H_2^+$ are computed using a quartic force field and the CCSD(T)-F12b method with cc-pVDZ-F12, cc-pVTZ-F12, and aug-cc-pVTZ basis sets. The first of these is shown to offer accuracy comparable to that of the latter two with a substantial reduction in computational time. Additionally, c-(CH)$C_3H_2^+$ is shown to have two fundamental frequencies at the onset of the interstellar unidentified infrared bands, at 5.134 and 6.088 μm or 1947.9 and 1642.6 cm^{-1}, respectively. This suggests that the results in the present study should assist in the attribution of parts of these aromatic bands, as well as provide data in support of the laboratory or astronomical detection of c-(CH)$C_3H_2^+$.

E-mail: r410@olemiss.edu

Phys. Chem. Chem. Phys. 22, 12951-12958 (2020)

https://pubs.rsc.org/en/content/articlelanding/2020/CP/D0CP01889A

Active Galactic Nuclei Winds as the Origin of the H_2 Emission Excess in Nearby Galaxies

Rogemar A. Riffel[1,2], **Nadia L. Zakamska**[2] **and Rogerio Riffel**[3]

[1] Department of Physics & Astronomy, Johns Hopkins University, Bloomberg Center, 3400 N. Charles St, Baltimore, MD 21218, USA

[2] Universidade Federal de Santa Maria, CCNE, Departamento de Física, 97105-900, Santa Maria, RS, Brazil

[3] Universidade Federal do Rio Grande do Sul, IF, CP 15051, Porto Alegre 91501-970, RS, Brazil

In most galaxies, the fluxes of rotational H_2 lines strongly correlate with star formation diagnostics (such as polycyclic aromatic hydrocarbons, PAH), suggesting that H_2 emission from warm molecular gas is a minor byproduct of star formation. We analyse the optical properties of a sample of 309 nearby galaxies derived from a parent sample of 2,015 objects observed with the *Spitzer Space Telescope*. We find a correlation between the [O I]λ6300 emission-line flux and kinematics and the H_2S(3) 9.665 μm/PAH 11.3 μm. The [O I]λ6300 kinematics in Active Galactic Nuclei (AGN) can not be explained only by gas motions due to the gravitational potential of their host galaxies, suggesting that AGN driven outflows are important to the observed kinematics. While H_2 excess also correlates with the fluxes and kinematics of ionized gas (probed by [O III]), the correlation with [O I] is much stronger, suggesting that H_2 and [O I] emission probe the same phase or tightly coupled phases of the wind. We conclude that the excess of H_2 emission seen in AGN is produced by shocks due to AGN driven outflows and in the same clouds that produce the [O I] emission. Our results provide an indirect detection of neutral and molecular winds and suggest a new way to select galaxies that likely host molecular outflows. Further ground- and space-based spatially resolved observations of different phases of the molecular gas (cold, warm and hot) are necessary to test our new selection method.

E-mail: rogemar@ufsm.br

Monthly Notices of the Royal Astronomical Society, 491, 1518 (2020)

https://ui.adsabs.harvard.edu/abs/2020MNRAS.491.1518R

Electronic Spectroscopy of He@C$_{60}^{+}$ for Astrochemical Consideration

E. K. Campbell[1], E. S. Reedy[1], J. Rademacher[1], R. J. Whitby[2], and G. Hoffman[2]

[1] School of Chemistry, University of Edinburgh, Joseph Black Building, Kings Buildings, David Brewster Road, Edinburgh EH9 3FJ, UK

[2] Chemistry, University of Southampton, Southampton, Hants, SO17 1BJ, UK

The electronic spectrum of the endohedral fullerene $\mathrm{He@C_{60}^{+}}$ observed by messenger spectroscopy in a cryogenic ion trap is presented. The role played by the messenger tag in the adopted experimental method is evaluated by recording spectra of $\mathrm{He@C_{60}^{+} - He}_n$ with $n = 1 - 4$. The results indicate a linear shift of $\sim 0.7\,\text{Å}$ in the wavelengths allowing accurate gas phase values to be reported. The presence of the helium inside the cage shifts the absorption bands by $2 - 3\,\text{Å}$ toward shorter wavelengths compared to $\mathrm{C_{60}^{+}}$. The magnitude of this displacement will enable searches for the spectral signatures of this fullerene analogue in interstellar environments by absorption spectroscopy. The implications for potential astronomical detection are discussed.

E-mail: e.k.campbell@ed.ac.uk

The Astrophysical Journal 897, 88 (2020)

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Astrochemical relevance of VUV ionization of large PAH cations

G. Wenzel[1], C. Joblin[1], A. Giuliani[2,3], S. Rodriguez Castillo[1,4], G. Mulas[1,5], M. Ji[1], H. Sabbah[1,6], S. Quiroga[7], D. Peña[7] and L. Nahon[2]

[1] Institut de Recherche en Astrophysique et Planétologie (IRAP), Université de Toulouse (UPS), CNRS, CNES, 9 Avenue du Colonel Roche, F-31028 Toulouse, France

[2] Synchrotron SOLEIL, L'Orme des Merisiers, F-91192 Saint Aubin, Gif-sur-Yvette, France

[3] INRAE, UAR1008, Transform Department, Rue de la Géraudière, BP 71627, F-44316 Nantes, France

[4] Laboratoire de Chimie et Physique Quantiques (LCPQ/IRSAMC), Université de Toulouse (UPS), CNRS, 118 Route de Narbonne, F-31062 Toulouse, France

[5] Istituto Nazionale di Astrofisica – Osservatorio Astronomico di Cagliari, Via della Scienza 5, I-09047 Selargius (CA), Italy

[6] Laboratoire Collisions Agrégats Réactivité (LCAR/IRSAMC), Université de Toulouse (UPS), CNRS, 118 Route de Narbonne, F-31062 Toulouse, France

[7] Centro de Investigación en Química Biolóxica e Materiais Moleculares (CiQUS) and Departamento de Química Orgánica, Universidade de Santiago de Compostela, E-15782 Santiago de Compostela, Spain

Context. As a part of interstellar dust, polycyclic aromatic hydrocarbons (PAHs) are processed by the interaction with vacuum ultraviolet (VUV) photons that are emitted by hot young stars. This interaction leads to the emission of the well-known aromatic infrared bands but also of electrons, which can significantly contribute to the heating of the interstellar gas.

Aims. Our aim is to investigate the impact of molecular size on the photoionization properties of cationic PAHs.

Methods. Trapped PAH cations of sizes between 30 and 48 carbon atoms were submitted to VUV photons in the range of 9 to 20 eV from the DESIRS beamline at the synchrotron SOLEIL. All resulting photoproducts including dications and fragment cations were mass-analyzed and recorded as a function of photon energy.

Results. Photoionization is found to be predominant over dissociation at all energies, which differs from an earlier study on smaller PAHs. The photoionization branching ratio reaches 0.98 at 20 eV for the largest studied PAH. The photoionization threshold is observed to be between 9.1 and 10.2 eV, in agreement with the evolution of the ionization potential with size. Ionization cross sections were indirectly obtained and photoionization yields extracted from their ratio with theoretical photoabsorption cross sections, which were calculated using time-dependent density functional theory. An analytical function was derived to calculate this yield for a given molecular size.

Conclusions. Large PAH cations could be efficiently ionized in H I regions and provide a contribution to the heating of the gas by photoelectric effect. Also, at the border of or in H II regions, PAHs could be exposed to photons of energy higher than 13.6 eV. Our work provides recipes to be used in astronomical models to quantify these points.

E-mail: christine.joblin@irap.omp.eu

In press in Astronomy and Astrophysics (A&A), arXiv:2005.02103

http://arxiv.org/abs/2005.02103

Microhydration of Protonated Biomolecular Building Blocks: Protonated Pyrimidine

Kuntal Chatterjee and Otto Dopfer

Institut für Optik und Atomare Physik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Protonation and hydration of biomolecules govern their structure, conformation, and function. Herein, we explore the microhydration structure in mass-selected protonated pyrimidine-water clusters (H^+Pym-W_n, n=1-4) by a combination of infrared photodissociation spectroscopy (IRPD) between 2450 and 3900 cm^{-1} and density functional theory (DFT) calculations at the dispersion-corrected B3LYP-D3/aug-cc-pVTZ level. We further present the IR spectrum of H^+Pym-N_2 to evaluate the effect of solvent polarity on the intrinsic molecular parameters of H^+Pym. Our combined spectroscopic and computational approach unequivocally shows that protonation of Pym occurs at one of the two equivalent basic ring N atoms and that the ligands in H^+Pym-L (L=N_2 or W) preferentially form linear H-bonds to the resulting acidic NH group. Successive addition of water ligands results in the formation of a H-bonded solvent network which increasingly weakens the NH group. Despite substantial activation of the N-H bond upon microhydration, no intracluster proton transfer occurs up to n=4 because of the balance of relative proton affinities of Pym and W_n and the involved solvation energies. Comparison to neutral Pym-W_n clusters reveals the drastic effects of protonation on microhydration with respect to both structure and interaction strength.

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

Physical Chemistry Chemical Physics 22, 13092-13107 (2020) [DOI: 10.1039/d0cp02110e]

https://pubs.rsc.org/en/content/articlelanding/2020/cp/d0cp02110e#!divAbstract

Announcements

Astrochemistry Discussions

With in-person conferences on-hold for the foreseeable future, we didn't want to miss out on the opportunity to see and hear from our colleagues around the world and find out what they're up to in the world of Astrochemistry. Since April, we've been hosting a 1.5 hour virtual webinar series every $\sim$2 weeks on topics across the board in Astrochemistry. We've had review talks by leaders in the field, themed days with several shorter research talks, largely from early-career folks, and several networking days where members of our community discuss their experiences in astrochemistry and academia in general.

Now, Astrochem Discussions is going on holiday... sort of. We'll be picking back up with our regularly scheduled seminars and workshops in September (look for more on that in the coming weeks!). There will be no regularly scheduled meetings in the remainder of July and throughout the month of August, as many of us are on extended vacations (whether we're actually leaving home or not). Instead, throughout the month of August we'll be releasing short videos from many of our participants giving you a taste of their research. Watch them on your own time, over coffee or on the couch, or catch up later when you're back from vacation! We'll send out e-mails every so often when a new batch of videos is up.

All of the information for Astrochemistry Discussions, including how to sign up for our mailing list (we send out $\sim$2 e-mails per webinar - 1 announcement and 1 reminder) and an archive of talks available for viewing whenever, is on our website at discussions.astrochem.net.

Please join us to watch, volunteer, or share your ideas for what you'd like to see from this free Astrochemistry webinar series this fall.

-The SOC
Andrew M. Burkhardt
Ilsa R. Cooke
Sommer L. Johansen
Thanja Lamberts
Nienke van der Marel
Brett A. McGuire

Astrochemistry Webinar Series
Now Available to Watch on Youtube

This past May and June, the Student Chapter of the American Vacuum Society at the University of Central Florida hosted the Astrochemistry Webinar Series, in which graduate students, postdocs, professors, and research scientists from various universities and NASA centers conducting astrochemical research in observations, theory, experiment, and missions gave talks intended for an audience with a broad range of expertise. Topics covered included interstellar chemistry, meteoritics, laboratory ice irradiation and ice irradiation modeling, space weathering, sample return missions, and applications of quantum chemistry. Many of these talks are now available to watch on Youtube on the following playlist:

https://www.youtube.com/playlist?list=PLs0-hejeR_o-xUuVdMLZJQl_Ljl_8lB5a

Talks made available in this playlist include:

Quantum Chemistry and Spectroscopy: A Match Made in the Heavens
Dr. Ryan Fortenberry
Assistant Professor of Chemistry & Biochemistry, University of Mississippi
https://youtu.be/jtaOtjghGc4

Radiation Processing of Dust, Asteroids and Moons: What does it do and what can it tell us?
Dr. Micah Schaible
NASA Postdoctoral Fellow, SSERVI REVEALS Team, Georgia Institute of Technology
https://youtu.be/ESkRxK3owkM

Dark Ice Chemistry in Interstellar Clouds
Danna Qasim
PhD Candidate, Leiden University
https://youtu.be/U8__mA36vLk

Cosmic Rays in Astrochemical Models
Dr. Christopher Shingledecker
Humboldt Research Fellow, Max Planck Institute for Extraterrestrial Physics
https://youtu.be/pSTWSV_2_bY

Probing the formation of complex organics in cometary ices: A New Laboratory Approach
Dr. Stefanie Milam
Research Physical Scientist and JWST Deputy Project Scientist, NASA Goddard Space Flight Center
https://youtu.be/e5UhxfwCVp8

The Unique Scientific Value of Returned Samples
Dr. Scott Sandford
Senior Laboratory Astrophysicist, NASA Ames Research Center
https://youtu.be/Vs4oKraKKO4

The Formation of the Building Blocks of Life in Astrophysical Environments
Dr. Michel Nuevo
BAER Institute Research Scientist, NASA Ames Research Center
https://youtu.be/oizVRM-1CBo

Formation and destruction of nucleobases in ices
Dr. Christopher Materese
Research Scientist, NASA Goddard Space Flight Center
https://youtu.be/G54k2Rh3exo

Delivery of PAHs in the Early Solar System: Forsterite as space shuttle
Dario Campisi
PhD Candidate, Leiden University
https://youtu.be/yJcAOz0qDOs

Searching for the chemical fingerprints of extraterrestrial life
Dr. Niels Ligterink
Research Scientist, Center for Space and Habitability, University of Bern
https://youtu.be/baOJpJK77rU

For more information about the event or the talks, please visit the following page:

https://ucf.avs.org/astrochem .

AstroPAH Newsletter

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astropah@strw.leidenuniv.nl — Submission deadline: 4 September 2020