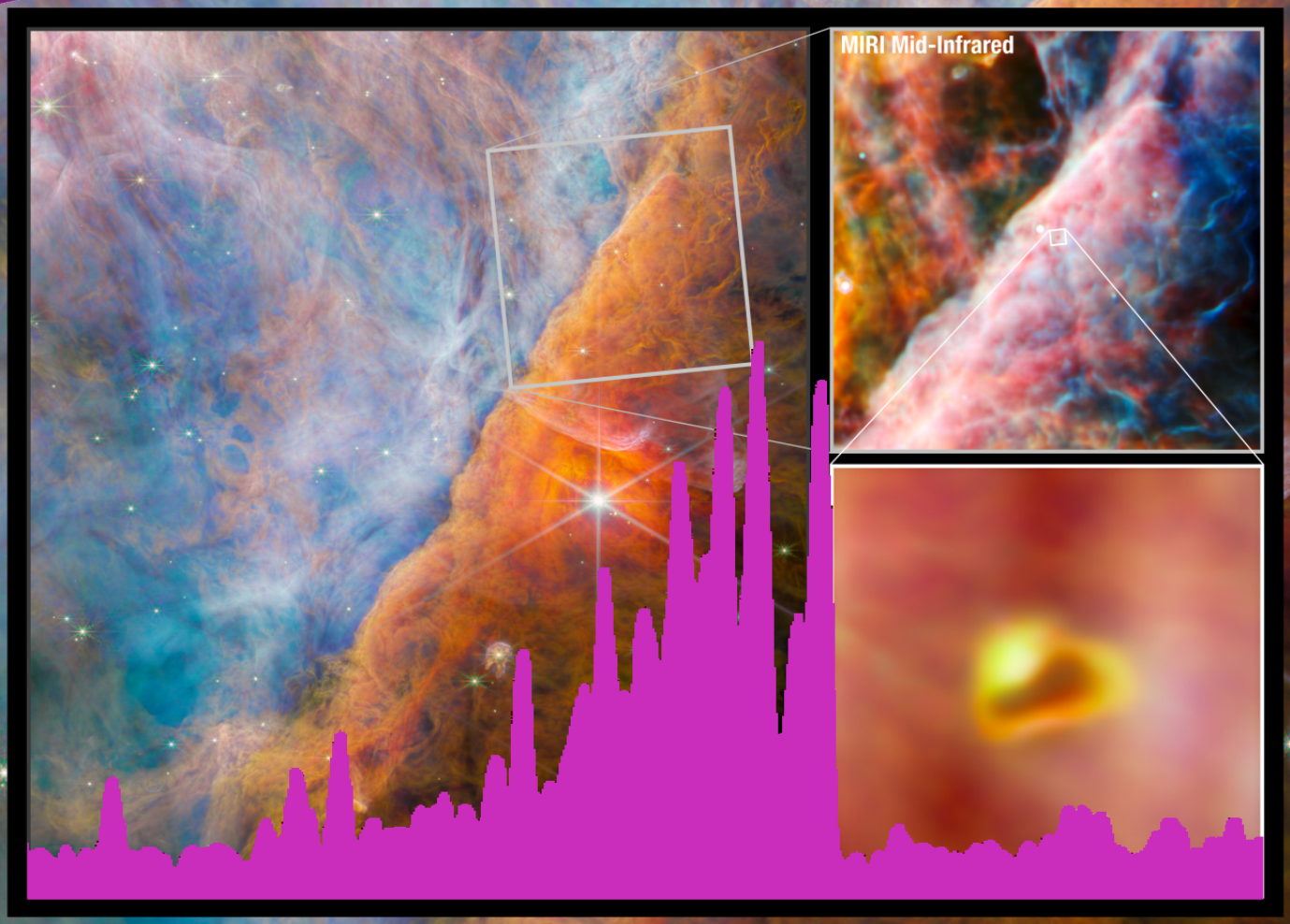
AstroPAH

A Newsletter on Astronomical PAHs

Issue 101 • September 2023



Methyl Cation in a Protoplantary Disc

Editorial

Dear Colleagues,

We are back from our August break with the 101st volume of AstroPAH! We hope you are all well and healthy.

Our cover illustrates the recent detection of the methyl cation (CH_3^+) in a planet-forming disc in the Orion Nebula. The link to the paper is available in the caption in the next page. This and other results were presented at the First Year of JWST results workshop and are accessible in the STSci Research Youtube channel.

Our In Focus this month is an interview with Dr. Jordy Bouwman, who recently joined the Institute for Modeling Plasma, Atmospheres, and Cosmic Dust at the University of Colorado Boulder.

In the Abstracts, you can find the latest publications on electronic spectroscopy, quantum tunneling, and gas-phase synthesis of coronene.

The next American Physical Society meeting next year will host a molecular astrophysics session covering interstellar molecules within the inventory of exoplanetary and solar system compounds. Abstract submission deadline is October 20. We also draw your attention to the Laboratory Astrophysics ICE 2024 Workshop in Kauai, Hawaii. Early registration closes October 30.

The Dutch Astrochemistry Network III (DAN-III) are advertising 4 PhD and 3 postdoc positions. See the announcement on page 15!

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: 19 October 2023.
Submission deadline: 6 October 2023.

Contact us:

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

First detection of methyl cation (CH_3^+) in the planet-forming disc known as d203-506, located about 1350 light years away from Earth, in the Orion Nebula. This carbon molecule was predicted by models to be a vital compound to the growth of larger carbon compounds. The full paper describing the discovery was published in Nature.

Credits: ESA/Webb, NASA, CSA, M. Zamani (ESA/Webb), the PDRs4All ERS Team. The images are available on this webpage.

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An Interview with
Jordy Bouwman

Figure 1 – *The Bouwman Group.*

Dr. Jordy Bouwman received his Bachelor in Applied Physics in 2004 at the TH Rijswijk, the Netherlands, and then obtained his MSc in Chemistry with specialization Laser Sciences in 2006 at the Free University in Amsterdam. After finishing his MSc, Dr. Bouwman moved to Leiden University to pursue his PhD in the field of Laboratory Astrochemistry in the group of Prof. Harold Linnartz, with whom Dr. Bouwman had already worked during his research projects in Amsterdam. His thesis work involved the photochemistry of PAHs in interstellar ices and was performed in strong collaboration with Dr. Lou Allamandola. After obtaining his PhD in 2010 he moved to University of California, Berkeley to work as a postdoc in the group of Prof. Stephen Leone. Here he studied reaction kinetics and branching fractions of low-temperature chemical reactions using multiplexed time of flight mass spectrometry at the Vacuum Ultraviolet (VUV) Beamline of the Advanced Light Source of Lawrence Berkeley

National Laboratory. Next, he moved to Radboud University Nijmegen on a personal NWO-VENI grant to study the dissociation of PAHs in the group of Prof. Jos Oomens at the Free Electron Laser for Infrared Radiation (FELIX). During his period in Nijmegen, he also build a strong collaboration with the Drs. András Bödi and Patrick Hemberger at the VUV beamline of the Swiss Light Source, with whom he investigated the formation of interstellar hydrocarbons using double imaging photoelectron photoion spectroscopy. He then won a NWO-VIDI grant that brought him back to the group of Prof. Harold Linnartz in Leiden to continue his work in this field as an assistant professor.

In 2021, Dr. Bouwman left Leiden University to take on a position as an Assistant Professor of Cosmochemistry at the Institute for Modeling Plasma, Atmospheres and Cosmic Dust (IMPACT) which is part of the Laboratory for Atmospheric and Space Physics (LASP) at the University of Colorado Boulder. His academic home at CU Boulder is the Chemistry Department. He investigates formation and dissociation of (aromatic) hydrocarbons in the interstellar medium using a variety of physico-chemical laboratory techniques combined with quantum chemical calculations. Moreover, his research supports the data analysis of the upcoming Europa-Clipper mission.

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What inspired you to become a scientist?

As a kid, I took electronic equipment apart to see what components it is made of and how it works. I was also interested in chemistry, but I always thought I was going to end up in the field of electronics and engineering. It was not until my bachelor research project at the Free University in Amsterdam that I realized that you can actually combine these skills and interests in the field of experimental physical chemistry. I was amazed by the fact that you can use lasers and sensitive detection techniques to study molecules, and this is what truly inspired me to become a scientist.

How did you get into astrochemistry research?

For my masters research project in Amsterdam, I performed cavity ringdown spectroscopy with the aim to characterize linear carbon chain radicals. The goal was to investigate if these species are carriers of the diffuse interstellar bands. The fact that laboratory measurements can help us shed light on chemical processes in space was fascinating to me. I then knew that I wanted to continue my career in the field of (laboratory) astrochemistry.

Can you tell us about your career path, the difficulties you have faced as a scientist to stay in the field and what has guided your current choice?

I did not land a tenure-track position for a very long time, but was employed on various temporary (independent) research positions. Jumping from one temporary job to another has not been easy. Looking back, however, it did allow me to work with many fantastic people in the field and it grew my network tremendously. Moreover, it exposed me to a large

variety of experimental and computational techniques and, in the end, this detour resulted in me being a well-rounded scientist.

In 2021, I accepted the position at CU Boulder. This position is a fantastic match, allowing me to teach topics that I sincerely care about (physical chemistry, spectroscopy, etc.) while conducting research in the fields of astrochemistry and planetary sciences that fascinate me. It has been a long journey to get where I am now, but every day I feel that I am exactly where I need to be.

What are your current research goals?

I am very excited about both astrochemistry and planetary sciences and hence my research goals are twofold. First, I want to continue our studies to shed light on the formation and (photo) dissociation of polycyclic aromatic hydrocarbons in the interstellar medium and link our findings to observations. Secondly, I want to identify molecules on- and assess the habitability of icy worlds in our Solar System. This field will get a huge boost with the soon to be launched Europa-Clipper mission and I am excited to be part of that team.

What was the most important advice somebody gave you?

The editor in chief of this journal always says “Make sure you do fun things with fun people”. Another important piece of advice I was given, was not to be frustrated by setbacks and to enjoy the journey.

How do you balance your professional and personal life?

Like most scientists, I love my job very much and therefore I easily put in too many hours. My wife and our two wonderful kids (2 and 9 y/o) force me to not always have work creep onto my schedule. Striking a good balance remains a challenge and I am not sure I master it (yet).

What do you do outside of work?

Our kids keep us very busy. We try to find time to enjoy the beautiful nature Colorado has to offer. Besides doing things with the family, I like to cook food, run, and play soccer. Over the years, I learned that the physical exercise is critical in keeping myself mentally strong.

What advice would you give a grad student who wants a career in academia?

Be sure to do what you love doing and to enjoy every step of your career.

Abstracts

Towards a reliable prediction of the infrared spectra of cosmic fullerenes and their derivatives in the JWST era

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Fullerenes, including C_{60}, C_{70}, and C_{60}^+, are widespread in space through their characteristic infrared vibrational features (C_{60}^+ also reveals its presence in the interstellar medium through its electronic transitions) and offer great insights into the carbon chemistry and stellar evolution. The potential existence of fullerene-related species in space has long been speculated and recently put forward by a set of laboratory experiments of C_{60}^+, $C_{60}H^+$, $C_{60}O^+$, $C_{60}OH^+$, $C_{70}H^+$, and [C_{60}-Metal]$^+$ complexes. The advent of the James Webb Space Telescope (JWST) provides a unique opportunity to search for these fullerene-related species in space. To facilitate JWST search, analysis, and interpretation, an accurate knowledge of their vibrational properties is essential. Here, we compile a VibFullerene database and conduct a systematic theoretical study on those species. We derive a set of range-specific scaling factors for vibrational frequencies, to account for the deficiency of density functional theory calculations in predicting the accurate frequencies. Scaling factors with low root-mean-square and median errors for the frequencies are obtained, and their performance is evaluated, from which the best-performing methods are recommended for calculating the infrared spectra of fullerene derivatives which balance the accuracy and computational cost. Finally, the recommended vibrational frequencies and intensities of fullerene derivatives are presented for future JWST detection.

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https://doi.org/10.1093/mnras/stad2335
https://arxiv.org/abs/2307.15668

Gas-Phase Synthesis of Coronene through Stepwise Directed Ring Annulation

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Molecular beam experiments together with electronic structure calculations provide the first evidence of a complex network of elementary gas-phase reactions culminating in the bottom-up preparation of the 24π aromatic coronene ($C_{24}HC_{12}$) molecule—a representative peri-fused polycyclic aromatic hydrocarbon (PAH) central to the complex chemistry of combustion systems and circumstellar envelopes of carbon stars. The gas-phase synthesis of coronene proceeds via aryl radical-mediated ring annulations through benzo[e]pyrene ($C_{20}HC_{12}$) and benzo[ghi]perylene ($C_{22}HC_{12}$) involving armchair-, zigzag-, and arm-zig-edged aromatic intermediates highlighting the chemical diversity of molecular mass growth processes to polycyclic aromatic hydrocarbons. The isomer-selective identification of five- to six-ringed aromatics culminating with the detection of coronene is accomplished through photoionization and is based upon photoionization efficiency curves along with photoion mass-selected threshold photoelectron spectra providing a versatile concept on molecular mass growth processes via aromatic and resonantly stabilized free radical intermediates to two-dimensional carbonaceous nanostructures.

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https://doi.org/10.1021/jacs.3c03816

Surface Diffusion of Carbon Atoms as a Driver of Interstellar Organic Chemistry

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Many interstellar complex organic molecules (COMs) are believed to be produced on the surfaces of icy grains at low temperatures. Atomic carbon is considered responsible for the skeletal evolution processes, such as C–C bond formation, via insertion or addition reactions. Before reactions, C atoms must diffuse on the surface to encounter reaction partners; therefore, information on their diffusion process is critically important for evaluating the role of C atoms in the formation of COMs. In situ detection of C atoms on ice was achieved by a combination of photostimulated desorption and resonance-enhanced multiphoton ionization methods. We found that C atoms weakly bound to the ice surface diffused above approximately 30 K and produced C_2 molecules. The activation energy for C-atom surface diffusion was experimentally determined to be 88 meV (1,020 K), indicating that the diffusive reaction of C atoms is activated at approximately 22 K on interstellar ice. The facile diffusion of C atoms at temperatures above 22 K on interstellar ice opens a previously overlooked chemical regime where the increase in complexity of COMs is driven by C atoms. Carbon addition chemistry can be an alternative source of chemical complexity in translucent clouds and protoplanetary disks with crucial implications in our current understanding on the origin and evolution of organic chemistry in our Universe.

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Nature Astronomy (2023)

https://doi.org/10.1038/s41550-023-02071-0
https://arxiv.org/abs/2308.02181

Quantum Tunneling Facilitates Water Motion across the Surface of Phenanthrene

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Understanding the diffusion of water monomers on carbon surfaces, like graphene, is a fundamental step towards comprehending various complex physical and chemical phenomena that occur in our everyday lives and in scientific and technological processes, such as corrosion, catalysis, electrochemistry, ice nucleation, and separation technologies, to name a few. However, studying the interaction between a single water molecule and a carbon surface has proven to be a challenging task due to the high propensity of water molecules to form hydrogen bonds, which results in rapid formation of water clusters, and the high mobility of water's protons. These factors make it difficult, for example, for imaging technique, to capture the water's behavior when interacting with such surfaces. We exploited the outstanding high resolution of broadband rotational spectroscopy to disentangle with an unparalleled level of detail the complex internal dynamics of a single water molecule when interacting with the planar carbon surface of phenanthrene, which served as a small-scale carbon-surface like model. Our findings revealed that the diffusion of a single water molecule on carbon surfaces occurs via quantum tunnelling of the water molecule between one aromatic ring of phenanthrene and the equivalent one. The water's migration pathway was disentangled with a remarkable level of detail by investigating the effect of isotopic substitution on the line splitting in the rotational spectra of the $H_2^{16}O$, $H_2^{18}O$, D_2O and HDO isotopologues of the monohydrated cluster of phenanthrene. This study shows that the water molecule diffuses via a concerted tunnelling motion which involves the simultaneous internal rotation of the water molecule and its translation between the two peripheral ring of phenanthrene. These findings provide a valuable small-scale model to help disentangle water's diffusion on more complex carbon surfaces, including those larger than phenanthrene, *i.e.*, large polycyclic aromatic hydrocarbons and graphene.

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https://doi.org/10.1021/jacs.3c04281

Electronic spectroscopy of 1-cyanonaphthalene cation for astrochemical consideration

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Context. Polycyclic aromatic hydrocarbons (PAHs) are believed to be the carriers of the aromatic infrared bands (AIBs) and have been proposed as candidates to explain other astronomical phenomena such as diffuse interstellar bands (DIBs). The first aromatic structures possessing more than one ring, 1- and 2-cyanonaphthalene (CNN), were recently detected by rotational spectroscopy in the dense molecular cloud TMC-1. Laboratory investigations have indicated that due to fast and efficient relaxation through recurrent fluorescence (RF), CNN^+ may be photostable in the harsh conditions of the lower density, more diffuse regions of the interstellar medium (ISM) exposed to ultraviolet (UV) radiation. As a result, it has been suggested that the widely held belief that small PAHs present in these regions are dissociated may need to be revisited. If 1-CNN^+ is able to survive in the diffuse ISM it may contribute to the population of 1-CNN observed in TMC-1. To investigate the abundance of 1-CNN^+ in diffuse clouds, laboratory spectroscopy is required. The present work concerns the electronic spectroscopy of 1-CNN^+ in absorption and the search for its spectroscopic fingerprints in diffuse clouds.

Aims. The aim is to obtain laboratory data on the electronic transitions of gas-phase 1-CNN^+ under conditions appropriate for comparison with DIBs and assess abundance in diffuse clouds.

Methods. Spectroscopic experiments are carried out using a cryogenic ion trapping apparatus in which gas-phase 1-CNN^+ is cooled to temperatures below 10 K through buffer gas cooling. Calculations are carried out using time-dependent density-functional theory.

Results. Experimental and theoretical data on the $D_2 \leftarrow D_0$ and $D_3 \leftarrow D_0$ electronic transitions of 1-CNN^+ are reported. The former transition has a calculated oscillator strength of $f = 0.075$ and possesses a pattern dominated by its origin band. The origin band is located at 7343 Å and has a full width at half maximum (FWHM) of 28 Å. In observational data, this falls in a region polluted by telluric water lines, hindering assessment of its abundance.

Conclusions. Space-based observations are required to search for the spectroscopic signatures of 1-CNN^+ and evaluate the hypothesis that this small aromatic system, stabilised by RF, may be able to survive in regions of the ISM exposed to UV photons.

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Astron. Astrophys., 677, A128 (2023)

https://doi.org/10.1051/0004-6361/202347199

Laboratory Astrophysics Workshop

ICE 2024

Kauai, Hawaii, USA
19–22 February, 2024

http://uhmreactiondynamics.org/ICE2024.html

Call for contributed presentations to ICE 2024.

Significant new experimental techniques have been developed to investigate the interaction of ionizing radiation (UV, VUV, gamma rays, charged particles) and of neutrals (atoms, radicals, molecules, grains) with surfaces of solids (ices, minerals, carbonaceous compounds) in the Solar System and in the Interstellar Medium (ISM). These processes provide new fundamental insights – sometimes on the molecular level – into the processes that are critical to the chemistry in the ISM, star and planet forming regions, and on/in icy objects in the Solar System from the formation of the simplest molecule (molecular hydrogen) to astrobiologically important species such as amino acids and sugars.

Based on the successful workshops in 2013 and 2015, the third workshop features invited as well as contributed talks covering the interaction of ionizing radiation (UV, VUV, gamma rays, charged particles) and neutrals (atoms, radicals, molecules, grains) with low temperature solids (ices, minerals, organics). The talks can be extended to observations, modeling, and electronic structure calculations, if these topics can be linked – as evident from the abstract – to laboratory experiments.

Accommodation: Several hotels are within walking distance of the conference center including the ISO Mokihana, Aston Islander on the Beach, Waipouli Beach Resort, Kauai Shores Hotel, and the Sheraton Coconut Beach Resort.

Conference: The workshop will take place in the Sheraton Coconut Beach Resort in Kapaa, Kauai, Hawaii, starting with a reception and registration on February 18, 2024, at 6 pm (Sunday) followed by presentations on February 19-22. Presenters may choose between oral or poster presentation formats. Early registration closes October 30, 2023. Please visit uhmreactiondynamics.org/ICE2024.html to register or email aturner7@hawaii.edu with questions.

E-mail for contact: aturner7@hawaii.edu

Molecular Astrophysics Symposium:

Linking Interstellar Molecules with the Organic Inventory of (Exo)-Planets and the Solar System

March meeting of the American Physical Society (APS)
Minneapolis, MN

3 - 8 March, 2024

https://ism2exoplanet.wordpress.com/

Abstract submission deadline: 20 October 2023, 5:00 pm ET

Organizers: Dr. P.P. Bera (NASA ARC) and Prof. A.G.G.M. Tielens (Leiden University)

With new results from the missions such as the James Webb Space Telescope and OSIRIS-REx, ground-based observatories such as ALMA, and new laboratory facilities and quantum chemistry studies and ever increasing sophisticated astronomical models providing deep insight into the role of molecules in the universe, molecular astrophysics is a rapidly developing field with potential to make significant contributions to our understanding of the universe. In this symposium, we will explore the organic inventory of regions of planet formation, the role of molecules in the formation of stellar and planetary systems, discuss the use of molecules to measure the universe, and deliberate on the future of molecular astrophysics. We will explore how molecules play a critical role by providing raw, prebiotic materials, by controlling the ionization balance and the coupling to magnetic fields, and by affecting the energy balance in regions of star and planet formation through their influence on heating and cooling processes.

We will cover the following topics in more detail:

- **The water trail:** from the dark cloud cores to comets and asteroids, to terrestrial planets
- **Hot Corinos and the organic inventory of regions of planet formation:** observations and chemical models of the organic inventory of protoplanetary disks with ALMA
- **The interstellar heritage of the organic inventory of exoplanets:** summarizing observations and models of exoplanet atmospheres, and the relative roles of interstellar, protoplanetary disks, and planetary processes
- **JWST's view of protoplanetary disks:** summarizing observations and chemical models of the organic inventory of the (inner) protoplanetary disks with JWST

We will have at least 4 sessions with 13 talks per session:

- Invited talks will be 24 minutes long (20+4 minutes for discussion) — max 2 invited talks for each 3-hour session.
- Contributed talks will be 12 minutes (10 + 2 for discussion).

There will also be two panel discussions and a poster session.

Session webpage: https://ism2exoplanet.wordpress.com/

General website of the APS Meeting: https://march.aps.org/

E-mail for contact: partha.bera@nasa.gov

Announcements

Dutch Astrochemistry Network (DAN-III) PhD and Postdoctoral Positions

Advertised by Alessandra Candian on behalf of DAN-III PIs and Co-Is

The launch of the James Webb Space Telescope (JWST) in 2022 opened a new window for the study of astrochemistry. JWST observes with unprecedented resolution different astronomical environments, thus permitting to study the ice composition in dense molecular clouds and protoplanetary disks but also the cycle of carbon through the phases of star and planet formation. Interpreting this novel data requires an interdisciplinary collaboration between astronomers, physicists and chemists to systematically collect and use key molecular data, such as gas and ice spectroscopy, collisional rate constants and/or reaction pathways.

Building on existing/long-standing successful collaborations of Dutch astronomers, laboratory/experimental and theoretical researchers - that led to the Dutch Astrochemistry Network (DAN) - we announce a focused research programme of 7 highly interwoven projects that aim to address the following astrochemical questions tightly linked to the new JWST data:

Inheritance versus Reset: How do ice and gas-molecules evolve together and get processed from molecular clouds to disks?

Carbon Cycle: How is carbon cycled through small gas-phase hydrocarbons and carbonaceous dust in different cosmic environments?

More information about the Dutch Astrochemistry Network can be found at https://www.nwo.nl/en/researchprogrammes/astrochemistry.

We are advertising seven between PhD and postdoc projects within this network to address the above questions. More details about each position can be found at the respective institutes vacancy webpages and/or by contacting the main supervisors.

1. **Probing spatially variable ice processing with radiative transfer** 3-yr postdoc position at Leiden University with Melissa McClure (Leiden University), Inga Kamp (University of Groningen), Stephanie Cazaux (TU Delft) and Rens Waters (Radboud University Nijmegen)
2. **Bridging the gap: modeling molecular ice abundances at the micro- and macro level** 4-yr PhD position at Leiden University with Thanja Lamberts (Leiden University), Herma Cuppen (Radboud University Nijmegen) and Serena Viti (Leiden University)
3. **Laboratory ice data in support of JWST ice observations** 1.5-yr postdoc position at Leiden University with Harold Linnartz and KoJu Chuang (both Leiden University)

4. **Energetic processing of ices** 1.5-yr postdoc position at Radboud University Nijmegen with Britta Redlich (Radboud University Nijmegen), Herma Cuppen (Radboud University Nijmegen) and Thanja Lamberts (Leiden University)
5. **Rovibrational emission spectra of small linear organics** 4-yr PhD position at University of Groningen with Floris van der Tak (SRON/University of Groningen), Gerrit Groenenboom (Radboud University Nijmegen), Inga Kamp (University of Groningen), Ewine van Dishoeck (Leiden University) and Ad van der Avoird (Radboud University Nijmegen)
6. **PAH spectroscopy for UV irradiated environments** 4-yr PhD position at Radboud University with Sandra Bruenken, Jos Oomens (both Radboud University Nijmegen), Wybren Jan Buma and Alessandra Candian (both University of Amsterdam)
7. **The contribution of PAHs to interstellar carbon chemistry** 4-yr PhD position at University of Amsterdam with Alessandra Candian, Wybren Jan Buma (both University of Amsterdam) and Inga Kamp (University of Groningen)

Deadline: See individual vacancies at Universities webpage

E-mail for contact: a.candian2@uva.nl; Main project advisors for details on positions.

Webpage: https://www.nwo.nl/en/researchprogrammes/astrochemistry/

AstroPAH Newsletter

http://astropah-news.strw.leidenuniv.nl
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Submission deadline: 6 October 2023