European Conference on Laboratory Astrophysics

ECLA 2026, “Exploring the cold Universe”

Scientific program

Monday, September 21

9:15 Welcome

Session 1: New Insights from JWST and ALMA - Setting the Stage (Chair: Annemieke Petrignani)

- 09:30 **Ewine van Dishoeck:** Laboratory astrophysics in the JWST and ALMA era (35+10)
- 10:15 **Inga Kamp:** A unique window into planet formation by combining JWST and ALMA (35+10)
- **11:00 Coffee break**
- 11:30 **Arshia Jacob:** Small molecules and its role in the Universe: A journey through its past and its exciting future (35+10)
- 12:15 **Maria Drozdovskaya**: First results from the COMPASS ALMA Large Program (12+3)
- 12:30 **Caroline Gieser:** A song of ice and fire: Linking ice and gas-phase chemistry in the high mass hot core IRAS 18089 (12+3)
- 12:45 **Yao Liu**: Dust Properties in Protoplanetary Disks Revealed by JWST/MIRI (12+3)

13:00 Lunch

Session 2: (Exo)-Planetary Atmospheres: A New Challenge (Chair: Thomas Henning)

- 14:30 **Christiane Helling**: Different chemical regime in exoplanet atmospheres: From plasma to cloud formation in one atmospheres (35+10)
- 15:15 **Antonio García Munoz:** Laboratory, theoretical and modelling needs for exo-aeronomy (25+5)
- 15:45 **Laura Schöller**: Pressure Broadening Coefficients of SO_2 by He for Studies of Exoplanetary atmospheres (12+3)
- **16:00 Coffee Break**
- 16:30 **Eva-Maria Ahrer:** Observations of Exoplanetary Atmospheres: From highlights and challenges with JWST to upcoming missions (25+5)
- 17:00 **Piero Ferrari**: Laboratory far-infrared spectra, fragmentation chemistry and cooling dynamics of sulfur allotropes (12+3)
- 17:15 **Jack Fulker**: Circular Dichroism Spectroscopy: Disentangling Intrinsic Molecular Chiroptical Response from Environment-Induced Effects (12+3)
- 17:30 **Maëva Louis:** Diving into the photochemistry of oxygen- and sulfur-bearing polycyclic aromatic hydrocarbons: oxanthrene and thianthrene (12+3)
- 17:45 **Sergio Ioppolo**: Formation and Stability of the Building Blocks of Life on Space-Relevant Ice Grain Analogs (12+3)

18:15 Bus to town

Tuesday, September 22

Session 3: Spectroscopic Characterization of Molecules and Solids (Chair: Holger Kreckel)

- 9:15 **Stephan Schlemmer:** Missing Ions in Laboratory and Space (35+10)
- 10:00 **Cornelia Jäger:** Astrochemical reactions on dust grains, chemical and spectral signatures (25+5)
- 10:30 **Luis Bonah:** Electronic spectra of mass- and shape-selected polycyclic aromatic hydrocarbons (12+3)
- 10:45 **Weslley Guilherme Silva**: Ground state rotational spectrum of protonated methanol ($CH_3OH_2^+$): The first step towards its interstellar detection (12+3)
- **11:00 Coffee break**
- 11:30 **Emmanuel Dartois:** Ice grains spectroscopy from dense cloud to protoplanetary discs: from laboratory to JWST observations. (25+5)
- 12:00 **Chiara Schleif:** High-resolution spectroscopy of HCN^+ and HNC^+ using an ion trap setup (12+3)
- 12:15 **Cristopher Kreuzig:** Measuring & Linking Mid-Infrared SiO_2 - Spectra to Dust Aggregate Growth in the GT4P Levitation Chamber – I. Scientific Approach (12+3)
- 12:30 **Karine Demyk:** Infrared spectroscopy of gas-phase hydrogenated and methylated pyrenes: from laboratory spectra to the simulated 3.4 μm emission band (12+3)
- 12:45 **Florian Foitzik:** Helium-Tagging Spectroscopy of PAH and Fullerene Cations (12+3)

13:00 Lunch

Session 4: Complex Organic Molecules (Chair: Christine Joblin)

- 14:30 **José Cernicharo:** Quijote: A new view of chemical complexity in space (35+10)
- 15:15 **Gabi Wenzel:** Aromatic Complexity in the Interstellar Medium (25+5)
- 15:45 **Laura Slumstrup:** The role of Interstellar Dust in the formation of Complex Organic Molecules (12+3)
- **16:00 Coffee Break**
- 16:30 **Cornelia Meinert:** Challenges in the detection of *chiral* COMs in interstellar ice analogues, meteorites and in the rationalization of their formation pathways (25+5)
- 17:00 **Frederik Eckhardt:** Ex-situ mass spectrometry analysis of organic residues from electron-irradiated ethanolamine ice (12+3)
- 17:15 **Sergiy Krasnokutski:** Formation of Carbonaceous Molecules and Peptides in Space from Formation to Spectroscopic Identification (12+3)
- 17:30 **Marissa Maney:** Isotopically Constrained Formation of Nitrogen-rich Organic Residues from UV Irradiation of CH_3OH:NH_3 Astrophysical Ice Analogs (12+3)
- 17:45 **Isabelle Fourré:** Gas-phase formation of sulphur-containing interstellar molecules of the HCS-R (R=CN, CCH) family: a computational study. (12+3)

18:00 – 19:00 Posters
19:15 Bus to town

Wednesday, September 23

Session 5: Gas Phase Reaction Rates (Chair: Sandra Brünken)

- 9:15 **Henning Zettergren:** Studies of gas phase reactions with cryogenic electrostatic storage rings (35+10)
- 10:00 **Ludovic Biennier:** Low-temperature gas-phase reactive collisions explored with uniform supersonic flows (25+5)
- 10:30 **Lukas Berger:** Fundamental ion-neutral reactions studied under interstellar conditions (12+3)
- 10:45 **Lucia Enzmann:** Low-energy electron collisions with C_{60}^+ in the Cryogenic Storage Ring (12+3)
- **11:00 Coffee break**
- 11:30 **Roland Wester:** Formation and destruction pathways of interstellar negative ions (25+5)
- 12:00 **Danial Mahan Mohammadi:** Gas-Phase Infrared Spectroscopy of Ethynyl-Bearing PAHs from Electrical Discharge using FELIX (12+3)
- 12:15 **Miguel Jiménez-Redondo:** Isomer-resolved ion-molecule reaction kinetics of HCO^+ and HOC^+ studied in a low-temperature ion trap (12+3)
- 12:30 **Marius Gerlach:** Spectroscopic product identification and kinetic modelling of the reaction of NCO^+ and $HNCO^+$ with H_2 at cryogenic temperatures (12+3)
- 12:45 **Ian Sims:** Product branching in the CN + propene reaction at very low temperatures probed by chirped-pulse millimeter wave spectroscopy (12+3)

13:00 Lunch

Lab Tours

Conference dinner
20:00 Tom Herbst: Enabling ELT: Two Technologies that Make it All Possible

Thursday, September 24

Session 6: Molecular Theory (Chair: Jonathan Tennyson)

- 9:15 **Alexandre Faure:** Molecular theory needs for astrochemical modeling (35+10)
- 10:00 **Jérôme Loreau:** Collisional excitation of interstellar organic molecules (25+5)
- 10:30 **Sándor Demes:** State-to-state collisional data from quantum scattering theories to simulate the rotational excitation of cyclopentadiene in interstellar environments (12+3)
- 10:45 **Stefan Bromley:** When Two Worlds Collide: How Dust Grain Collisions can Drive Complex Chemistry (12+3)
- **11:00 Coffee break**
- 11:30 **Sergey Yurchenko:** ExoMol at All Wavelengths: Spectroscopic Data for Exoplanet Atmospheres from JWST and Ariel to the ELTs (25+5)
- 12:00 **Zsolt Mezei:** Electron-driven reactivity of molecular cations: from mechanisms to cross sections (12+3)
- 12:15 **Tobe Vorsselmans:** Binding Energies of Sulfur-Bearing Species on Charged Interstellar Ice: A Density Functional Theory Study (12+3)
- 12:30 **Niccolò Bancone:** TD-DFT Modeling of ECD in Chiral Alcohols: Conformation and Solvation (12+3)

13:00 Lunch

Session 7: Surface and Ice Chemistry (Chair: Tushar Suhasaria)

- 14:30 **Liv Hornekaer:** Novel Pathways to Complex Organic Molecule Formation in Space (35+10)
- 15:15 **Rafael Martín-Doménech:** Exploring the chemical evolution of sulfur in the laboratory (25+5)
- 15:45 **Eddy Abdo:** Heavy-ion irradiation of interstellar dust analogs -interaction at the nanometer scale (12+3)
- **16:00 Coffee Break**
- 16:30 **Ko-Ju Chuang:** Unlocking the Interstellar Sulfur Puzzle: Laboratory Constraints from Interstellar Ice Chemistry (25+5)
- 17:00 **Frederik Doktor:** Are interstellar PAHs more deuterated than they should be? (12+3)
- 17:15 **Alfred Thomas Hopkinson:** Non-aqueous peptide creation via the energetic processing of glycine (12+3)
- 17:30 **Lawry Honold:** Advanced Analytical Workflow to Characterize Organic Residue Generated from Astrophysical Ice Analogues (12+3)
- 17:45 **Antoine Hacquard:** Impact of Oxygen on Carbonaceous Dust Formation in the presence of Iron under Circumstellar-like Conditions (12+3)

18:00 – 19:00 Posters

19:15 Bus to town

Friday, September 25

Session 8: New Experimental Techniques (Chair: Thomas Henning)

- 9:15 **Stephan Schlemmer and Inga Kamp**: Discussion on future directions (45)
- 10:00 **Deepak Sharma**: Toward gas phase spectroscopy of complex molecular ions in a cryogenic ion trap (25+5)
- 10:30 **Christine Joblin:** Ion-Molecule Reactions: Efficient Pathways for PAH Growth (12+3)
- 10:45 **Selina Gaisser:** A new 4k-pixel microcalorimeter detector MOCCA for molecular fragment mass measurements at CSR (12+3)
- **11:00 Coffee break**
- 11:30 **Jérôme Bernard**: Polar Mini-Ring @ SOLEIL: A Cryogenic Electrostatic Ion Storage Ring to Quantify the Relaxation Dynamics of VUV-Excited PAHs (25+5)
- 12:00 **Suvasthika Indrajith:** Probing Charge-Transfer and Ion-Neutral Reactions at Low Energy with a Cryogenic Merged-Beam Device (12+3)
- 12:15 **Thibault Nguyen Trung:** Heavy ion irradiation of astrophysical ice analogs: Forthcoming improvements at GANIL facilities (12+3)

13:00 Departure / Bus to town

Conference dinner talk (Wednesday, 23rd)

Enabling ELT: Two Technologies that Make it All Possible

Tom Herbst

In a very few years, European astronomers will begin using the 39-meter Extremely Large Telescope (ELT). This facility represents a quantum leap in collecting area and spatial resolution, and it will likely spark a revolution in our understanding of the Universe. Two critical technologies, Mirror Segmentation and Adaptive Optics are at the heart of this breakthrough. In this talk, I will outline how we got here in terms of large telescopes and explain the how's and why's of these two essential innovations.

Abstracts: Oral contributions

Heavy-ion irradiation of interstellar dust analogs -interaction at the nanometer scale-

Eddy Abdo[1], Emmanuel Dartois[1], Marin Chabot[2], Olivier Sublemontier[3], Thibault Nguyen Trung[4], Emeline Charon[3], Frieder Koch[5], Pascal Simon[5], Ina Schubert[5], Marie Godard[1], Thomas Pino[1], Cécile Engrand[2], David Troadec[6], Sandra Casale[7], and Joffrey Frereux[8, 9]

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4 Centre de recherche sur les Ions, les Matériaux et la Photonique Université Caen Normandie, ENSICAEN, CNRS, CEA, Normandie
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6 University Lille, CNRS, Centrale Lille, Junia, University Polytechnique Hauts de France, UMR 8520-IEMN, F59000 Lille, France
7 Laboratoire de Réactivité de Surface (LRS), UMR7197, Sorbonne Université, Campus Pierre et Marie Curie, 75005 Paris, France
8 Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, 1348 Louvain-la-Neuve, Belgium
9 DAAA, ONERA, Institut Polytechnique de Paris, 92190 Meudon, France

Carbonaceous and siliceous interstellar dust grains are exposed to cosmic rays in the diffuse and dense interstellar medium. This interaction alters the morphology and surface and bulk chemistry of the grains, playing a role in the interstellar medium matter cycle evolution. To better understand the effect of cosmic rays on interstellar dust, we produced two types of analogs in the laboratory: hydrogenated amorphous carbon samples, and polystyrene-SiO_2 composite samples. Irradiations of these samples were carried out at the GSI UNILAC accelerator (Darmstadt, Germany) using a heavy-ion beam, simulating the irradiation by Galactic cosmic rays. The irradiation's chemical and physical effects were studied by following the infrared features of the samples throughout irradiation, and by imaging them post-irradiation using transmission electron microscopy and energy dispersive X-ray imaging. We were able to determine the C-H destruction cross sections of the different analogs, the size of tracks produced by the ions in the matrices, as well as the ion-induced morphological changes at the nanoscale. Such irradiated grains might promote the chemistry and thus help in the complex molecules budget in the interstellar medium.

Observations of Exoplanetary Atmospheres: From highlights and challenges with JWST to upcoming missions

Eva-Maria Ahrer[1]

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Observations of directly imaged and transiting exoplanets provide the opportunity to probe the atmospheric compositions of a diversity of exoplanets. Direct imaging allows us to measure their spectra directly, while for the transiting exoplanet we use the starlight transmitted through the exoplanet's limb during transit. By analysing these subtle spectral variations, we can identify the presence and abundance of various species, including water vapour, methane, alkali metals, as well as clouds and hazes.

In this talk, I will first review recent scientific highlights regarding the atmospheres of Jupiter-sized planets, as giant planets are particularly amenable targets for both directly imaged and transiting planets as they are large and tend to have extended atmospheres. In particular JWST's infrared capabilities have revealed a breadth of new scientific advances: absorption features from molecules such as H_2O, CO_2, NH_3 and CO with exquisite precision, detections of cloud properties, and constraints on the photochemistry at play in giant planet atmospheres (e.g., see also review from Espinoza & Perrin, 2025).

While JWST has advanced our understanding of exoplanet atmospheres, the data are not without their challenges, especially for smaller planets. So in the second half, I will discuss instrumental and astrophysical limits faced by the exoplanet community - from detector problems to stellar activity - while also giving an overview of the lessons learned by the community thus far.

Finally, I will discuss the links between JWST and current and upcoming instruments and missions. I hope to provide the audience with new discussion points regarding the study of exoplanet atmospheres and the link to laboratory astrophysics.

References:

Espinoza, N., Perrin, M. (2025), Highlights from Exoplanet Observations by the James Webb Space Telescope. In: Deeg, H.J., Belmonte, J.A. (eds) Handbook of Exoplanets . Springer, Cham. https://doi.org/10.1007/978-3-319-30648-3_216-1

TD-DFT Modeling of ECD in Chiral Alcohols: Conformation and Solvation

Niccolò Bancone,[1] Jana Bocková,[1] Jack E. Fulker,[1] Jérémie Topin,[1] Nykola C. Jones,[2] Søren V. Hoffman,[2] Cornelia Meinert.[1]

1 Institut de Chimie de Nice, University Côte d'Azur, France
2 ISA, Department of Physics and Astronomy, Aarhus University, Denmark

Electronic Circular Dichroism (ECD) is a spectroscopic technique with exceptional sensitivity to molecular conformation and chemical environment.[1,2] Gas-phase ECD measurements grant direct access to the intrinsic conformational properties of isolated molecular systems, while solution-phase experiments reveal how those conformations, and their associated chiroptical responses, are modulated by the surrounding medium. Because most chemical structures are sufficiently flexible to populate multiple conformational states, the chiroptical response of a real macroscopic system reflects a conformational ensemble rather than a single, well-defined geometry. Aqueous solvation can further reshape chiroptical properties through two principal, non-mutually exclusive mechanisms:

1. Redistribution of conformational populations
2. Modification of the chiroptical response of individual conformers

Assigning spectral bands, identifying the relevant conformational populations and electronic transitions, and disentangling solvent contributions are all inherently challenging tasks that cannot be fully resolved on a purely experimental basis. Atomistic simulations can bridge this gap, connecting macroscopic spectral observables to their molecular-level interpretation and enabling band-structure assignment and the characterization of excited states in both the gas and liquid phases.
This work presents the spectral deconvolution of the gas-phase and aqueous solution ECD and anisotropy spectra of the chiral alcohols *R*-glycidol and (2*R*,3*R*)-butanediol, using Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT). The computational strategies employed to model conformational distributions, chiroptical spectra, and water solvation are described in detail, with a critical discussion of their limitations and inherent system dependence.

References:
[1] Padula, D., Pescitelli, G. *Molecules*, 23(1), 128 (2018).
[2] Macleod, N. A., Butz, P., Simons, J. P., Grant, G. H., Baker, C. M., & Tranter, G. E. *Phys. Chem. Chem. Phys.* 7(7), 1432 (2005).

Fundamental ion-neutral reactions studied under interstellar conditions

Lukas Berger[1], Florian Grussie[1], Manfred Grieser[1], Leonard Isberner[1,2], Oldrich Novotny[1], Xavier Urbain[3], and Holger Kreckel[1]

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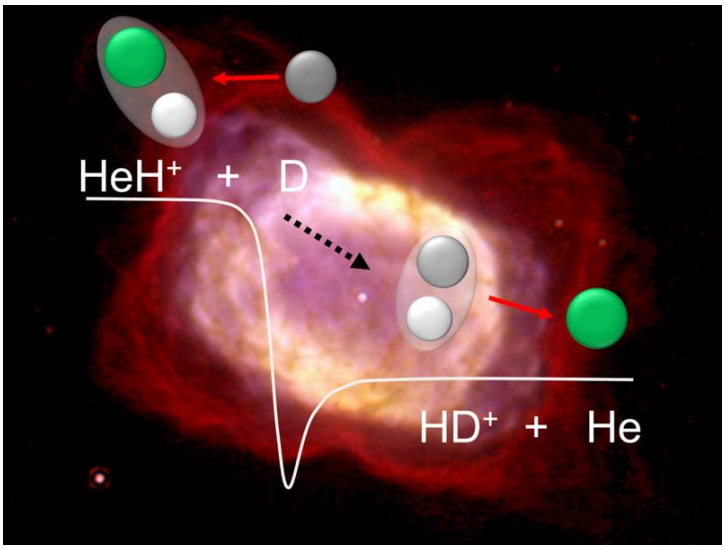
2 Columbia Astrophysics Laboratory, Columbia University, New York, USA
3 Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Louvain-la-Neuve, Belgium

Ion-neutral reactions are the main driver of cold gas-phase chemistry in the interstellar medium (ISM), and reliable rate coefficient data for key molecular systems require measurements performed under conditions that closely approach the ISM's low temperatures and densities [1,2]. The Cryogenic Storage Ring (CSR) at the Max Planck Institute for Nuclear Physics provides a unique platform for such measurements. Cooled to ~5 K by a closed-cycle liquid-helium system, it provides an environment with strongly suppressed blackbody radiation and residual gas densities as low as 10^3 cm^{-3}, while the ion-optical lattice stores ions with kinetic energies of 20–300 keV per unit charge [3]. A dedicated neutral-beam line merges stored ions with a fast beam of ground-term atoms produced by photodetachment of negative ions [4]. Independent control of the ion and neutral beam velocities enables absolute, energy-resolved reaction rate coefficient measurements with cold molecular ions.



We present the CSR setup together with recent merged-beam measurements of the reaction $HeH^+ + D \rightarrow HD^+ + He$ [5]. We find the reaction to be barrierless and to remain fast at low collision energies, showing that previous studies severely underestimated the low-temperature rate coefficient due to an artifact in a widely used potential-energy surface. Since HeH^+ is considered a potential coolant during the epoch of the formation of the first stars in the early Universe, this result calls for a reassessment of primordial helium chemistry.

References

[1] Grussie et al., Phys. Rev. Lett. 132.24 (2024)
[2] Grussie et al., Phys. Rev. A 109.6 (2024)
[3] von Hahn et al., Rev. Sci. Instrum. 87.6 (2016)
[4] Grussie et al., Rev. Sci. Instrum. 93.5 (2022)
[5] Grussie et al., A&A 699 (2025)

Polar Mini-Ring @ SOLEIL: A Cryogenic Electrostatic Ion Storage Ring to Quantify the Relaxation Dynamics of VUV-Excited PAHs

Jérôme Bernard[1], Suvasthika Indrajith[1], Guillaume Montagne[1], Laurent Nahon[2], Alexandre Giuliani[2], J.-F. Gil[2], Anthony Bonnamy[3], Ana I. Lozano[3], Christine Joblin[3]

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2 Synchrotron Soleil, L'Orme des Merisiers, St. Aubin BP48, F-91190, Gif sur Yvette, France
3 Université de Toulouse, CNES, CNRS, Institut de Recherche en Astrophysique et Planétologie (IRAP), F-31028 Toulouse, France

Polycyclic aromatic hydrocarbons (PAHs) are key components in photodissociation regions. However, the dynamics of internal energy relaxation following ultraviolet excitation remains incompletely understood due to limited experiments under well-controlled conditions. In particular, disentangling the roles of initial excitation, internal energy redistribution, isomerization, radiative cooling, and unimolecular dissociation on their survival remains challenging, as these processes span a broad range of overlapping dynamical timescales depending on molecular structure, electronic structure and internal energy.

A new cryogenic version of the Mini-Ring electrostatic ion storage ring has recently been commissioned for these studies. Its interfacing with the DESIRS beamline at the SOLEIL synchrotron facility is currently underway (cf. Figure 1). Particular attention has been paid to synchronizing the photon excitation with the ion motion in the ring. A dedicated VUV photon beam chopper has been designed to provide adjustable pulse structures with variable duty cycles.

Using this combination, we expect to prepare cold PAH ions and subsequently induce

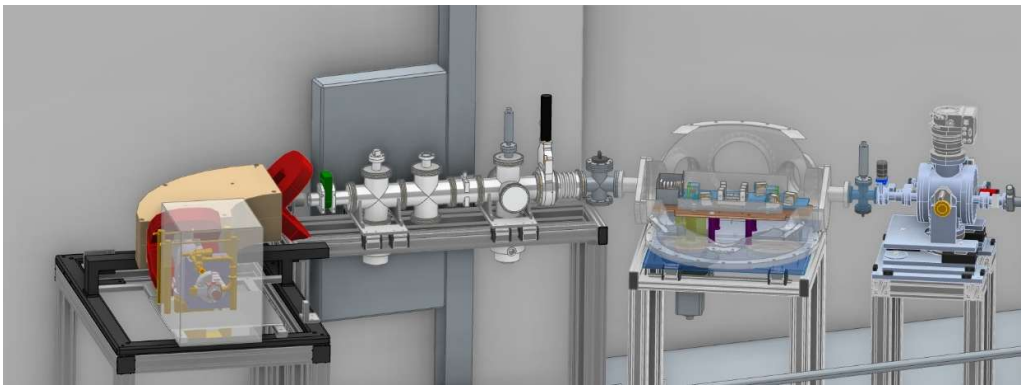

Figure 1: Schematic view of the experimental setup, including the Polar Mini-Ring and its ion beamline, together with the VUV photon-beam chopper developed for the coupling with the DESIRS beamline at the SOLEIL synchrotron facility.

dissociation via single VUV-photon absorption. This well-defined configuration should provide direct access to unimolecular fragmentation rates, offering stringent constraints on statistical models based on RRKM and Arrhenius-type descriptions. Polar Mini-Ring will also enable VUV action spectroscopy and investigations of radiative cooling in competition with fragmentation.

Acknowledgments: This work is supported by l'Agence Nationale de la Recherche in France (Project SynPAHcool under grant ANR-21-CE30-0010).

Low-temperature gas-phase reactive collisions explored with uniform supersonic flows

Ludovic Biennier

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One of the major questions in astrophysics is to understand how the cycle of interstellar matter leads to an increase in molecular complexity. The role played by gas-phase and surface processes in this cycle remains debated. One of the challenges is to determine the nature and abundance of the molecules observed, almost exclusively in the gas-phase, in a wide variety of astrophysical environments, from interstellar clouds, star-forming regions, to planetary atmospheres. Among the key mechanisms governing the gas-phase chemistry of these objects are bimolecular reactions.

The elucidation of the mechanisms of the underlying elementary reactions, in particular at low collision energies, provides crucial information for modeling the chemistry of these environments. Despite long-term efforts, the kinetics and nature of the products of many key gas-phase reactions remain poorly understood at relevant temperatures.

In our laboratory, we have developed an original method associating the CRESU technique to generate cold uniform supersonic flows, a mass selective source of ions (SIS), and mass spectrometry to study reactive collisions between molecular ions and neutral species at low temperature down to 15 K [1]. The CRESU-SIS instrument has been applied to the study of elementary reactions of the methyl cation with small hydrocarbons. Our experimental measurements combined with quantum calculations confirm that CH_3^+ is a vector of complexity in the interstellar medium through ion-molecule reactions, thereby highlighting the role of ionic processes in such cold environments.

Neutral processes play a key role as well in the build-up of molecular complexity. The latest upgrade of the CRESUSOL machine [2], which combines the CRESU method with photoionization coincidence mass spectrometry and the tunable synchrotron VUV radiation will be presented. This facility can be used to explore reaction products of radical-neutral reactions down temperatures as low as 20 K. CRESUSOL is expected to pave the way to the systematic investigation of radical-neutral reaction products. To date, only a handful of these has been examined below 50 K.

References:
[1] B. Joalland et al., "A mass-selective ion transfer line coupled with a uniform supersonic flow for studying ion–molecule reactions at low temperatures," J. Chem. Phys. **150**, 164201 (2019).

[2] O. Durif et al. , “A new instrument for kinetics and branching ratio studies of gas phase collisional processes at very low temperatures” Rev. Sci. Instrum. **92**, 1, 014102 (2021).

Electronic spectra of mass- and shape-selected polycyclic aromatic hydrocarbons

Luis Bonah[1], Anne P. Rasmussen[1,2], Zekai Li[1], Corentin Rossi[1], Uma Namangalam[1], Bérenger Gans[1], Ugo Jacovella[1]

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The more than 340 molecules detected in space range from small, two-atomic molecules, such as CH^+, all the way up to C_{60}^+, C_{60}, and C_{70}. However, except for cyanocoronene ($C_{24}H_{11}CN$), there is a large gap of molecules containing 18 to 59 carbon atoms. This gap is due to the lack of laboratory fingerprints to identify these molecules in space—even though this gap is considered crucial for solving a variety of astronomical questions, like understanding the astronomical carbon budget or solving the origin of the diffuse interstellar bands.
Therefore, we aim to record the electronic spectra of mass- and shape-selected polycyclic aromatic hydrocarbons (PAHs). The ions are created via laser ablation in a hydrogen-rich region and then shape-selected via a drift tube. The latter exploits the fact that different shapes have different collisional cross sections (CCS) with the buffer gas and thus take different times to travel through the drift tube. Then, the molecules are mass-selected and stored in a cryogenically cooled 3D Paul trap for spectroscopic interrogation.
Electronic spectra of first hydrocarbons have been recorded with resonance-enhanced photodissociation (REPD) methods and will be presented. For future measurements, implementing the recently developed leak-out spectroscopy (LOS) could provide an additional degree of filtering to nicely complement the existing capabilities of the setup.

Dunham, *Publ. Astron. Soc. Pac.* **49** (1937) 26
Foing & Ehrenfreund, *Nature* **369** (1994) 296
Cami *et al.*, *Science* **5996** (2010) 1180
Wenzel *et al.*, *Astrophys. J. Lett.* **984** (2025) L36
Rossi *et al.*, *Chem. Methods* **9** (2025) e202500013

When Two Worlds Collide:
How Dust Grain Collisions can Drive Complex Chemistry

Alexandros Kyriazis[1,2], Albert Rimola[2,3], Stefan T. Bromley[1,4]★

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4 Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain

Although observations reveal the presence of silicate and carbonaceous material in interstellar grains, these components are generally interpreted as belonging to distinct dust populations. While some dust models incorporate aggregated silicate-carbonaceous grains, there is little direct evidence for such mixed grains. Here, we use the Nucleated Atomistic Grain Growth Simulator (NAGGS) to prepare realistic silicate and hydrogenated carbonaceous nanograins that have structures and compositions that are consistent with observations (Guiu et al. 2026). We then accurately simulate collisions between these grains at velocities representative of a range of astrophysical environments to determine the physical and chemical outcomes of these nanograin interactions (Kyriazis et al. 2026). We find that only very specific collisional velocities can induce aggregation, with bouncing/weak interactions (< 3.5 km s^{-1}) or fragmentation ($\gtrsim 7.5$ km s^{-1}) being the more likely outcomes. Carefully tracking the chemical species resulting from fragmentation we find a high fraction of CO molecules, along with hydrocarbons, complex organic molecules, molecular silicates, and mixed carbonaceous-silicate clusters - many of which have been observationally detected. We note that most of these species are not simply mechanical fragments of the original grains but follow from reactions involving grain material that are enabled using the collisional energy. We thus suggest that collisions between thermally cold grains could provide a viable pathway for generating wide range of molecular species. We thus provide a simple credible mechanism linking the physics of grain processing with observed complex interstellar chemistry. Finally, we discuss how laboratory experiments could be employed to explore our proposed collisional grain chemistry.

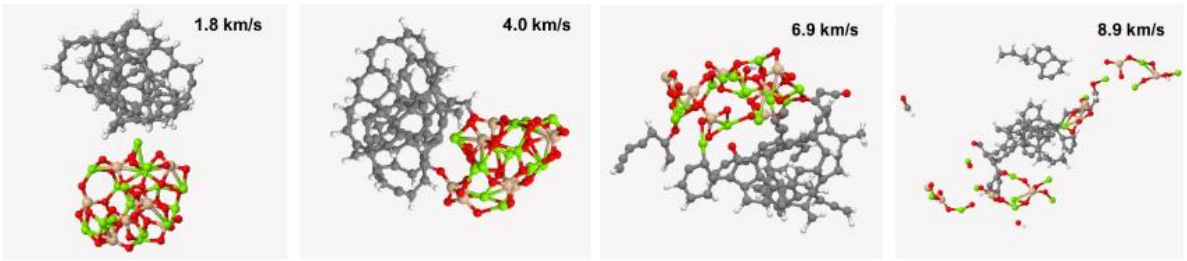

Figure 1. Results of collisions between hydrogenated carbonaceous and silicate nanograins at a range of velocities.

References

J. Mariñoso Guiu, A. Maciá Escatllar, S. T. Bromley, The Nucleated Atomistic Grain Growth Simulator (NAGGS): application to the size-dependent structural and physical properties of nanosilicate dust, A&A, 706, A303 (2026).

A. Kyriazis, A. Rimola, S. T. Bromley, When Two Worlds Collide: How Collisions Between Silicate and Carbonaceous Nanograins can Drive Complex Chemistry, A&A (2026) under revision.

QUIJOTE: A NEW VIEW OF CHEMICAL COMPLEXITY IN SPACE

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This talk is devoted to the analysis of chemical complexity in interstellar and circumstellar clouds. In particular, I will present the recent results obtained with the QUIJOTE line survey of the cold dark core TMC-1 and of the carbon-rich evolved star IRC+10216. The observations have been carried out with the YEBES (Spain) 40m radio telescope in the Q-band. A new set of receivers have been installed in the telescope within the frame of the ERC synergy Nanocosmos project that allows to cover the whole 31-50 GHz band in dual polarization with a spectral resolution of 38.15 kHz. The survey in TMC-1 reaches an unprecedented sensitivity varying between 0.06 and 0.20 mK, and allows to search for new molecules in a line by line (no stacking) detection procedure. These new data have permitted to detect many protonated species of abundant molecules, several sulfur-bearing species, cycles (benzyne, cyclopentadiene, indene, acenaphthylene, phenalene), radicals, and long hydrocarbon chains. I will show the present chemical models we have performed to explain the chemistry of these species and in particular the possible reactions leading to the formation of these cycles. We suggest that a bottom-up approach starting with reactions of simple radicals, such as propargyl and the vinyl radical, with vinyl and allyl acetylene and other hydrocarbons could reproduce satisfactorily well the observed abundances. **None** of the new molecules found in TMC-1 are detected towards the carbon-rich evolved star IRC+10216, in particular the PAHs which were expected to be formed in this type of stars.

Unlocking the Interstellar Sulfur Puzzle: Laboratory Constraints from Interstellar Ice Chemistry

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The "missing sulfur" problem is a long-standing challenge in star-forming regions, particularly in dark, cold molecular clouds where interstellar ice mantles form. Although these icy mantles are widely regarded as a possible sulfur reservoir, the underlying solid-state chemical networks and their spectroscopic signatures remain poorly constrained. This talk highlights recent laboratory advances tracing the chemical evolution of sulfur in interstellar ices, from simple precursor species to complex sulfur-bearing molecules.

By reproducing molecular-cloud conditions in the laboratory, we investigate the mechanisms governing sulfur chemistry on icy dust grains. Particular attention is given to H_2S, one of the earliest sulfur-bearing species expected to form on grain surfaces, and to its interactions with astrophysically relevant atoms and molecules in the absence of external radiation. These non-energetic processes show that repeated hydrogenation–dehydrogenation cycles efficiently drive SH-radical chemistry, leading to substantial chemical desorption in H-rich environments and the formation of OCS through reactions with accreted CO ice, consistent with astronomical spectroscopic evidence.[1–4] For sulfur-bearing organic molecules, reactions involving atomic carbon provide additional pathways to H_2CS and CH_3SH, species that have traditionally been linked to the hydrogenation of CS, an analog of CO. Furthermore, low-temperature acid–base chemistry between H_2S and NH_3 leads to efficient formation of ammonium hydrosulfide (NH_4SH), identifying it as a promising carrier of the ubiquitous 6.85 μm absorption feature and a potential precursor to material incorporated into cometary ices.[5,6]

Beyond these non-energetic pathways, energetic processing, such as UV photons and cosmic rays, initiates more extensive reaction networks that generate a diverse population of sulfur-bearing complex organic molecules.[7] Together, these results demonstrate how sulfur can be incorporated into increasingly complex species and transformed throughout the evolution of star-forming environments. The resulting laboratory framework provides critical constraints on the interpretation of ice observations and offers new insights into the chemical evolution of the hidden sulfur reservoir in the interstellar medium.

References:
[1] Oba et al. Nat. Astron., 2, 228 (2018)
[2] Santos et al. A&A, 678, A112, (2023)
[3] Santos et al. A&A, 690, A24, (2024)
[4] Slavicinska et al. ACS-ESC, 9, 8, 2148, (2025)
[5] Slavicinska et al. A&A, 693, A146, (2025)
[6] Vitorino et al. MNRAS, 533, 52 (2024)
[7] Muñoz Caro et al. Nat. Rev. Chem., 9, 537 (2025)

Ice grains spectroscopy from dense cloud to protoplanetary discs: from laboratory to JWST observations.

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Interstellar clouds are the cradles of star and planet formation, where gas and dust evolve from diffuse ISM conditions toward protoplanetary discs. JWST spectroscopy of dense clouds now demonstrates that grain growth to micron scales begins before the protostellar phase. This early aggregation modifies ice absorption profiles, reshaping the band structure in ways that directly affect abundance determinations. The inferred size distribution implies efficient mass transfer from small to large grains, a reduction in reactive surface area, and alters radiative transfer through cloud material. JWST observations provide constraints on the extent of icy grain growth in dense environments, with critical consequences for both astrochemistry and the initial conditions of disc formation. At later evolutionary stages, JWST spectra of nearly edge-on protoplanetary discs reveal ice absorption bands with diverse optical depths and atypical profiles, posing significant challenges for radiative transfer modelling and for our current picture of dust and ice in disc environments.

To interpret these features and constrain disc evolutionary state, we'll discuss models relying on laboratory measured optical constants and accounting for dust grain size distributions, shapes, and compositions, aiming to reproduce the observed JWST spectra. The goal is to constrain dense clouds/disc icy grains properties by reproducing observed SEDs, dust–ice spatial distributions observed, and key spectral features.

References:
Dartois, E., Noble, J.A., Bergner, J.B., et al., 2026, A&A, 705, L14. doi:10.1051/0004-6361/202557177
Dartois, E., Noble, J.A., McClure, M.K., et al., 2025, A&A, 698, A8. doi:10.1051/0004-6361/202452966
Dartois, E., Noble, J.A., Caselli, P., et al., 2024, Nature Astronomy, 8, 359. doi:10.1038/s41550-023-02155-x
Dartois, E., Noble, J.A., Ysard, N., et al., 2022, A&A, 666, A153. doi:10.1051/0004-6361/202243929

State-to-state collisional data from quantum scattering theories to simulate the rotational excitation of cyclopentadiene in interstellar environments

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Recent observations revealed an amazing molecular complexity in space through the detection of a series of complex organic molecules and large carbon cycles, mostly in cold interstellar clouds [1]. However, to properly interpret the detected observational spectra, a complex physico-chemical analysis is often needed, which accounts the non-local thermodynamic equilibrium (non-LTE) properties of the astronomical source. This can be only carried our through incorporating state-to-state collisional excitation data for the particular species in radiative transfer models, since their population in this regime is governed by two competing processes: collisional and radiative.

Cyclopentadiene (C_5H_6) has recently been detected in several cold molecular clouds, such as TMC-1 [2] and L1495B [3]. Since there were no collisional data available at the time of these observations, the authors have assumed LTE-conditions. Motivated by this, we have carried out quantum scattering calculations to derive accurate state-to-state rate coefficients for the rotational excitation of C_5H_6 in collisions by helium. These are performed on a new 3-dimensional rigid rotor potential energy surface [4]. We have incorporated the close-coupling for low-lying and coupled-states scattering method for higher-lying rotational states. Our study covers a total of about 225 *ortho*- and *para*-C_5H_6 states, separately, with rotational quantum numbers reaching $j \leq 25$. The calculated collisional data were implemented into non-LTE radiative transfer codes, allowing a proper astrophysical modeling of C_5H_6 in a wider range of interstellar environments, with kinetic temperatures ranging from 10 to 50 K.

The first radiative transfer simulations indicate that most cyclopentadiene rotational levels are thermalized under typical conditions of cold interstellar clouds (~10 K), and only exhibit negligible non-LTE effects. Nevertheless, we have some very important findings regarding the general collisional excitation mechanisms of larger cyclic and aromatic species in space, which can have an impact on the upcoming molecular surveys in cold environments.

References

[1] B. A. McGuire. ApJS, 259, 30 (2022).
[2] J. Cernicharo, M. Agúndez et al. A&A, 649, L15 (2021).
[3] M. Agundez, N. Marcelino et al. A&A, 677, L13 (2023).
[4] S. Demes, C.T. Bop, M.B. Khalifa and F. Lique. PCCP, 26, 16829 (2024).

Infrared spectroscopy of gas-phase hydrogenated and methylated pyrenes: from laboratory spectra to the simulated 3.4 µm emission band

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Polycyclic aromatic hydrocarbons (PAHs), composed of several aromatic rings, are good candidates for the Aromatic infrared bands (AIBs) observed in emission in a wide range of environments dominated by UV photons. Following excitation by UV photons, PAHs cool radiatively by emitting photons in the infrared and the AIBs are due to vibrations of aromatic CH and CC bonds. In addition to the main aromatic CH stretching band at 3.3 µm, some minor bands observed in the 3.4-3.6 µm range are assigned to aliphatic CH stretching modes. Hydrogenated and methylated PAHs have been proposed as carriers of these bands.

The identification of the carriers of spectroscopic features observed in astronomical spectra relies on experimental and theoretical works that provide spectra of dust and molecules to compare with the observations. However, because the emitting PAHs are hot, anharmonic effects should be considered in generating synthetic IR spectra that can be compared with astronomical AIB spectra.

In this talk we present new absorption spectroscopic measurements of gas-phase pyrene, methylated pyrene (Me-pyrene), and hydrogenated pyrene (Hn-pyrene) in the 1.4-15 µm wavelength range at various temperatures between 373 and 673 K. Detailed anharmonic calculations at 0 K are performed to support the band analysis. The analysis of the temperature dependence of the experimental IR spectra enables us to derive empirical anharmonicity factors. These factors are then incorporated into an emission model to generate synthetic spectra that can be compared with JWST observations.

Based on these state-of-the-art simulated spectra, we propose 1,2,3,6,7,8-hexahydropyrene as the carrier of the red component of the 3.4 µm band observed at 3.403 µm. While 1-methylpyrene may also contribute to the underlying emission plateau, it lacks a strong specific infrared band, which complicates detection in observed spectra, unlike hexahydropyrene. All experimental spectra and their temperature-dependent analyses are available in the new cosmicPAH database of anharmonic infrared spectra (cosmicPAH-IRD, https://www.cosmicpah-irdb.ovgso.fr/).

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Are interstellar PAHs more deuterated than they should be?

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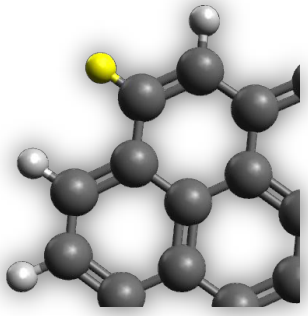
Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous to the interstellar medium (ISM) and are believed to be the carriers of the famous aromatic infra-red (IR) bands (AIBs) [1]. Especially in photodissociation regions (PDRs), such as the Orion Bar, will PAHs get excited from absorption of UV light and cool through their vibrational manifold via IR emission. Recent James Webb Space Telescope (JWST) observations reveal ***a local deuterium enrichment of PAHs*** within PDR fronts [2], where high gas temperatures should diminish any significant isotope effects. Hence, we explore how this local enrichment could occur and consider regions deeper in the PDR where PAHs will exist in a superhydrogenated state.

Through a combination of experimental techniques (temperature programmed desorption and scanning tunneling microscopy) and kinetic Monte Carlo simulations (KMC), we set out to characterize key reactions dynamics between PAHs and atomic hydrogen/deuterium such as the kinetic isotope effect (KIE), scrambling [3] and addition-abstraction reaction cycles [4]. We study four isotopically different systems, i.e. coronene ($C_{24}H_{12}$) and d-coronene ($C_{24}D_{12}$) exposed to either H or D atoms, hereby revealing reactions otherwise hidden to usual experimental techniques. Exchange reactions on coronene lead to fully deuterated coronene ($C_{24}H_{12} \rightarrow C_{24}D_{36}$) and vice versa, hence the KMC simulations are needed to untangle the various reactions cross sections across the entire superhydrogenation/deuteration process. Furthermore, the current values for H_2 formation, catalyzed by PAHs [5], may underestimated. We use χ^2 to fit the KMC simulations to the experimental data and find well defined minima for the important reaction cross sections. An ***apparent inverse KIE*** is explored in detail, and we compare the data for coronene to superhydrogenation/deuteration of corannulene, a curved PAH with a 5-membered ring. Corannulene shows no sign of an inverse KIE which helps the understanding of the exact reaction processes that govern the route towards deuterated PAHs in the ISM.



References:
[1] ARAA, 46.1 (2008): 289-337.
[2] A&A, 685 (2024): A74.
[3] A&A, 635 (2020): A9.
[4] ApJ, 679.1 (2008): 531-536.
[5] A&A, 595 (2016): A23.

First results from the COMPASS ALMA Large Program

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Complex Organic Molecules in Protostars with ALMA Spectral Surveys (COMPASS) is a Large Program tailored to systematically characterize complex organic chemistry in a sample of 11 deeply embedded Solar-type (low-mass) protostars known to harbor warm gas that shows emission from complex organic molecules. Its main aims are to understand what the physical, environmental, and evolutionary regulators of the formation of complex organics are? Is there a universal outcome of interstellar chemistry in terms of complex organics? And ultimately: how much diversity in organic inventories do we expect for planetary systems?

The international team of around 30 researchers is about to release a series of papers presenting the first results from COMPASS. In this talk, I will present COMPASS and its unique approach of "unbiased spectral surveys". I will also showcase the first results from the team and demonstrate the wealth of information in the data set on the chemical inventory of the targeted protostars. I will highlight that the power of the program lies in understanding the entire sample of observed protostars and tease upcoming synergies with follow-up JWST observations.

More information about the program:
https://erda.ku.dk/vgrid/COMPASS/index.html

Ex-situ mass spectrometry analysis of organic residues from electron-irradiated ethanolamine ice

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Ethanolamine (EA), a potential precursor of simple amino acids, was recently detected in molecular clouds of the interstellar medium (ISM) [1, 2]. This discovery raises key questions about EA's formation, stability and its possible contribution to the synthesis of more complex organics. To investigate the latter two aspects, we studied the photo processing of EA ice at 10 K under electron gun irradiation to simulate secondary electrons generated by galactic cosmic rays (GCR) in the ISM. After irradiation, the ice was gradually warmed to room temperature, leaving an organic residue that was further analyzed using wet chemical methods. Via retention times and fragmentation patterns, we identified several amino acids and (cyclic) dipeptides. Adhering to the highest mass spectrometry identification standards for unambiguous molecular assignments was of top priority [3]. A primary goal was to establish a reliable ex-situ identification method that minimizes chemical alteration and avoids additional derivatization. Our experiments proved that amino acids and (cyclic) dipeptides can be nearly unambiguously identified without the use of harsh chemical processing. In addition, we expanded the current list of formed (cyclic) dipeptides in such systems. We also discuss likely reasons why some expected amino acids are absent, which might have ended up in dead-end reaction sinks. Overall, the product data obtained via this ex-situ approach provides a robust basis for direct use in future in-situ experiments.

[1] T. Suhasaria *et al.*, *ApJ* **2025**, *982*, 48.

[2] V. M. Rivilla *et al.*, *PNAS* **2021**, *118*.

[3] E. L. Schymanski *et al.*, *ES&T* **2014**, *48*, 2097

Low-energy electron collisions with C_{60}^+ in the Cryogenic Storage Ring

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The interstellar medium (ISM) is characterized by a diverse molecular landscape. In particular, carbon-rich molecules such as fullerenes and polycyclic aromatic hydrocarbons (PAHs) are important in astrochemical processes. While the presence of C_{60}^+ in the cold ISM is well-established [1], its formation and destruction mechanisms remain a puzzle. Dissociative recombination (DR) in low-energy electron collisions is a significant destruction pathway for small molecules in the ISM [2], but studies on large molecules at those collision energies are limited and challenging. We investigate low-energy electron collisions with C_{60}^+ using the Cryogenic Storage Ring (CSR) at the Max Planck Institute for Nuclear Physics [3].

The CSR operates at temperatures below 10 K and thus offers an ideal environment to study these reactions at conditions mimicking the ISM. The cryogenic beam environment enables to store an ion beam for hundreds of seconds such that reaction dynamics can be investigated as the stored ions cool internally. By overlapping the stored beam with an electron beam in a merged-beams setup, we study electron collisions with C_{60}^+ at energies ranging from a few meV to approximately 85 eV. We observed various collisional processes and determined absolute rate coefficients. In comparison to collisions of smaller cationic molecules with electrons, C_{60}^+ exhibits a dominant non-dissociative recombination channel with high recombination rates at low collision energies. These results shed a light on the destruction mechanisms of C_{60}^+ in the ISM and provide data for modeling the chemistry of complex carbon-rich molecules in space. Building on this work, we have recently measured electron collisions with C_{70}^+. Future experiments at the CSR will focus on studying electron collisions with PAHs, further contributing to our understanding of the complex chemistry in the ISM.

[1] Campbell, E., Holz, M., Gerlich, D. et al., Nature 523, pp. 322–323 (2015)
[2] Geppert, W.D. and Larsson, M., Molecular Physics, 106(16–18), 2199–2226 (2010)
[3] von Hahn, R. et al., Rev. Sci. Instrum. 87, 063115 (2016)

Molecular theory needs for astrochemical modeling

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Astrochemistry is largely driven by observations, but laboratory experiments and theoretical calculations play a crucial role. Our understanding of interstellar chemistry thus relies on chemical networks that require knowledge of thousands of *reaction* rate coefficients. In addition, because the pressure in the interstellar medium is extremely low, state-to-state *inelastic collision* rate coefficients are needed to derive accurate non-LTE column densities and abundances. Despite significant experimental advances in recent years, astrochemical models rely heavily on theory, which alone can meet the ever-growing data requirements of astrochemistry.

I will provide an overview of recent progress in the theoretical determination of gas-phase reactive and collisional rate coefficients. The major role of the potential energy surfaces will be emphasized, together with the high computational cost of "exact" quantum calculations and the resulting need for approximate, accelerated, and machine-learning-based methods. A selection of recent results will be presented for key processes, including the rovibrational excitation and rotational-state-selective destruction of polyatomic molecules. Detailed comparisons between theory and experiment will be reported for benchmark species such as CO [1], H_2O [2, 3] and H_3^+ [4]. Finally, astrochemical models of strongly non-equilibrium processes – such as maser action, chemical pumping, and nuclear-spin-state chemistry – will be presented, with illustrative comparisons to ALMA and JWST observations and future prospects.

References:
[1] Labiad et al., PRA, 112, 062816 (2025)
[2] Garcia-Vazquez et al., Faraday Discuss., 251, 205 (2024)
[3] Garcia-Vazquez et al., CPC 25, e202300698 (2024)
[4] Znotins et al. PRA, 112, 052819 (2025)

Laboratory far-infrared spectra, fragmentation chemistry and cooling dynamics of sulfur allotropes

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Understanding the chemical pathways of sulfur in the interstellar medium (ISM) remains a puzzle [1]. Whereas in diffuse low-density interstellar environments the abundance of atomic sulfur roughly corresponds to the known cosmic value, in dense molecular clouds, star-forming regions, and planet-forming disks there is a major depletion of gas phase atomic sulfur, by up to two orders of magnitude [2]. Gas phase sulfur-bearing molecules, such as HCS, OCS, and SO_2 have been detected, but at concentrations too low to account for the missing sulfur. Moreover, sulfur can be present in volatile ices, salts, or in more refractory species, such as FeS. Nevertheless, another class of molecules proposed as a possible sink for the missing sulfur is composed by sulfur allotropes, of which S_8 stands out as a prominent candidate, given its higher relative stability. Still, crucial to explore this alternative is to have laboratory spectroscopic data under astrochemically relevant conditions. In this contribution, we discuss the current efforts undertaken at HFML-FELIX (Nijmegen, The Netherlands), to provide such missing data for a variety of sulfur allotropes. In particular, using the light of the free electron laser FELIX in combination with molecular beams and ion traps, we have investigated neutral and charged sulfur allotropes [3], focusing on the infrared range where the James Webb Space Telescope (JWST) is most sensitive. In addition, experiments at the cryogenic ion beam storage ring DESIREE at Stockholm University are used to address the competition between fragmentation, vibrational cooling, and recurrent fluorescence on the octasulfur cation, S_8^+, thus elucidating on its survival probability under energetic interstellar environments [4].

References:
[1] Space Sci. Rev., 217, 14, (2021)
[2] A&A, 687, A87 (2024)
[3] Nat. Commun. 15, 5928 (2024)
[4] A&A, 709, A136 (2026)

Helium-Tagging Spectroscopy of PAH and Fullerene Cations

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Helium-tagging spectroscopy has emerged as a sensitive method for probing the intrinsic optical properties of cold molecular ions and ionic clusters under well-controlled conditions, while introducing only minimal perturbations to the investigated species. In our approach, ions are generated and efficiently cooled inside multiply charged helium nanodroplets. Controlled collisional heating of the droplets with helium buffer gas enables the controlled formation of helium-solvated ions and ionic complexes at low temperatures. Upon mass selection, resonant photoexcitation of the target ions leads to the evaporation of one or more weakly bound helium atoms. The resulting helium loss is monitored by time-of-flight mass spectrometry and provides an action spectroscopy scheme for recording electronic and vibrational spectra [1]. This technique allows the production and spectroscopic investigation of a broad range of species, including isolated molecular ions, weakly bound ionic complexes, and size-selected ionic clusters. In addition, the implementation of a second ion source makes it possible to generate multiply charged ions, extending the accessible systems also to higher charge states [2].

In this contribution, we focus on the spectroscopy of polycyclic aromatic hydrocarbons (PAHs) and fullerenes in both the visible and infrared spectral regions [3,4]. These carbonaceous molecules are of fundamental interest in molecular physics, materials science, and especially in astrochemistry, as they are considered potential carriers of diffuse interstellar bands and infrared emission features observed in space. We present spectra of PAH and fullerene cations, as well as the corresponding cationic clusters, providing insight into their electronic transitions and vibrational fingerprints.

References:

1. Bergmeister et al., *Rev. Sci. Instrum.* **94**, 055105 (2023)
2. Ganner et al., *Phys. Rev. Lett.* **133**, 023001 (2024)
3. Ganner et al., *ACS Earth Space Chem.* **9**, 11, 2694 (2025)
4. Ganner et al., *Astrophys. J.* **993**, 47 (2025)

Gas-phase formation of sulphur-containing interstellar molecules of the HCS-R (R=CN, CCH) family: a computational study.

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The cold, dense molecular cloud TMC-1 (T=10 K, molecular density around 10^4 cm^{-3}) has been dubbed a 'sulphur factory' (Cernicharo, Cabezas, Agúndez, et al. 2021): indeed, some twenty sulphur-containing molecules have been discovered there since 2021.

The molecules cyanothioformaldehyde (HCSCN) and propynethial (HCSCCH), which share the same HCS group, are the sulphur analogues of HCOCN and HCOCCH, also detected in this cloud (Cernicharo, Cabezas, Endo, et al. 2021). The formation reactions that feed into the gas-phase kinetic model used by astrochemists are (where X = O, S):

$X + CH_2CCH^{\bullet}/CH_2CN^{\bullet} = HCXCCH/HCXCN + H^{\bullet}$

$H_2CX + CCH^{\bullet}/CN^{\bullet} = HCXCCH/HCXCN + H^{\bullet}$

Whilst the abundances of oxygen-bearing molecules are well reproduced, those of sulphur-bearing species are underestimated by two orders of magnitude. The authors suggest that the network of chemical reactions is incomplete.

We investigated the reactivity of these species using the automated reaction discovery software AutoMeKin (AMK) at the ωB97XD/Def2-TZVPP level of theory, and filtering our results according to the detection status in TMC-1 of the reactants (Martínez-Núñez, Barnes, Glowacki et al 2021). We show that the formation reactions proposed by astrochemists are viable in TMC-1 (Figure 1 for HCSCN).

As far as neutral-neutral reactions are concerned, we find that HCSCN can also be formed by the reaction $N+H_2CCS$, in only three steps (Figure 1). AMK also discovered an ion-neutral reaction pathway toward protonated forms of HCSCN, $HCS + HCNH^+ = HCSCNH^+ + H$.

Concerning HCSCCH, the only new reaction with H as a by-product is $C_2H_2S + CH_2^+$ which forms the protonated species $HCCCHSH^+$.

AutoMeKin's automated and exhaustive exploration of the potential energy surface can reveal unexpected products beyond chemical intuition. This capability provides new targets for astronomical searches. Illustrative examples of candidate molecules emerging from this approach will be discussed.

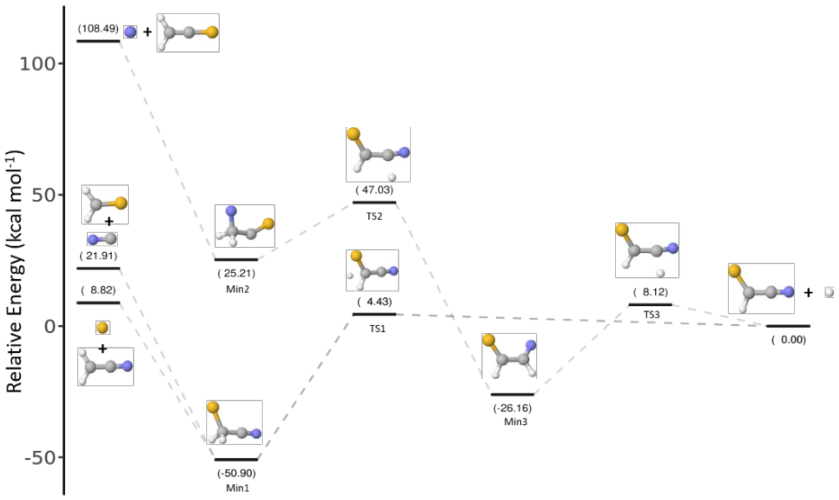

Figure 1 : DFT-computed energy profiles for the formation of HCSCN.

References

J. Cernicharo, C. Cabezas, M. Agúndez et al. A&A 648, L3 (2021)

J. Cernicharo, C. Cabezas, Y. Endo et al. A&A 650, L14 (2021)

E. Martínez-Núñez, G. L. Barnes, D. R. Glowacki et al. J. Comp. Chem. 42, 2036 (2021).

Circular Dichroism Spectroscopy: Disentangling Intrinsic Molecular Chiroptical Response from Environment-Induced Effects

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Amorphous solid water (ASW) and complex organic molecules (COMs) coexist in environments from interstellar molecular clouds through to evolved solar systems. It is theorised that primordial ice *may* have brought the molecules of life to Earth four billion years ago, which could have kickstarted the origin of life on Earth. Furthermore, L-enrichments of amino acids found in carbonaceous chondrites provide a strong hint that the phenomenon of life's homochirality, the exclusive use of left-handed amino acids in proteins, originated in these environments. The enantiomeric excess observed in these samples is generally believed to have arisen from asymmetric UV photolysis, making the study of chiral photon-matter interactions crucial. Despite ASW being such an important component of these interstellar ices, the effects of ASW on the chiroptical properties of COMs are not well understood, and so combined experimental and theoretical studies of ice:COM mixtures aim to better constrain these effects.

Circular dichroism (CD) spectroscopy reveals the wavelength-dependent, differential absorption of circularly polarised light (CPL) by chiral molecules. In the gas phase, this offers a unique route to probe the intrinsic chiroptical response of isolated molecules, free from environmental perturbations, and provides exceptional conformational sensitivity.[1,2] On the other hand, solution phase data show pronounced spectral changes arising from solvation, giving insight to how the local environment can influence chiroptical response.[3,4] Through these studies, we can identify and benchmark molecular properties from environmental effects with a view to understanding the influence of ASW on CPL induced photochemistry within astrochemically relevant molecular ices.

The electronic CD and absorption spectra of chiral COMs in the gas and condensed phase have been recorded using dedicated vacuum chambers at the AU-CD beam line at the ASTRID2 synchrotron, Aarhus University. Interpretation of these experimental data is supported by quantum chemical calculations (TDDFT) including hydration models to determine the effects of hydrogen bonding through the surrounding water molecules. We show that solvation can reshape the CD spectra (band positioning and/or inversion) through a combined effect of conformer redistribution and modification of the electronic nature of low-lying excited states.[5] As such, we highlight the importance of investigating the CD spectra of chiral COMs within amorphous ices so that the realistic local environment can be accounted for and studied.

References:

[1] Garcia A *et al.*, *Science Advances,* 8, eadd4614 (2022).
[2] Meinert C *et al., Nature Comm.* 13, 502 (2022).
[3] Meinert C *et al., J. Photochem. Photobio. A: Chem.*, 331, 130-137 (2016).
[4] Bredehöft JH *et al.*, *Chirality,* 26, 373-378 (2014).
[5] Bancone N *et al.*, *in preparation for 2026.*

A new 4k-pixel microcalorimeter detector MOCCA for molecular fragment mass measurements at CSR

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A wide variety of molecules have been discovered in the interstellar medium (ISM) [1]. The formation of many of these molecules remains a subject of debate and ongoing research. One of the processes thought to play a role in the formation of these molecules is dissociative recombination (DR) [2]. In this process, a positive molecular ion captures a free electron, causing the molecule to break apart into two or more neutral fragments. Investigating these processes in a laboratory setting presents a significant challenge, requiring highly specialized experimental facilities designed to reproduce the extreme conditions characteristic of the ISM.

One such facility is the cryogenic storage ring (CSR) at the Max Planck Institute for Nuclear Physics in Heidelberg, Germany [3]. The CSR enables operation in a temperature range below 10 K and at a residual gas density below 10^4 cm^{-3}. Molecular ions circulate in the ring with beam energies ranging from 20 keV to 300 keV per unit charge, for periods of up to several thousand seconds. A collinear electron beam is merged with the circulating molecular ions, allowing DR to be studied under well-controlled laboratory conditions. Precise investigation of these processes within the CSR demands a detector that combines high mass resolution, high time resolution, and position sensitivity, while capturing every neutral product from each individual reaction event.

For this purpose, the 4k-pixel molecular camera array (MOCCA) detector was developed at the Kirchhoff Institute for Physics in Heidelberg, Germany. MOCCA is an array of 64 × 64 metallic magnetic calorimeters (MMCs). The signals are read out via 32 superconducting quantum interference devices (SQUIDs) employing a novel multiplex readout system. This configuration provides both positional sensitivity and high energy resolution, the latter facilitating the mass identification of incoming neutral fragments.

In addition to MOCCA, nanosecond time resolution is achieved through a secondary electron readout. Prior to installation at the CSR, the full detector configuration will be implemented and commissioned in a standalone setup, enabling studies of molecular ion collisions with a neutral gas jet target as well as with laser photons. Ongoing commissioning measurements are paving the way towards first tests with molecular fragments. An overview of the current project status and progress will be presented.

References:
[1] B. A. McGuire, Astrophys. J. Suppl. Ser. 259, 30 (2022),
[2] D. R. Bates, Phys. Rev. 78, 492 (1950),
[3] R. von Hahn, Rev. Sci. Instrum. 87, 063115 (2016).

Laboratory, theoretical and modelling needs for exo-aeronomy

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The recent years have experienced a rapid development in the field of aeronomy – the investigation of planets' upper atmospheres –, driven by contemporaneous advances in the characterization of exoplanets. There is by now a consolidated set of atmospheric tracers with which to probe exoplanets' upper atmospheres, and that can be monitored over a diverse population of such objects. Indeed, aeronomy has opened new avenues for characterizing low-mass exoplanets having atmospheres whose compositions could range from being hydrogen-dominated to steam-rich. These tracers often occur in the low-density atmospheric layers of the planets, where the gas departs from equilibrium in various ways (e.g. non-Maxwellian velocities, non-Boltzmann populations). This talk provides context to understand the astrophysical relevance of exo-aeronomy observations and their model-based interpretations in the bigger picture of exoplanets and their long-term evolution. We will identify critical processes that need to be revised and the critical needs (e.g. cross sections, rate coefficients, chemical networks) that are limiting further progress.

Spectroscopic product identification and kinetic modelling of the reaction of NCO^+ and $HNCO^+$ with H_2 at cryogenic temperatures

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Isocyanic acid, HNCO, is ubiquitous in the interstellar medium (ISM) having been detected in over 50 astronomical objects.[1] Its composition of the essential atoms for organic life also suggests a potential role as a prebiotic intermediate for the formation of formamide, NH_2CHO, which itself may be linked to the abiotic synthesis of amino acids and DNA bases.[2] Despite the potential importance of HNCO, its chemistry and formation mechanism in the ISM remain experimentally unknown. A suggested gas-phase mechanism proceeds via two subsequent hydrogenations of NCO^+ leading to H_2NCO^+ and $HNCOH^+$ which may form neutral HNCO via dissociative recombination.[3]

In this contribution, we explore the chemistry and spectroscopy of these ions using the 22-pole cryogenic ion trap instrument FELion[4] coupled to the infrared free-electron lasers at HFML-FELIX. Employing cryogenic infrared action spectroscopy,[5,6] we were able to spectroscopically identify the reaction products of NCO^+ and $HNCO^+$ with H_2, while kinetic modelling allowed us to extract experimental reaction rates at 19K. We find significant differences between the experimental results and both the previously theoretically predicted rates and branching ratios to the reaction products, showing the importance of the experimental verification of these estimated parameters. Employing astrochemical models, we then explore the impact of these revised kinetic rates on the predicted abundances of these ions and neutral HNCO.

References:

(1) Zinchenko, I.; Henkel, C.; Mao, R. Q. *Astron. Astrophys.* **2000**, *361*, 1079–1094.
(2) López-Sepulcre, A.; Balucani, N.; Ceccarelli, C.; Codella, C.; Dulieu, F.; Theulé, P. *ACS Earth Space Chem.* **2019**, *3* (10), 2122–2137.
(3) Iglesias, E. *Astrophys. J.* **1977**, *218*, 697–715.
(4) Jusko, P.; Brünken, S.; Asvany, O.; Thorwirth, S.; Stoffels, A.; van der Meer, L.; Berden, G.; Redlich, B.; Oomens, J.; Schlemmer, S. *Faraday Discuss.* **2019**, *217* (0), 172–202.
(5) Schmid, P. C.; Asvany, O.; Salomon, T.; Thorwirth, S.; Schlemmer, S. *J. Phys. Chem. A* **2022**, *126* (43), 8111–8117.
(6) Steenbakkers, K.; van Boxtel, T.; Groenenboom, G. C.; Asvany, O.; Redlich, B.; Schlemmer, S.; Brunken, S. *Phys. Chem. Chem. Phys.* **2024**, *26* (3), 2692–2703.

A song of ice and fire: Linking ice and gas-phase chemistry in the high-mass hot core IRAS 18089

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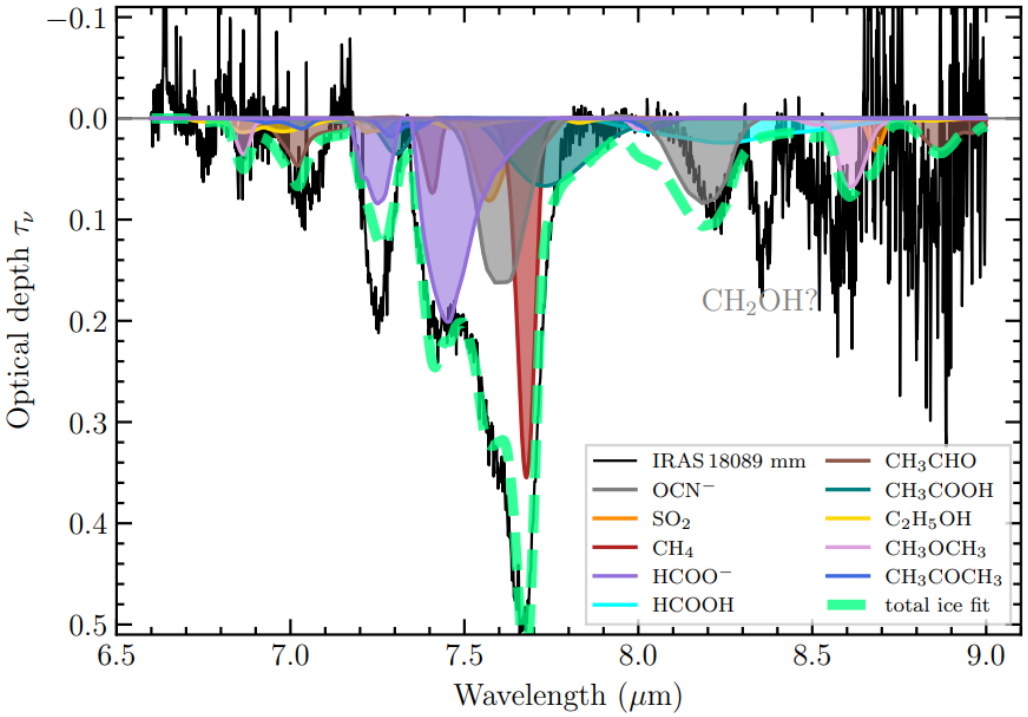
The formation and destruction of molecules in the interstellar medium result from a complex interplay between gas-phase chemistry and processes on dust grains and within icy mantles. Using mid-infrared spectroscopy from JWST (5–28 μm) and sensitive 3 mm molecular line observations from ALMA, we investigate the molecular content on the ices and in the gas-phase toward the embedded high-mass hot core IRAS 18089 on ∼5000 au scales. While some species show comparable abundances in both phases, others exhibit significant phase-dependent differences, indicating additional gas-phase formation routes or inefficient desorption from the ices. Ice abundances are broadly consistent with those towards other Galactic low-mass protostars, with tentative trends with Galactocentric distance. These results highlight the importance of combined ice and gas-phase studies to constrain chemical pathways in star-forming regions.



References:
Gieser, Rocha, Chen, et al. 2026, Astronomy & Astrophysics, Volume 709, A235

Impact of Oxygen on Carbonaceous Dust Formation in the presence of Iron under Circumstellar-like Conditions

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In astrophysical environments, the carbon-to-oxygen (C/O) ratio is a key parameter determining gas-phase chemistry and dust formation pathways. Dust formation involves the nucleation of condensation nuclei and their growth by accreting key molecules from the gas phase [1]. Equilibrium condensation models predict abrupt transitions in condensate composition between carbon-rich and oxygen-rich regimes [2]. However, the role of the C/O ratio should be investigated beyond thermodynamic models.

Cold plasma experiments offer a valuable laboratory framework to probe dust formation under simplified circumstellar-like environments [3-5]. In addition, such approach allows introducing metallic atoms such as iron atoms in the gas phase. In this work, we investigate the formation of iron-containing carbonaceous dust in a low-pressure argon RF capacitively-coupled plasma. Iron atoms are introduced by sputtering of a metallic target. The other elements (C, O, H, Si) are provided by decomposition in the plasma of hexamethyldisiloxane (HMDSO) precursor. Additional oxygen is injected to probe the carbon-rich to oxygen-rich transition. The elementary processes occurring into the plasma are followed *in situ* by optical emission spectroscopy (OES) and measurements of the electrical parameters. The formed dust and molecular content are analyzed *ex situ* by laser-desorption-ionization mass spectrometry (AROMA setup) and secondary electron microscopy (SEM).
OES measurements on the plasma emission reveal the presence of Fe atomic lines in addition to the rich Ar spectrum. Increasing the amount of HMDSO leads to a progressive decrease of Fe emission lines, indicative of efficient transformation into other iron-containing species. Mass spectrometry analysis reveals the presence of complex organic and organometallic species. SEM images shows dust morphology and the presence of iron at nanoscale.

The impact of oxygen on the formation of large organic/organometallic species and Fe-containing carbonaceous dust is investigated for various C/O conditions.
Taken together, these analyses provide new experimental insights on the formation and chemical evolution of dust analogues and complex organics around the carbon-rich to oxygen-rich transition region under non-equilibrium conditions.

Acknowledgements
This work was supported by l'Agence Nationale de la Recherche in France through project ANR GROWNANO under grant ANR-21-CE29-0001.

References:
[1] T. Yamamoto & H. Hasegawa, Prog. Theor. Phys., 58, 816-828 (1977)
[2] D. S. Ebel, J. Geophys. Res., 105, A5, 10363,(2000)
[3] L. Martínez et al., Nat. Astron., 4, 97-105 (2000)
[4] R. Bérard et al., Front. Astron. Space Sci., 8, 654879, (2021)
[5] G. Tajuelo-Castilla et al., Nat. Astron., arXiv:2605.03575 (2026)

Different chemical regime in exoplanet atmospheres: From plasma to cloud formation in one atmospheres

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The ensemble of the more than 6000 known extrasolar planets in our galaxy exhibits a diversity of objects unseen in our solar system. With space missions like HST, CHEOPS, JWST and soon also PLATO, exoplanet research has turned from discovering such planets to characterizing these objects that orbit stars other than our Sun.

Recent progress in characterizing exoplanets has demonstrated that extrasolar gas giants exhibit climate regimes ranging from ultra-hot to rather cold (1). Ultra-hot Jupiters like WASP-18b (2) host vastly different chemical regimes in their atmospheres because they exhibit enormous day-night temperature differences of more than 2000K, but colder gas giants appear more homogenous. The atmosphere's thermo- and hydrodynamics drive a rich gas phase chemistry, including gas – solid phase transitions (cloud formation) that always occur on the nightside and large-scale gas – plasma phase transitions that may be confined to the dayside only. In order to physically interpret such complex atmosphere behavior that is imprinted in exoplanet observations, our virtual laboratories predict temperature, velocity, cloud and chemistry maps for planets orbiting different host stars. Complemented with chemical and spectral material properties, virtual laboratories are applied to explore the atmosphere structure and cloud formation of specific planets (e.g. the JWST target WASP-39b) as well as to ensemble studies in preparation of observational campaigns (3). Future progress is hampered by missing material properties for metal oxide clusters, complex hydrocarbons and ions (4,5). Machine learning techniques are helping to fill gaps where deterministic modelling is too time-consuming (6).

References:

(1) Helling et al. 2023, A&A 671, 122
(2) Helling et al. 2019, A&A 626, 133
(3) Carone et al. 2026, A&A 708, 185
(4) Bisht et al. 2026, ApJ, accepted for publication
(5) Helling et al. 2020, A&A 614, 178
(6) Plaschzug et al. 2026, A&A 706, 157

Advanced Analytical Workflow to Characterize Organic Residue Generated from Astrophysical Ice Analogues

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Understanding the formation and evolution of organic compounds in hot molecular cores is crucial to determine the origins of a fraction of the chemical diversity observed in interplanetary objects. These cold and dense regions of the interstellar medium (ISM) provide unique physical and chemical conditions that enable the growth of icy mantles around dust grains, hosting a rich organic chemistry [1], which may later be incorporated into interplanetary object during the accretion phase [2].

To investigate these processes, we used the MICMOC setup [3] at PIIM laboratory to simulate the pressure (10-7 - 10-8 mbar) and temperature (77 - 300 K) conditions of ices at the edge of a protoplanetary disk. We studied the photochemical evolution of ice analogues, specifically focusing on the alteration of ices formed from a H2O:CH3OH:NH3 mixture. After vacuum ultraviolet (VUV) irradiation and warming up to room temperature, these ices yield complex organic residues. High-resolution mass spectrometry (HRMS) analyses have revealed the presence of thousands of compounds, with molecular masses reaching up to 4000 Da [4], while targeted analyses highlighted the presence of a wide range of key chemical moieties.

To pursue the characterisation of such complex samples, we developed a multi-chromatographic analytical strategy inspired by meteorite organic matter extraction protocols [1, 5]. By combining multi-solvent extraction (hexane, dichloromethane, acetonitrile, and methanol) with diverse chromatographic columns, data deconvolution, and molecular networking, we constructed a comprehensive cartography of the sample composition. This approach revealed chemical families such as hydrocarbons, acidic compounds, O- and N-heterocycles, imidazoles, pyridine-like structures, nitriles, amides, and carbamates-like, some of which were previously undetected. This complementary analytical approach provides new insights into the molecular complexity and chemical processes in icy astrophysical environments, advancing our understanding of organic matter evolution within the Solar System.

[1] Arumainayagam, C. R. et al., Chem. Soc. Rev., 2019, 48, 2293–2314.
[2] Schmitt-Kopplin, P. et al., Proc. Natl. Acad. Sci., 2010, 107, 2763–2768.
[3] Javelle, T. et al., Com. Chem., 2025, 8(1), 306.
[4] Danger, G. et al., Geochim. Cosmochim. 2016, Acta 189, 184–196.
[5] Schmitt-Kopplin, P. et al., Nat. Com., 2023, 14(1), 6525.

Non-aqueous peptide creation via the energetic processing of glycine

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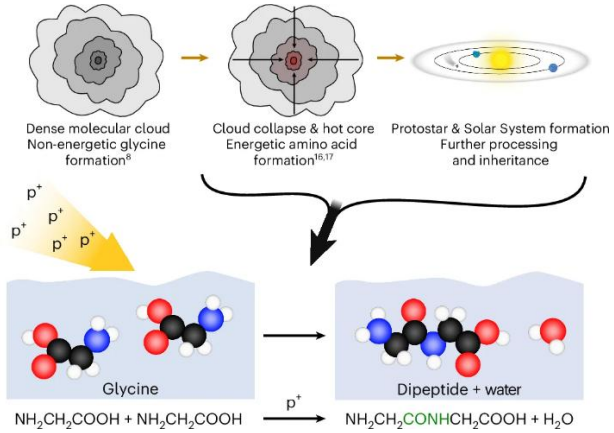

Figure showing an overview of the energetic processing of glycine to form peptides [1]

The detection of glycine in the coma of comet 67P/Churyumov-Gerasimenko [2] and its laboratory-simulated formation under interstellar conditions [3] suggest that simple amino acids may be widespread in space. However, the fate of glycine under astrophysical energetic processing remains largely unexplored. In a recent publication [1], we investigated the radiolytic processing of glycine isotopologues under simulated space conditions, demonstrating the formation of complex organic molecules, including species containing peptide bonds. Using proton irradiation combined with *in situ* spectroscopic analysis, we provide direct evidence for the formation of peptide bonds with water formation as a side product. Through the use of *ex situ* electrospray ionisation mass spectrometry, glycylglycine, the simplest peptide, was detected. This supports a potential extraterrestrial pathway for peptide synthesis. Our findings suggest that energetic processing of glycine in interstellar clouds, protoplanetary disks, and planetary bodies could contribute to the inventory of prebiotic molecules available for planetary accretion. This work advances our understanding of the astrochemical complexity and molecular inheritance of biologically relevant compounds with implications for the origins of life.

[1] A.T. Hopkinson, et al., Nature Astronomy (2026)
[2] K. Hadraoui, et al., A&A, 32, 630 (2019)
[3] S. Ioppolo, et al., Nature Astronomy, 5, 197-205 (2021)

Novel Pathways to Complex Organic Molecule Formation in Space

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Interstellar dust and molecular clouds, the regions where new stars and planetary systems form, are home to surprisingly complex chemistry. In spite of the very low temperatures and pressures characterizing these clouds more than 340 different molecules have so far been detected. Nanoscale dust grains are expected to play a dominant role as catalysts for this molecular complexity. The last 20 years have seen major advancements in our understanding of interstellar reactions, specifically with regards to simple molecules, however, the degree of chemical complexity attainable via such reactions is still under exploration. Recently it was shown that the simplest amino acid, glycine, can form under interstellar conditions. In this case a non-diffusive reaction mechanism was proposed. Erosion reactions directly involving carbonaceous dust grain surfaces provide an alternative pathway to complex molecule formation under interstellar conditions. Here I discuss recent advances in experimental surface and solid-state astrochemistry with focus on such alternative formation pathways to interstellar complex organic molecules.

Probing Charge-Transfer and Ion-Neutral Reactions at Low Energy with a Cryogenic Merged-Beam Device

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Under low density and temperature conditions, only ion-neutral and ion-ion reactions are fast enough to affect the local chemistry. Such processes take place in environments as varied as the Earth's ionosphere, the interstellar medium, and stellar atmospheres, where they govern charge balance and influence models of elemental abundances.

In this context, we plan to study several low-energy ion-neutral reactions of astrophysical and planetary importance. These include deuteration of H_3^+ in collisions with D atoms [1], the proton transfer between H_3^+ and CO [2] — one of the most abundant molecular species in the Universe after H_2 and He —, the proton-oxygen charge-transfer reaction that triggers oxygen chemistry in diffuse clouds [3-4], and the carbon ion-oxygen reaction occurring in the upper atmosphere of Venus [5].

To this end, we are assembling and commissioning a next-generation merged-beam apparatus featuring improved high vacuum and a cryogenic section in the collision region where beams of cations, anions, or neutral species will be merged. The device also includes an automated control system, multi-particle detection capabilities, an ion beam trap, and several types of ion sources: a high-repetition-rate supersonic expansion source, an Electron Cyclotron Resonance (ECR) source, a duoplasmatron source, a cesium sputter source, and a thermionic emission source. These may be supplemented with a sodium double charge exchange cell. The production of a cold H_3^+ quasi-continuous beam is achieved through supersonic expansion, as already tested at UCLouvain [6]. The production of neutral species will be carried out by selective photodetachment of an anion beam or neutralization of a cation beam on a target gas.

[1] P.-M. Hillenbrand, K. P. Bowen, J. Liévin, X. Urbain, and D. W. Savin, The Astrophysical Journal, 877:38 (2019)
[2] E. Herbst, W. Klemperer, Astrophys. J. 185, 505 (1973).
[3] P.C. Stancil, D.R.Schultz, M.Kimura, J.-P.Gu, G.Hirsch and R.J.Buenker Astron. Astrophys. Suppl. Ser. 140, 225 (1999);
[4] J. A. Spirko, J. Zirbel, and A. P. Hickman, J. Phys. B: At. Mol. Opt. Phys. 36, 1645 (2003)
[5] J. L. Fox and L. J. Paxton, J. Geophys. Res. 110, A01311 (2005)
[6] L. Berger, F. Grussie, F. Nuesslein, O. Novotný, A. Znotins, J. Fréreux, X. Urbain, H. Kreckel, Review of Scientific Instruments, 96, 013301 (2025)

Formation and Stability of the Building Blocks of Life on Space-Relevant Ice Grain Analogs

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Complex organic molecules are thought to form on icy dust grains in interstellar environments through a combination of energetic and non-energetic processes driven by photons, electrons, ions, and atoms. Thanks to the James Webb Space Telescope, JWST, and the Atacama Large Millimeter/submillimeter Array, ALMA, we can now map and characterize ices and gases across a wide range of star-forming regions, providing new insight into star formation and chemical evolution.

European large-scale experimental facilities play a crucial role in interpreting these observations by enabling the simulation of space-like conditions in the laboratory. In this presentation, I will discuss recent laboratory findings on the formation and stability of prebiotic molecules on ice-grain analogues, which mimic icy surfaces in space. These studies are key to understanding potential pathways toward the origin of life on Earth and to bridging the gap between experimental data and astrochemical theory.

References:
Hopkinson et al. (2026), Nature Astronomy, 10, 531-539
Mifsud et al. (2026), Phys. Chem. Chem. Phys., 28, 3642-3655
Kaňuchová et al. (2025), A&A, 700, A115

Small molecules and its role in the Universe: A journey through its past and its exciting future

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For much of history, the interstellar medium (ISM) was assumed to be empty. Only in the late 19th century did observations, such as spectral lines in nebulae like the Orion Nebula, reveal it as a diffuse gaseous medium. Today, we know the ISM is a complex, inhomogeneous mixture of gas, dust, radiation, and energetic particles. While hot, ionised gas fills most of its volume, most of its mass resides in cooler, denser neutral regions (Draine, 2011; Tielens, 2005).

These neutral regions are key sites for astrophysical processes. They provide the raw material for star formation and connect the scales between stars and galaxies. Despite their low heavy-element content, they host a surprising chemical diversity: nearly 300 molecular species have been detected, from simple diatomics to large carbon structures like fullerenes (McGuire, 2022). These molecules appear across many environments, from interstellar clouds to external galaxies.

Progress in astrochemistry has been driven by advances in radio and submillimetre observations and laboratory spectroscopy, making it a strongly interdisciplinary field (Herbst & van Dishoeck, 2009). Molecules act as powerful probes of physical conditions through their distinct spectral signatures, while also influencing their environments by shaping thermal balance, ionisation, and the onset of star formation (Snow & McCall, 2006).

Interpreting these signals requires detailed chemical understanding, often limited to simpler systems. For this reason, small molecules, well understood and foundational to more complex chemistry, offer a crucial pathway forward. This talk explores recent discoveries of simple molecules, advances in laboratory astrophysics, and how new observations, including those from James Webb Space Telescope, are reshaping our view of the chemical Universe (Bialy et al., 2026).

References:

Bialy, S., et al. (2026), "*Direct detection of cosmic-ray-excited H_2 in the interstellar medium", Nature Astronomy*

Draine, B. T. (2011), "*Physics of the Interstellar and Intergalactic Medium"*, Princeton University Press

Herbst, E., & van Dishoeck, E. F. (2009), "*Complex Organic Interstellar Molecules,*" *Annual Review of Astronomy and Astrophysics*, 47, 427–480

McGuire, B. A. (2022), "*2021 Census of Interstellar, Circumstellar, Extragalactic, Protoplanetary Disk, and Exoplanetary Molecules*," *The Astrophysical Journal Supplement Series*, 259, 30

Snow, T. P., & McCall, B. J. (2006), "*Diffuse Atomic and Molecular Clouds*," *Annual Review of Astronomy and Astrophysics*, 44, 367–414

Tielens, A. G. G. M. (2005), "*The Physics and Chemistry of the Interstellar Medium"*, Cambridge University Press

Astrochemical reactions on dust grains, chemical and spectral signatures

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Refractory cosmic dust grains and molecular ices, formed through the accretion of gases such as H_2O, CO_2, CO, NH_3, CH_4, and CH_3OH onto cold dust surfaces, are fundamental chemical constituents of molecular clouds, high- and low-mass protostellar environments, protoplanetary disks, and the Solar System. Complex organic and prebiotic molecules have been identified in all of these environments. Dust grains contribute to molecular complexity through both catalytic activity and erosive processes.

Laboratory studies of astrophysical ice analogues under interstellar conditions have demonstrated the efficient formation of complex nitrogen- and oxygen-bearing molecules. Reactions involving ice constituents, as well as interactions between dust grains and ice species, are initiated by energetic photons and lead to the synthesis of a wide range of organic compounds, including aldehydes, carboxylic acids, simple carbohydrates, amides, isocyanides, nitriles, and even amino acids.

Advanced laboratory experiments are essential for understanding the evolution of dust grains and grain–ice mixtures in astrophysical environments. To address this need, we have developed experimental approaches that simulate the condensation and processing of major dust components, as well as the formation of complex organic molecules within ice layers deposited on cold refractory grains. In my presentation, experimental results will be presented which demonstrate the importance of dust/ice interactions and the complex astrochemical formation pathways to organic and prebiotic molecules. Furthermore, the necessity of employing a variety of analytical approaches to identify complex prebiotic species within ice mixtures will be demonstrated.

Isomer-resolved ion-molecule reaction kinetics of HCO^+ and HOC^+ studied in a low-temperature ion trap

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HCO^+ and its higher energy isomer, HOC^+, are one of the simplest pairs of molecular ion isomers. HCO^+ was detected in the interstellar medium more than 50 years ago [1, 2], with HOC^+ following a decade later [3]. The HCO^+/HOC^+ column density ratio could potentially become an important diagnostic tool for different interstellar environments, varying from ~1000-9000 in dense molecular clouds to ~50-120 in diffuse clouds and photodissociation regions. However, uncertainties in the reaction rates and branching ratios of key reactions involving these ions have limited their quantitative use. We present isomer-resolved ion-molecule reaction rate coefficients measured in a cryogenic 22-pole radio frequency ion trap [4], using chemical probing with $^{15}N_2H^+$ to distinguish HOC^+ from its lower-energy isomer HCO^+.

We report rate coefficients for the isomerization of HOC^+ to HCO^+ with H_2 and CO, and for three reactions producing both isomers: $CO^+ + H_2$, $H_3^+ + CO$, and $ArH^+ + CO$. Our results demonstrate that the reaction $CO^+ + H_2$ produces HCO^+ with near-unity yield and a negligible fraction of HOC^+ (<0.2%), in agreement with recent theoretical predictions but contradicting earlier experimental results that assumed a ~1:1 branching ratio [5]. We also find that HOC^+ isomerization to HCO^+ is efficient with both H_2 and CO. These new rate coefficients are incorporated into a state-of-the-art astrochemical model to assess their impact on the HCO^+/HOC^+ ratio in both dark cloud and diffuse cloud conditions.

References:
[1] D. Buhl, L. E. Snyder, Nature, 228, 267 (1970)
[2] R. C. Woods et al., Phys. Rev. Lett., 35, 1269 (1975)
[3] R. C. Woods et al., ApJ, 270, 583 (1983)
[4] P. Jusko et al., Mol. Phys., 122, e2217744 (2024)
[5] M. A. Smith et al., ApJ, 578, L87 (2002)

Ion-Molecule Reactions: Efficient Pathways for PAH Growth

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Ion-molecule reactions offer rapid pathways for molecular growth. Here, we explore their potential role in the formation of polycyclic aromatic hydrocarbons (PAHs), from single-ring to two- or three-ring systems. These processes are relevant in natural astrophysical and planetological environments, such as cold molecular clouds, photodissociation regions in star- and planet-forming regions, and (exo)planetary atmospheres (e.g., Titan). They also apply to the interpretation of laboratory simulations involving flames, plasmas, or photochemical reactors. The broad interest in ion-molecule reactions stems from their generally barrierless nature, making them temperature-independent.

The experimental work was conducted using the PIRENEA setup, a dedicated platform for laboratory astrophysics. PIRENEA operates under ultra-low-pressure conditions and over extended timescales, enabling radiative cooling—particularly slow infrared emission. While it can function at cryogenic temperatures (30 K), the experiments reported here were performed at room temperature. Equipped with multiple photon sources, PIRENEA supports photoprocessing and spectroscopic characterization. Its multiplex capabilities, including the ability to isolate single masses, allow for well-controlled conditions and for mimicking interstellar environments.

We investigated the reactivity of three key ions—c-$C_5H_5^+$ (cyclopentadienyl cation), $C_9H_7^+$ (indenyl cation), and $C_{11}H_9^+$ (1- and 2-naphthylmethylium)—with simple aromatic species, including C_6H_6 (benzene), C_7H_8 (toluene), $C_{10}H_8$ (naphthalene), and $C_{11}H_{10}$/$C_{12}H_{12}$ (methyl/dimethyl-naphthalene).
Most of the studied reactions resulted in the formation of long-lived ion-molecule complexes (adducts), highlighting the importance of studying these complexes under conditions where they can stabilize via radiative cooling. Formation of larger PAHs was observed upon irradiation of the adducts with visible photons from a Xe lamp equipped with different color filters. For a few cases, it was observed directly without further irradiation, suggesting that the adduct could not stabilize. Small neutral fragments, such as CH_3, C_2H_4, and C_6H_6, are expected to be produced in all cases.

We demonstrate that this chemistry provides efficient pathways for PAH growth, from one- to two-ring systems and from two- to three-ring systems, involving both hexagonal and pentagonal rings. Complementary density functional theory calculations and molecular dynamics simulations suggest that these pathways are driven by C–C bond formation between the reactants and by isomerization processes.

Acknowledgements
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References:
A. I. Lozano et al., ACS Earth Space Chem. 9, 2017-2032 (2025)
A. I. Lozano et al., ACS Earth Space Chem.10, 1254-1266 (2026)

A unique window into planet formation by combining JWST and ALMA

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Planet formation likely starts early, meaning that the building blocks of planets likely exist in young protoplanetary disks of 1 to a few Myr.
These disks span a huge range of physical conditions of molecular clouds. With the simultaneous access to JWST infrared spectra and ALMA submm observations, we thus have for the first time access to the complete radial inventory of these disks - from the warm rocky planet forming region to the cold outer regions that harbour the supply for further planet growth. I will provide an overview of recent new insights from advances in warm disk chemistry, showcase examples of the use of recent theoretical and laboratory data for the quantitative interpretation of mid-IR spectra, as well as challenges in chemical-dynamical modeling of disk processes linking the outer and inner disk composition.

Formation of Carbonaceous Molecules and Peptides in Space from Formation to Spectroscopic Identification

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4 Laboratory for Astrophysics, Leiden Observatory, Leiden University, Netherlands

This presentation highlights two closely interconnected research directions: low-temperature chemistry and spectroscopy ultra-cold ions. Investigating chemistry at ultralow temperatures helps identify which species can form and persist in the low-temperature areas of space, thereby contributing to their observed abundances. Complementary spectroscopic studies yield experimental spectra that can be directly compared with astronomical observations, enabling the identification of these species in space.

He-tagging spectroscopy has been employed to record UV–VIS–NIR spectra of several carbonaceous ions. The resulting absorption features were compared with diffuse interstellar bands (DIBs), which are a long-standing mystery in astronomy. As shown in Figure 1, the laboratory spectrum of C_4^+ exhibits a close match with the DIB at 503.9 nm [1].

Studies of low-temperature chemistry reveal efficient formation pathways for peptides including cyclic dipeptide diketopiperazine (DKP) [2,3]. As illustrated in Figure 1, DKP^+ is predicted to exhibit exceptionally strong absorption in the visible range. Furthermore, DKP has also been detected in meteorites. Given that nitrogen-containing PAHs are believed to be prevalent in space, DKP^+ is a promising candidate for DIB carrier molecules.

Adding atomic hydrogen as a reactant to the chemistry described in references 2 and 3 increases molecular diversity, yielding peptides containing glycine, alanine, serine and threonine residues. Furthermore, the presence of H atoms greatly enhances polymerization efficiency, considerably increasing the length of the formed peptides.

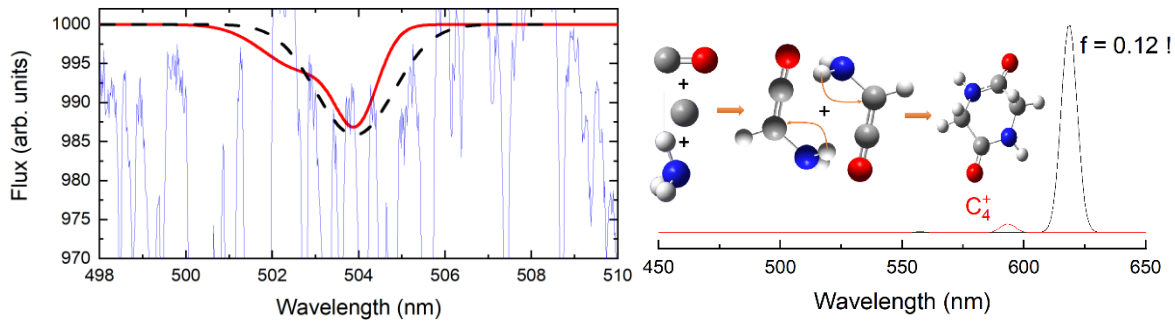

Fig 1. Left: Comparison of laboratory and astronomical spectra. The solid red trace shows the attenuation of flux due to absorption by C_4^+ The solid blue trace represents the observational spectrum, while the dashed black trace corresponds to the DIB profile reported in previous studies. **Right:** Comparison of calculated spectra for C_4^+ (red) and DKP^+ (black), together with the proposed mechanism for DKP formation in the ISM.

References:

[1] S.A. Krasnokutski, L. Ganner, M. Ončák, F. Foitzik, S. Bergmeister, F. Zappa, P. Scheier, E. Gruber, APJ, 34, 982 (2025).
[2] S.A., Krasnokutski, K.J. Chuang, C. Jäger, N. Ueberschaar, T. Henning, Nat Astron, 6, 381 (2022)
[3] S.A. Krasnokutski, C. Jäger, T. Henning, C. Geffroy, Q.B. Remaury, P. Poinot, Sci. Adv., eadj7179, 10 (2024)

Measuring & Linking Mid-Infrared SiO_2 - Spectra to Dust Aggregate Growth in the GT4P Levitation Chamber – I. Scientific Approach

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The growth of µm-sized dust grains into larger aggregates is one of the key steps in planet formation[1], yet the direct interpretation of astronomical dust spectra remains challenging. In protoplanetary disks, the SiO_2 emission around 10 µm is widely used as a tracer of dust processing and grain growth[2]. However, variations in the band strength, peak position and spectral shape are not uniquely controlled by particle size alone, but also depend on aggregation. Laboratory experiments that follow dust growth under controlled conditions are therefore essential to connect observable mid-infrared spectra to the physical evolution of aggregates.

The GT4Pebbles experiment, “Ground Truth for Pebbles in Planet Formation”, is designed to provide such a laboratory reference. In a large rotating, gas-filled levitation chamber, silicate dust particles will be injected into a controlled low-pressure environment, where they can remain suspended and undergo low-velocity collisions. This enables the study of spectral evolution from initially µm-sized monomers toward increasingly porous aggregates of up to dm-size. The experiment can be stopped at selected stages, allowing aggregates to be sampled and analyzed via THz-Spectroscopy and mechanical measurements.

A central diagnostic of GT4P is mid-infrared spectroscopy. We will monitor the evolution of the SiO_2 features initially in the 7-13 µm range, with a planned extension toward 2-20 µm, covering both the prominent 10 µm SiO_2 stretching band and additional spectral information at neighboring wavelengths. The scientific goal is to determine how the band shape, peak position and continuum behavior evolve as aggregates grow and restructure. These spectra will be combined with the Overview Observation System, which provides optical imaging, cloud morphology, aggregate tracking and independent size information. This combined approach will allow us to link spectral changes to aggregate size, porosity and morphology instead of relying on spectral interpretation alone.

In addition, sampled aggregates can be investigated with complementary methods such as microscopy and THz spectroscopy. Polarization-dependent measurements may further constrain the scattering behavior and internal structure of the aggregates. GT4P will therefore provide a controlled experimental bridge between astronomical observations of silicate dust in protoplanetary disks and the underlying physical properties of growing dust aggregates.

References:
[1]Jürgen Blum Dust agglomeration, Advances in Physics, 55:7-8, 881-947(2006)
[2] J. Varga, MINDS survey of silicates in T Tauri disks: Correlation between dust and gas, A&A, (2026)

Dust Properties in Protoplanetary Disks Revealed by JWST/MIRI

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Dust grains in protoplanetary disks are the building blocks of planets, and characterizing their mineralogy and size distribution is crucial for understanding the earliest stages of planet formation. Mid-infrared spectroscopy offers a powerful tool for probing the composition and size of dust grains in the terrestrial planet-forming regions of disks. In this talk, I will present our recent studies of dust properties in protoplanetary disks based on observations from Spitzer/IRS and JWST/MIRI. By combining spectral decomposition techniques with radiative transfer modeling, we investigate the mineralogical properties and evolution of dust grains across a range of disk environments and evolutionary stages.

References:
Yao Liu, et al. 2025, SCPMA, 68, 259511
Fei Gao, Yao Liu, et al. 2026, RAA, 26, 075005
Yao Liu, et al. 2026, ApJ, 1004, 162

Collisional excitation of interstellar organic molecules

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Molecular spectra from various astrophysical environments often display significant deviations from the local thermodynamic equilibrium (LTE) assumption due to the low gas densities. A complete interpretation of such spectra and the retrieval of accurate column densities require a radiative transfer model and thus the knowledge of the rate coefficients corresponding to the collisional excitation of molecules by the background gas, composed mainly of H_2 molecules and He atoms. However, at present time, the collisional properties of many molecules detected in the interstellar medium remain unknown due to the complexity of the underlying calculations and measurements.
I will review recent theoretical efforts to compute rate coefficients for the excitation of organic molecules of various sizes induced by collisions with He or H_2. I will discuss the current theoretical and numerical challenges through several examples such as HCOOH, *c*-C_3H_2, CH_3CN, or C_6H_5CN [1-5], and I will also highlight the impact of these collisional data on the interpretation of observations in environments such as TMC-1 or Sgr B2 using non-LTE models.

References:
[1] M. Ben Khalifa and J. Loreau, *MNRAS* **527** 846 (2024)
[2] M. Ben Khalifa, B. Darna, and J. Loreau, *A&A* **683** A53 (2024)
[3] K. Sogomonyan, M. Ben Khalifa, and J. Loreau, *ACS Earth and Space Chemistry*, **9** 394 (2025)
[4] M. Ben Khalifa, L. Wiesenfeld, and J. Loreau, *Phys. Chem. Chem. Phys*., **27** 9876 (2026)
[5] K. Sogomonyan, A. Veselinova-Marinova, F. Lique, and J. Loreau, *Phys. Chem. Chem. Phys*., *accepted* (2026)

Diving into the photochemistry of oxygen- and sulfur-bearing polycyclic aromatic hydrocarbons: oxanthrene and thianthrene.

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Polycyclic aromatic hydrocarbons (PAHs) are well-established components of the interstellar medium [1,2]. In recent years, a specific focus is given to functionalized PAH derivatives, particularly with the discovery of cyano-PAHs [3,4]. These functionalized PAHs show distinct photochemical behaviors that can influence their stability and detectability in space. Among them, oxygenated PAHs (OPAHs) and sulfur-bearing PAHs (SPAHs) [5] have attracted increasing interest due to their potential role in astrochemistry, with studies highlighting their unique electronic, vibrational, and rotational signatures [6,7]. In this study, we aim to investigate the photochemical properties of substituted three-ring PAHs, including the rovibrational electronic spectra, with a specific focus on oxanthrene and its sulfurated counterpart thianthrenene using both theoretical calculations and high-resolution experimental techniques. The incorporation of heteroatoms into PAHs affects their photochemical behavior. These species have efficient intersystem crossing [8,9], resulting in higher population of triplet states that may impact their stability under astrophysical conditions and increase their chemical reactivity. Special attention is given to understanding the photochemical properties of these molecules.

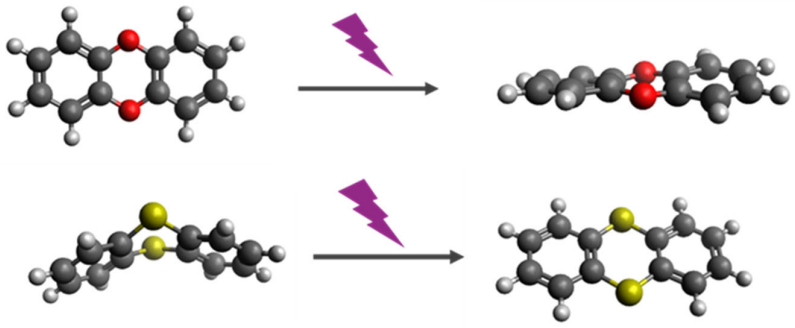

Figure 1: Above, oxanthrene in its groundstate (planar, top left) and its first excited stateconfiguration (twisted, top left) abd below, thianthrene in its groundstate (folded, bottom left) and first excited state (planar, bottom right) configuration.

References:

[1] E. Peeters et al., A&A (2002).
[2] R. Chown et al., A&A (2024).
[3] B. A. McGuire et al., Science (2021).
[4] G. Wenzel et al., Nature Astronomy (2025).
[5] Araki, M., Sanz-Novo et al., Nature Astronomy (2026).
[6] A. P. Rasmussen et al., A&A (2023).
[7] S. Mishra et al., MNRAS (2025).
[8] E. A. Gastilovich et al., Optics and Spectroscopy (2002).
[9] Y. Wen et al., CCS Chemistry (2021).

Gas-Phase Infrared Spectroscopy of Ethynyl-Bearing PAHs from Electrical Discharge using FELIX

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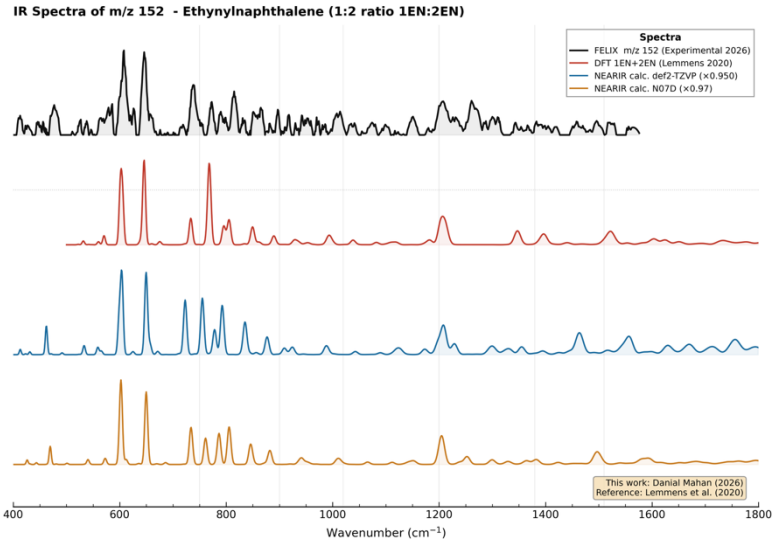
Reactions of the interstellar C_2H radical with aromatic hydrocarbons represent an efficient growth pathway toward molecular complexity in cold clouds [1], a mechanism supported by radio-astronomical detections of several ethynyl- and cyano-substituted aromatics in TMC-1, including ethynylbenzene [2], cyanonaphthalene [3], and recent detection of a $C_{11}H_8$ species [4]. Gas-phase infrared fingerprint spectra of these molecules are essential complements to radio detections, enabling structural identification in infrared observations with JWST.

We apply IR-UV ion dip spectroscopy using Free electron laser (FELIX) coupled with mass-selective two colour 1+1' Resonant Enhanced Multi Photon Ionization, to characterize vibrational fingerprint spectra of ethynyl aromatic products generated by the electrical discharge of bromobenzene and 1,2 -dibromopropane precursors in a supersonic free-jet expansion.

Ethynylnaphthalene (m/z 152) serves as both a confirmed spectral assignment [3] and a DFT calibration anchor. Notably, its formation here proceeds via a radical-induced pathway from the discharge precursors, itself astrochemically relevant given the role of radical-driven PAH synthesis in the cold ISM. Multiple computational protocols are benchmarked against this reference, including DFT and machine learning methods.



Our experiments additionally yield a range of higher-mass products arising from distinct radical pathways, with distributions that partly overlap and partly diverge from those observed in naphthalene-based discharge experiments [5,6]. Structural assignments for these additional species are ongoing. The validated framework is being applied to $C_{11}H_8$ (m/z 140), directly motivated by the recent TMC-1 detection [4], using a spectral unmixing pipeline to disentangle isomeric contributions.

References:
[1] F. Goulay & S.R. Leone, J. Phys. Chem. A 110, 1875 (2006)
[2] D. Loru, C. Cabezas, J. Cernicharo et al., A&A 677, A166 (2023)
[3] B.A. McGuire et al., Science 371, 1265 (2021)
[4] Fuentetaja et al., Astron. Astrophys. (2026)
[5] A.K.F. Lemmens et al., Nat. Commun. 11, 269 (2020)
[6] D. Loru et al., J. Mol. Spectrosc. 386, 111629 (2022)

Isotopically Constrained Formation of Nitrogen-rich Organic Residues from UV Irradiation of CH_3OH:NH_3 Astrophysical Ice Analogs

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Primitive asteroids contain diverse organic molecules, including amino acids and other soluble compounds. Recent analyses of samples returned from asteroid Bennu have revealed a rich inventory of nitrogen-bearing organic matter preserved in primitive Solar System materials. While parent-body processes can modify and generate organic matter after accretion, interstellar and protostellar ice mantles are potential sources of this molecular inventory. Determining the contribution of ice photochemistry to the organic matter observed in primitive bodies remains a key challenge linking astrochemistry and Solar System evolution.

We present results from SPACEMOUSE (Surface Processing Apparatus for Chemical Exploration of Meteoritic Organics Under Simulated Environments), a new ultra-high-vacuum laboratory instrument for investigating ultraviolet (UV) processing of astrophysical ice analogs and the formation of refractory organic residues. The system combines cryogenic ice deposition, UV irradiation, temperature-programmed desorption monitored by quadrupole mass spectrometry, and contamination-controlled residue recovery for ex situ ultra-high-resolution Orbitrap mass spectrometry.

Using CH_3OH:NH_3 ice mixtures, we investigate molecular complexity generated by UV irradiation at cryogenic temperatures. Recovered residues contain hundreds to thousands of molecular formulas spanning a broad range of elemental compositions. Isotopic labeling with $^{13}CH_3OH$ and $^{15}NH_3$ traces carbon and nitrogen incorporation into photochemical products and strengthens molecular formula assignments. The resulting molecular inventories include numerous formulas consistent with amino acids and other nitrogen-bearing organic compounds.

These results demonstrate the capability of SPACEMOUSE for laboratory studies of organic synthesis in astrophysical ices and provide new constraints on the formation of nitrogen-rich organic matter during the early stages of star and planet formation.

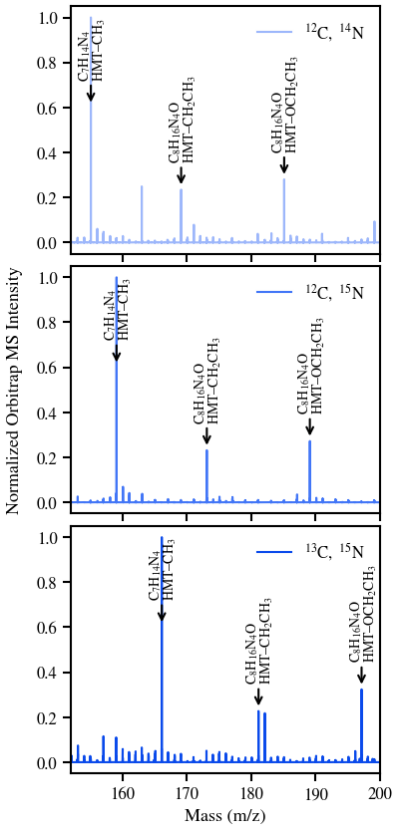

Figure 1. Representative Orbitrap spectra demonstrating carbon and nitrogen incorporation into HMT-related photoproducts through isotopic labeling.

References:
Muñoz Caro, G. M., et al., Nature, 416, 403-406 (2002).
Nuevo, M., et al., Origins Life Evol. Biosph., 38, 37-56 (2008)
Elsila, J. E., et al., ApJ, 660, 911-918 (2007).
Glavin, D. P., et al., Nat. Astron., 9, 199-210 (2025).

Exploring the chemical evolution of sulfur in the laboratory

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Interstellar ice chemistry constitutes a key contribution to the chemical evolution of star-forming regions, specifically to the growth of chemical complexity within these environments, with implications to the origin of prebiotic molecules [1]. Unfortunately, the chemical evolution of sulfur (one of the six essential elements essential to life) is currently unconstrained, because observed abundances of S-bearing molecules are up to two orders of magnitude lower than expected [2]. A significant fraction of this missing sulfur is expected to be locked in icy dust grains [3]. However, observations of interstellar ice mantles have only detected OCS [4] and, tentatively, SO_2 [5] accounting for <5% of the sulfur abundance.

Ice chemistry can be studied in the laboratory under conditions relevant to the interstellar medium. In this talk I will present laboratory experiments exploring the energetic processing of ice analogs containing potential S-carriers.

First I will present a series of experiments studying the chemistry of binary mixtures containing a major ice component (H_2O, CO, or CO_2) and CS_2 (a S-bearing molecule detected in comets that could also be present in interstellar ices). These experiments allowed us not only to address the chemistry of a potential S-carrier in a realistic ice environment, but also to evaluate the formation of OCS through the CO+S and CS+O pathways proposed in the literature [6]. We subsequently used the *pyRate* astrochemical model to theoretically reproduce the laboratory results. The goal was twofold: to test our current understanding of the sulfur evolution in interstellar ices, and to support the interpretation of the experimental results [7]. This work highlighted the complementary nature of theoretical and experimental astrochemistry in our efforts to understand the chemical evolution in star-forming regions.

A significant fraction of the initial sulfur was missing after irradiation of CS_2-bearing ices in the laboratory, suggesting that it could be locked in undetectable sulfur allotropes. These are one of the potential carriers of the missing sulfur in the interstellar medium, and their formation had been previously characterized also in H_2S-bearing ices [8].

Finally, we have recently performed laboratory experiments to study nonthermal desorption processes of SO_2-bearing ices. Nonthermal desorption processes play an important role in the chemical evolution of ices in cold regions of the interstellar medium. The laboratory-derived photodesorption yields can be included in gas-grain chemical models such as NAUTILUS to evaluate their contribution to the gas-phase abundances in astrophysical environments [9].

[1] Herbst & van Dishoeck, ARAA, 47, 1, 427 (2009)
[2] Fuente et al., A&A, 624, A105 (2019)
[3] Laas & Caselli, A&A, 624, A108 (2019)
[4] McClure et al., Nature Astronomy, 7, 421 (2023)
[5] Rocha et al., A&A, 683, A124 (2024)
[6] Martín-Doménech et al.. MNRAS, 535, 1, 807 (2024)
[7] Sipillä et al., A&A, *accepted* (2026)
[8] Carrascosa et al., MNRAS, 533, 1, 967 (2024)
[9] Martín-Doménech et al., MNRAS, 541, 4, 2992 (2025)

Challenges in the detection of *chiral* COMs in interstellar ice analogues, meteorites and in the rationalization of their formation pathways

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Complex organic molecules (COMs) formed in cold astrophysical environments are key molecular witnesses of the chemical evolution that links interstellar clouds, icy grains, comets, asteroids, and ultimately planetary surfaces. Among them, chiral COMs such as amino acids and sugars are of particular interest because they may connect astrochemical synthesis with the emergence of biological homochirality. However, their detection in laboratory ice analogues, as well as meteorite and asteroid return samples, remains analytically challenging, especially when multiple structural isomers, stereoisomers, low-abundance products, refractory residues, and possible contamination sources must be disentangled [1].

In this contribution, I will discuss recent laboratory simulations of interstellar and outer Solar System ice chemistry aimed at understanding the formation of biologically relevant sugars and other chiral COMs under astrophysically relevant conditions. UV and cosmic-ray processing of simple ice mixtures containing H_2O, CO, CO_2, CH_3OH, NH_3 and related precursors produces complex organic residues in which sugars, sugar alcohols, and sugar acids can be detected after careful analytical *in situ* and *ex situ* analyses [2–4]. Recent experiments on ammonia-doped methanol ices irradiated at low temperature further show that fundamental sugars, including ribose, 2-deoxyribose, glucose, and a suite of C_3–C_6 sugar derivatives, may form efficiently under conditions relevant to icy bodies and cold molecular environments [5].

Beyond detection, a major challenge is to rationalize the underlying formation pathways. Combining high-sensitivity molecular analysis with electronic-structure calculations allows us to identify the role of ice composition, temperature, radiation chemistry, and pre-reactive complexes in promoting carbon–carbon bond formation. Ammonia appears to facilitate low-temperature radical coupling by stabilizing molecular arrangements that shorten the distance between reactive carbon centers, thereby enhancing sugar yields. Together, these results highlight the capacity of laboratory astrophysics to bridge molecular inventories, mechanistic insight, and extraterrestrial observations, while emphasizing the need for reproducible ice-irradiation experiments and robust enantioselective analytical approaches for future studies of chiral COMs in ice analogues simulating cold cosmic environments.

References:

[1] V. Leyva, et al., Nat. Commun., 17, 2060 (2026),
[2] C. Meinert, et al., Science, 352, 208 (2016),
[3] M. Nuevo, et al., Nat. Commun., 9, 5276 (2018),
[4] C. Zhang, et al. PNAS, 121, e2320215121 (2024),
[5] C. Zhang, et al. *under revisions*

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Electron-driven reactivity of molecular cations: from mechanisms to cross sections

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Electron impact recombination, (ro-)vibrational-, electronic- and dissociative excitation of molecular cations are in the heart of the molecular reactivity in the cold interstellar medium [1], being major charged particles destruction reactions and producing often atomic species in metastable states, inaccessible through optical excitations. They involve super-excited molecular states undergoing predissociation and autoionization, having thus strong resonant character.

The Multichannel Quantum Defect Theory (MQDT) [1, 2] or MQDT based methods are the most suitable approaches for these processes, capable to account the strong mixing between ionization and dissociative channels, open - direct mechanism - and closed - indirect mechanism, via capture into prominent Rydberg resonances correlating to the ground and excited ionic states, and the rotational effects. These features will be illustrated for several cations of high astrophysical relevance such as NS^+ [3], H_2^+ and isotopologues [4], NeH^+ [5]. Advancement in the theoretical treatment, isotopic effects for small polyatomic systems like N_2H^+ [6], and C_2H^+ [7] will also be presented.

[1] I. F. Schneider, O. Dulieu, J. Robert, eds., EPJ Web of Conferences 84 (2015).
[2] J. Zs. Mezei et al, ACS Earth and Space Chem 3, 2276 (2019).
[3] R. Hassaine et al, J. Phys. B At. Mol. Opt. Phys. 57, 165201 (2024).
[4] R. Hassaine et al, A&A 703 A220 (2025).
[5] R. Hassaine et al, Phys. Rev. A 113, 032820 (2026).
[6] J. Zs. Mezei et al, to be submitted to A&A (2026).
[7] J. Zs. Mezei et al, submitted to Atoms (2026).

High-resolution spectroscopy of HCN^+ and HNC^+ using an ion trap setup

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High resolution spectroscopy is not only an important tool to obtain spectroscopic fingerprints of molecules, but it helps revealing and understanding intramolecular energetic structures and dynamics.

Using a 22-pole cryogenic ion trap, rotationally resolved spectra of small molecular ions can be measured by applying in-house customised/developed action spectroscopy methods like zero-background “kick-out” Laser Induced Reaction (LIR) [1] and Leak-Out Spectroscopy (LOS) [2]. The focus is here in particular on species that are known or expected to play important roles in chemical processes in the interstellar medium (ISM).

One of the most recent projects deals with one of the simplest yet important isomeric systems, HCN^+/HNC^+. Building on the previous publication [3], the latest measurements cover regions in the near-infrared and visible energy range, unveiling dense spectra containing transitions to the first electronically excited states and higher order overtone and combination bands.

This contribution will give an overview of the experimental setup and the applied action spectroscopy methods, and insight into the analysis of the obtained spectra.

[1] P. C. Schmid et al., J. Phys. Chem. A, 126, 8111–8117, (2022)
[2] S. Schlemmer et al., IJMS, 185-187, 589–602, (1999)
[3] M. Jiménez-Redondo et al., Spectrochim. Acta A, 349, 127359, (2026)

Missing Ions in Laboratory and Space

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Action spectroscopy in cryogenic radio-frequency traps is a well-established tool for the study of molecular ions. Over the past 30 years many light induced processes which lead to a change of the mass of the ion of interest have been used to detect the initial absorption of a photon employing a mass spectrometer [1]. The development of the novel technique of leak-out spectroscopy (LOS) in cryogenic ion traps allows us to record broad-band high-resolution spectra of many elusive ions [2]. The method will be introduced briefly.
Rotationally resolved vibrational spectra of astrophysically relevant ions such as small hydrocarbons or protonated versions of abundant neutral species in space, e.g., methanol, will be reported. Rotational lines of these species are recorded by employing millimeter wave-infrared double-resonance spectroscopy [3]. As a result, several molecular ions could be found recently in space based on newly obtained laboratory spectra. Also first medium resolution electronic spectra of such molecules will be presented [4]. LOS is a mass selective and intrinsically background-free technique which sets new standards in spectral quality and scanning speed. Moreover, this method allows a new class of studies because the leak-out process ultimately leads to the preparation of a spectroscopically and mass selected sample. As an illustration I will show direct measurements of the ortho to para ratio for CH_3^+ as well as for its isotopologs CH_2D^+ and CD_2H^+. But also structural isomers can be selected. Examples and future perspectives of the unique features of LOS will be discussed.

Acknowledgement: The work presented summarizes many important contributions by Oskar Asvany[1], Weslley Silva[1], Philip Schmid[1], Thomas Salomon[1], Sven Thorwirth[1], Samuel Marlton[1], Divita Gupta[1] and many doctoral students.

References:
[1] B. A. McGuire, O. Asvany, S. Brünken, S. Schlemmer, Nat. Rev. Phys., 2, 402–410, (2020)
[2] P.C. Schmid, O. Asvany, T. Salomon, S. Thorwirth, and S. Schlemmer, J. Phys. Chem. A, 126, 8111–8117 (2022)
[3] O. Asvany and S. Schlemmer, Phys. Chem. Chem. Phys., **23**, 26602–26622 (2021);
[4] S. J. P. Marlton, P. C. Schmid, T. Salomon, O. Asvany, and S. Schlemmer, J. Phys. Chem. Lett., **16**, 8758–8763 (2025)

Pressure Broadening Coefficients of SO_2 by He for Studies of Exoplanetary Atmospheres

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Over the past few years, the focus of exoplanetary science has shifted from their detection to the characterization of their atmospheres. A major contributor to this transition has been the James Webb Space Telescope (JWST), which has provided the first detailed constraints on the chemical composition of a wide range of exoplanets, from rocky worlds such as 55 Cnc-e to gas giants like WASP-39b. With the recent first light of GRAVITY+ and upcoming facilities such as ARIEL and the Extremely Large Telescope (ELT), capabilities are expected to improve significantly by delivering spectra with even higher spectral resolution and signal-to-noise ratios.

As a result, the accurate interpretation of these spectra strongly depends on precise spectroscopic reference data, which are typically provided by databases such as HITRAN [1] and ExoMol [2]. While these databases contain extensive molecular line lists and spectroscopic parameters, important data relevant under exoplanetary conditions, particularly pressure-broadening coefficients, are still missing for many species. This limitation becomes especially relevant for molecules such as sulfur dioxide (SO_2), which has been discussed as a molecule of astrobiological interest due to its links to geological activity, atmospheric photochemistry, and, in some contexts, potential biosignature scenarios [3,4] in rocky planets. With its detection in the atmosphere of the hot Saturn WASP-39b [5,6], it has been interpreted as the first clear evidence for photochemistry in an exoplanetary atmosphere. Given that H_2 and He dominate the atmospheres of gas giants, we focus here on He-induced broadening of SO_2 as a collisional partner for interpreting these atmospheres over a relevant pressure range (up to 1 bar).

We perform high-resolution gas-phase spectroscopy using a Bruker 120/5 HR FTIR spectrometer in the mid-infrared spectral region. In particular, we determine pressure-broadening coefficients of SO_2 at room temperature for pressures up to 1000 mbar. In this talk, I will present first results on He-induced pressure broadening of SO_2, focusing on the ν_3 and $\nu_1+\nu_3$ bands, and compare them with existing values in the HITRAN database.

References:
[1] Gordon et al. 2026, JQSRT 353, 109807
[2] Tennyson et al. 2016, J. Mol. Spectrosc. 327, 73
[3] Seager et al. 2016, Astrobiology, 16(6), 465
[4] Schwieterman et al. 2018, Astrobiology, 18(7), 663
[5] Alderson et al. 2023, Nature, 614, 664
[6] Rustamkulov et al. 2023, Nature, 614, 659

Toward gas phase spectroscopy of complex molecular ions in a cryogenic ion trap

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The diffuse interstellar bands (DIBs) and unidentified mid-infrared emission (UIE) are two of the most intriguing spectroscopic phenomena linked to complex molecules in interstellar space. DIBs are absorption features originating from interstellar matter that have so far resisted assignment to any known atomic or molecular transitions, while UIE lines are infrared emission features detected across a wide range of interstellar environments. Molecular ions are considered likely carriers of both DIBs and UIEs, with polycyclic aromatic hydrocarbons (PAHs) being among the most promising candidates [1]. A landmark study by Campbell et al. identified two DIB features at 9632 Å and 9577 Å as belonging to C_{60}^+, based on laboratory studies obtained via helium-tagging spectroscopy [2]. Despite these advances, the intrinsic difficulty of gas phase spectroscopy with complex molecular ions continues to hinder the unambiguous assignment of interstellar features to specific species, and the characteristics and origins of both DIBs and UIEs remain amongst the longest-standing open problems in molecular astrophysics.

To address some of these issues, we are presently developing a novel gas phase spectroscopy setup for complex molecular ions. The technique relies on laser-driven excitation of electronic transitions in complex molecules, followed by intramolecular vibrational energy redistribution and subsequent mid-infrared photon emission [3]. Detection is achieved using a sensitive mid-infrared sensor (2-30 μm). Experimentally, we will couple a cryogenic electrostatic ion beam trap [4] with a mid-infrared detector module based on blocked-impurity-band (BIB) technology [5]. In this talk, we outline the current status of the experiment and discuss prospects for future developments.

References

[1] S. Schlemmer et al., Science 265,1686-1689 (1994)
[2] E. Campbell et al., Nature 523, 322–323 (2015)
[3] L. J. Allamandola, et al., Astrophys. J. Suppl.71, 733 (1989)
[4] D. Zajfman, et al., Physical Review A. 55, 3, p. R1577-R1580 (1997)
[5] Petroff et al., United States Patent, US4568960A (1980)

Ground state rotational spectrum of protonated methanol ($CH_3OH_2^+$): The first step towards its interstellar detection

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Protonated methanol ($CH_3OH_2^+$) has long been suggested as an important intermediate species driving chemical complexity in the interstellar medium. Yet, its high-resolution spectra, crucial for enabling its eventual interstellar detection, remain unknown. Using the recently developed leak-out spectroscopy (LOS) method [1], the first high-resolution spectroscopic data for $CH_3OH_2^+$ are reported here. The measurements were performed at cryogenic temperatures using an ion trap apparatus. Rovibrational transitions within the fundamental C–H and O–H stretching modes were initially measured near 3000 cm^{-1} and 3500 cm^{-1}, respectively. Because $CH_3OH_2^+$ exhibits two large-amplitude motions (CH_3 rotation and OH_2 inversion), the observed spectra are extremely dense, containing more than 6,000 transitions arising from multiple tunneling components. Despite this complexity, several series of lines could be assigned, providing the first set of ground state parameters for $CH_3OH_2^+$. These rovibrational data were subsequently used to search for pure rotational transitions of $CH_3OH_2^+$ in the millimeter-wave range using an infrared/millimeter-wave double resonance scheme [2]. So far, this combined experimental approach enabled the measurement of more than 25 rotational transitions in the 40–350 GHz frequency range from four different tunneling species. Based on the accurate transition frequencies derived in this work, first searches for this important cation in space are now in progress.

References:
[1] J. Phys. Chem. A, 126, 8111 (2022)
[2] Phys. Chem. Chem. Phys., 25, 19740 (2023)

Product branching in the CN + propene reaction at very low temperatures probed by chirped-pulse millimeter wave spectroscopy

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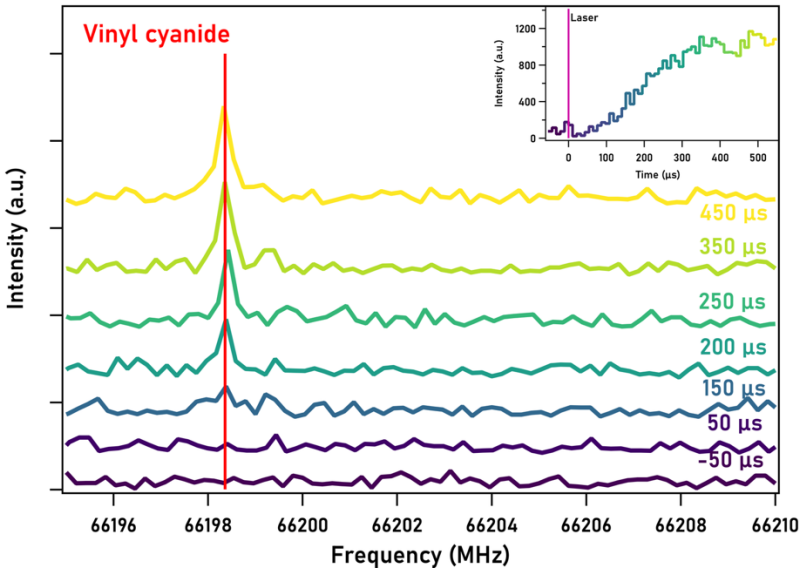
Propene was first detected in 2007 in the cold dark interstellar cloud TMC-1[1] and has since been observed in a range of interstellar sources at high abundance. Recent observations have also detected some potential products of its reaction with CN radicals.[2] In this work, we employ the CPUF (Chirped Pulse in Uniform supersonic Flow) technique,[1,2] which is a combination of the CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme or Reaction Kinetics in Supersonic Uniform Flow) method to provide a low temperature gas phase environment and a chirped-pulse Fourier transform millimeter spectroscopic detection method. This CRESU flow has been modified with an additional expansion chamber to enhance the detection of a wider variety of species and to overcome pressure effects in the flow. The branching fraction of the reaction between CN radicals and propene to yield acrylonitrile plus methyl radicals was measured at 35 K and 52 K for the first time. No pressure dependence was found. Upper limits for the different cyanopropene isomers were also determined. The results are compared to RRKM / Master Equation calculations on a new potential energy surface. Time / space permitting, new developments of the CRESU method enabling lower temperature flows (5 K and below) for the study of barrierless reactions and energy transfer will also be detailed.



References :
[1] N. Marcelino, J. Cernicharo, M. Agundez, E. Roueff, M. Gerin, J. Martin-Pintado, R. Mauersberger, and C. Thum, *Astrophys. J.*, **665**, L127 (2007).
[2] J. Cernicharo, R. Fuentetaja, C. Cabezas, M. Agundez, N. Marcelino, B. Tercero, J. R. Pardo, and P. de Vicente, *Astron Astrophys*, **663**, 11, L5 (2022).
[3] C. Abeysekera, B. Joalland, N. Ariyasingha, L. N. Zack, I. R. Sims, R. W. Field, and A. G. Suits, *J. Phys. Chem. Lett.*, **6**, 1599 (2015).
[4] T. Guillaume, B. M. Hays, D. Gupta, I. R. Cooke, O. Abdelkader Khedaoui, T. S. Hearne, M. Drissi, and I. R. Sims, *J. Chem. Phys.*, **160**, 204201 (2024).

The role of Interstellar Dust in the formation of Complex Organic Molecules

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Interstellar dust grains play a vital role in the physics and chemistry of the interstellar medium (ISM). Formed in the outflows of evolved stars, these carbon and/or silicate rich grains are ejected into the ISM and provide surfaces upon which molecules and atoms accrete and react. In the coldest, densest regions, the grains reach temperatures as low as 10 K and get covered in icy mantles of H_2O, CO, CO_2, etc. Interactions between the ice, dust, and interstellar radiation can lead to the formation of complex organic molecules (COMs) of which some are biologically relevant species, which are later inherited by stellar and planetary systems.

The experiments presented here aim to study such formation processes. For the first time, the interaction with atomic beams, ices, and radiation is investigated for the realistic carbonaceous dust analogues synthesised at the Stardust facility in Madrid, an ultra-high vacuum (UHV) setup dedicated to directly mimicking the interstellar formation of dust grains. This carbonaceous dust comprises a range of nanometer-sized hydrocarbon particles, pure carbon clusters, and aliphatic carbon chains [1].

Previous experiments have shown that a range of COMs can be formed when complex ices containing hydrocarbon molecules undergo energetic processing [2, 3]. Since the dust grains synthesised at Stardust already contain various reactive carbon species, we propose that interstellar dust can be a direct precursor to complex molecules such as fatty acids. We expose the dust grains to atomic beams, interstellar relevant ices and energetic ultraviolet (UV) radiation, mimicking several astrochemical processes.

The results, as presented here, give new insights into the role of carbonaceous dust in interstellar chemistry and investigate novel pathways to the formation of prebiotic fatty acids.

[1] L. Martínez, G. Santoro, P. Merino, et al., Nature Astronomy, 4, 97-105 (2020)
[2] J. Noble, E. Michoulier, C. Aupetit and J. Mascetti, Astronomy & Astrophysics, 644, A22 (2020)
[3] M. Nuevo, S. N. Milam, S. A. Sandford et al., Advances in Space Research, 48, 1126-1135 (2011)

Heavy ion irradiation of astrophysical ice analogs: Forthcoming improvements at GANIL facilities

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Complex organic molecules (COMs) are widespread across the Universe, from interstellar clouds to planetary atmospheres. In the cold, dense regions of space, simple molecules such as H_2O and CO condense onto dust grains, forming icy mantles that act as reservoirs for more complex chemistry. Cosmic rays, as a dominant external energy source, trigger the release of these molecules into the gas phase, driving the evolution of interstellar and planetary organic inventories.

For laboratory astrophysics applications, we replicate the radiative conditions of cosmic rays in astrophysical environments using heavy ions accelerated at GANIL (Grand Accelerateur national d'Ions Lourds, in Caen, France) [1]. Through the IGLIAS setup, we irradiate low-temperature ices and organic materials, employing infrared absorption spectroscopy and QMS mass spectrometry to detect and characterize the physico-chemical evolution of molecules under heavy ion bombardment [2]. This approach provides unique insights into the transformation mechanisms of matter under extreme conditions, directly relevant to interstellar and planetary chemistry.

In this context, we investigated the evolution of propionitrile (CH_3CH_2CN) ice mixed with water, irradiated by keV–MeV heavy ions to simulate cosmic ray interactions. Propionitrile is a relevant molecule for astrochemistry, as it has been detected in the interstellar medium [3] as well as in Titan's atmosphere [4]. We will present the results of this experiment and an overview of the new MIRRPLA (Multiple-beam Irradiation Platform) [5], currently commissioned at CIMAP-GANIL. This platform enables simultaneous irradiation with UV photons, keV electrons, and keV–GeV ions, allowing the study of synergistic reactions in ices through a multi-analytical approach combining QMS, FTIR spectroscopy, and high-resolution Orbitrap mass spectrometry.

[1] Rangama, J.& al, Nucl. Phys. News. 32, No. 2 29-33 (2022)
[2] Rothard, H. & al, J. Phys. B: At. Mol. Opt. Phys. 50, 062001 (2017).
[3] Johnson, D.R. APJ 1 218, 370-376 (1977)
[4] Khanna R. K. Icarus 177,1 (2005)
[5] Domaracka and Danger, Nuclear Physics News 33(4), 36–37 (2023).

Laboratory astrophysics in the JWST and ALMA era

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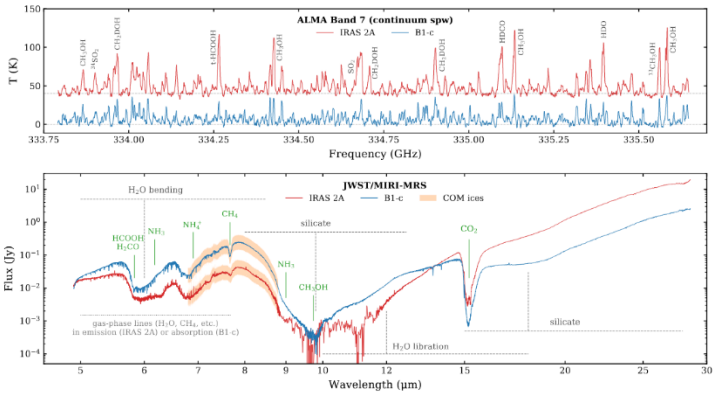
Astronomy is driven by new observational facilities that open up wavelength ranges with unprecedented sensitivity, spectral and spatial resolution. Over the past decade, the Atacama Large Millimeter/submillimeter Array (ALMA), together with other radio facilities at millimeter and centimeter wavelengths, combined with the James Webb Space Telescope (JWST) at infrared wavelengths, have greatly expanded the opportunities to observe molecules both in the gas as well as in ices and solid state. However, the scientific harvest from those spectra relies heavily on "laboratory" measurements (i.e., experiments and theory) that provide the basic molecular data and underlying chemical reactions. In this talk, a brief overview and examples will be presented of recent developments where observations and laboratory astrophysics go hand in hand.



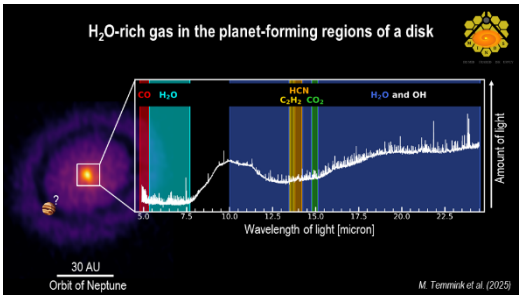


Figure Left: ALMA spectrum of complex organic molecules toward the low-mass hot core protostars B1c and NGC 1333 IRAS2A (top) and JWST spectra of ices (including the same complex molecules) toward these sources (bottom) (Chen et al. 2024, A&A 690, A205). Right: JWST spectrum of a planet-forming disk showing broad silicate emission as well as a rich forest of H_2O lines together with CO, C_2H_2 HCN and CO_2 (Temmink et al. 2025, A&A 699, A134). These data come from the JWST-MIRI JOYS (miri.strw.leidenuniv.nl) and MINDS (https://minds.cab.inta-csic.es/) programs.

Binding Energies of Sulfur-Bearing Species on Charged Interstellar Ice: A Density Functional Theory Study

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The chemically rich nature of the interstellar medium (ISM) is intrinsically linked to the presence of dust grains, where amorphous solid water (ASW) icy mantles act as active catalytic surfaces.[1] A crucial parameter in astrochemical modeling is the binding energy of molecular species to these ices, which dictates vital processes such as surface diffusion, reaction efficiency, and thermal desorption. Despite its importance as an essential element for the basis of life on earth, sulfur presents a long-standing paradox in astrochemistry: its observed gas-phase abundance drops drastically in dense clouds, a phenomenon known as the "sulfur depletion problem".[2] While efficient hydrogenation to H_2S on grain surfaces is theoretically expected, there are at present no direct observations of H_2S on interstellar ices, leaving the dominant chemical reservoirs of sulfur under debate.

Standard computational models often treat interstellar ice as an electronically neutral surface. However, cosmic rays and radiation may cause grain charging to be present in the ISM. Building upon recent insights that surface charging can influence molecular desorption in a highly species-dependent manner, this work investigates the binding energies of key sulfur-bearing species: S, H_2S, SO_2, and OCS, on both neutral and singly negatively charged ASW surfaces using Density Functional Theory (DFT).[3]

Through a detailed statistical analysis of the binding energy distributions, we demonstrate that surface charging alters the desorption energetics in a non-uniform way. Specifically, we find that the binding energy of OCS does not change, while the binding energy of H_2S increases slightly resulting in a broadening of the binding energy distribution. In contrast, the binding energies of S and SO_2 on a charged surface increase significantly, by an order of magnitude.

These results will not only have a direct implication for astrochemical modeling, but also offer a novel framework that could shed new light on the mechanisms driving the missing sulfur budget in the dense interstellar medium.

References:

1. E. Herbst, E. F. van Dishoeck, *ARA&A* **2009**, 47, 427.
2. T. H. G. Vidal, J.-C. Loison, A. Y. Jaziri, et al., *MNRAS* **2017**, 469, 435.
3. T. Vorsselmans, E. C. Neyts, *ApJ* **2025**, 986, 30.

Aromatic Complexity in the Interstellar Medium

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Complex carbon-bearing molecules such as polycyclic aromatic hydrocarbons (PAHs) play a central role in interstellar chemistry, and their identification requires a close interplay between laboratory spectroscopy and astronomical observations. In this talk, I will show how the interplay of high-resolution rotational spectroscopy and radio astronomy uncovers previously uncharacterized aromatic molecules in astronomical sources such as the cold, dark molecular cloud TMC-1. I will highlight recent detections and non-detections, and discuss what they reveal about the evolution of complex cosmic carbon, its role in interstellar chemistry, and its connection to the organic material that seeds forming planetary systems. I will further outline key open questions in PAH chemistry and the opportunities ahead for advancing our laboratory and astronomical understanding of these molecules.

Formation and destruction pathways of interstellar negative ions

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Negatively charged ions have been observed in the interstellar medium for the first time in 2006 [1]. Since then their role in interstellar chemistry and their relevant formation and destruction processes have seen a lot of attention [2,3]. We study ion-molecule reactions and photodetachment spectroscopy of negative ions using cryogenic radiofrequency ion traps. We have probed absolute detachment cross sections [4,5], which could be used to benchmark theoretical cross sections for radiative association [6]. By adding a source for cold atomic hydrogen to our ion trap, we have determined absolute reaction rate coefficients for reactions of several negative ions, CN^-. C_3N^-. C_2^-, C_4^-, C_2H^-, C_4H^- with atomic hydrogen in the low-temperature range relevant for interstellar molecular clouds [7,8]. In addition, we have numerically studied the expected abundance of the simplest of all negative ions, H^-, in a prototypal dense molecular cloud [9]. Recently, we started to study anion-cation mutual neutralization reactions at low temperature, another important and largely unstudied loss channel for interstellar negative ions.

[1] M. C. McCarthy, C. A. Gottlieb, H. Gupta, P. Thaddeus, Ap. J. 652, L141 (2006)
[2] T. J. Millar, C. Walsh, T. A. Field, Chem. Rev. 117, 1765 (2017)
[3] M. Agúndez, N. Marcelino, B. Tercero, I. Jiménez-Serra, J. Cernicharo, Astron. Astrophys. 677, A106 (2023)
[4] T. Best, R. Otto, S. Trippel, P. Hlavenka, A. von Zastrow, S. Eisenbach, S. Jezouin, R. Wester, E. Vigren, M. Hamberg, W. D. Geppert, Ap. J. 742, 63 (2011)
[5] S. S. Kumar, D. Hauser, R. Jindra, T. Best, Š. Roučka, W. D. Geppert, T. J. Millar, R. Wester, Ap. J. 776, 25 (2013)
[6] M. Khamesian, N. Douguet, S. F. dos Santos, O. Dulieu, M. Raoult, W. J. Brigg, V. Kokoouline, Phys. Rev. Lett. 117, 123001 (2016)
[7] C. Lochmann, S. Purushu Melath, M. Hauck, R. Wild, R. Wester, J. Phys. Chem. A 129, 103 (2024)
[8] C. Lochmann, S. Purushu Melath, R. Wild, E. Yurtsever, A. Martín Santa Daría, L. González-Sánchez, F. A. Gianturco, R. Wester, Ap. J. 976,114 (2024)
[9] N. Meindl. F. A. Gianturco, R. Wester, Mon. Not. R. Astron. Soc. (in press)

ExoMol at All Wavelengths: Spectroscopic Data for Exoplanet Atmospheres from JWST and Ariel to the ELTs

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Accurate and comprehensive spectroscopic data are essential for interpreting the atmospheres of exoplanets, from low-resolution space observations with JWST and the future Ariel mission to high-resolution ground-based studies with current and next-generation telescopes. Over the past 15 years, the ExoMol project has developed into a major international resource for molecular line lists, cross sections and opacity data, supporting a broad community working on exoplanets, cool stars, brown dwarfs and atmospheric chemistry.

In this talk I will review the scientific motivation behind ExoMol, its mission to provide open, high-quality spectroscopic data for the community, and some of its key successes to date. I will then discuss the current and urgent data needs emerging from exoplanet spectroscopy: broad wavelength coverage from the UV to the infrared, reliable high-temperature opacities, photodissociation and chemical data, and line lists suitable for both low-resolution retrievals and high-resolution cross-correlation spectroscopy. Finally, I will outline the future direction of ExoMol, which aims to deliver all-wavelength molecular data for the next generation of exoplanet observations, including Ariel, JWST follow-up studies, atmospheric-chemistry applications, and the coming era of extremely large telescopes.

Studies of gas phase reactions with cryogenic electrostatic storage rings

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Cryogenic electrostatic ion-beam storage rings provide unique opportunities to investigate the properties of gas-phase ions and their reactions under conditions that closely resemble those found in space. The Cryogenic Storage Ring (CSR) [1] at the Max Planck Institute for Nuclear Physics in Heidelberg is designed for merged-beams studies of ion–electron recombination [2-6] and ion–neutral reactions [7-8] involving internally cooled ions. The DESIREE facility at Stockholm University [9] enables studies of collisions between oppositely charged internally cooled ions with precise control of the collision energy down to the sub-electronvolt regime [10-16]. Such low-energy ion–ion reactions are expected to play a significant role in the chemistry of dilute environments where anions, rather than electrons, serve as the dominant negative charge carriers [17]. In addition, the exceptional vacuum conditions achieved in CSR, DESIREE, and other cryogenic ion-storage devices worldwide enable investigations of the intrinsic properties and dynamics of atomic, molecular, and cluster ions on timescales exceeding minutes and in unprecedented detail [18-23].

In this overview talk, I will present recent results obtained with cryogenic electrostatic ion-beam storage rings and discuss how these facilities contribute to our understanding of the formation, evolution, and survival of molecules in astrophysical environments.

References:
[1] R. v. Hahn et al, Rev. Sci. Instrum. **87**, 063115 (2016).
[2] A Znotins, et al, Nat. Commun. 16, 7738 (2025)
[3] Á Kálosi et al, ApJ Lett. 955, L26 (2024)
[4] D Paul et al, ApJ 939, 122 (2022)
[5] Á Kálosi et al, PRL 128, 183402 (2022)
[6] O. Novotny et al, Science 365, 6454, 676 (2019)
[7] F Grussie et al A&A, 699, L12 (2025)
[8] F Grussie et al PRL 132, 243001 (2024)
[9] R. D. Thomas et al, Rev. Sci. Instrum. 82, 0655112 (2011); H. T. Schmidt et al, Rev. Sci. Instrum. 84, 055115 (2013).
[10] M. Poline et al, PNAS, accepted (2026)
[11] M. Gatchell et al, A&A 694, A43 (2025).
[12] A. Bogot et al, Nat. Chem. 17, 541 (2025).
[13] M. Poline et al, Nat. Commun. 16, 8528 (2025).
[14] M. Poline et al, PRL 132, 023001 (2024).
[15] A. Bogot et al, Science 383, 285-289 (2024).
[16] J. Grumer et al, PRL 128, 033401 (2022).
[17] T. J. Millar, C Walsh, & T. A. Field, Chem. Rev. 117, 1765 (2017)
[18] V. C. Schmidt et al, PRL 133 , 183001 ()
[19] J. E. N. Navarrete, et al, PRL 135, 213001 (2025).
[20] J. N. Bull et al. PRL. 134, 228002 (2025).
[21] P K Najeeb et al. PRL 131, 113003 (2023).
[22] M. Stockett et al, Nat. Commun. 14 395 (2023).
[23] M. Gatchell et al, Nat. Commun. 12, 6646 (2021).

Abstracts: Posters

Synchrotron Vacuum-Ultraviolet Scattering Measurements of Interstellar Ice Analogues

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Amorphous water ice plays a critical role in astrochemistry and is found throughout the interstellar medium, planet forming regions, and cometary bodies. Its amorphous and porous structure[1] influences its microphysical molecular behaviour, including processes like adsorption, desorption and chemical reactivity. Indeed, the degree of surface porosity controls the availability of surface sites for adsorption and reactions of different volatile species.[2] In previous lab experiments, the porosity of vapor-deposited amorphous water ices have been characterized indirectly using infrared vibrational spectroscopy, focused on the appearance of dangling O-H bands from undercoordinated water molecules, and through adsorption isotherms of small guest molecules such as methane.[2] These studies, alongside theoretical work, show the surface porosity of water ice is highly dependent on deposition angle[3] and can evolve through thermal[4] and irradiation processing.[5]

Light scattering has been used to characterize a variety of other materials with interesting small-scale structure. This method relies on inhomogeneities between the refractive index of the bulk material compared to its pores, suspended particles or other structural elements.[6] Vacuum ultraviolet (VUV) wavelengths provide access to pores and structures on size scales of tens to hundreds of nanometers,[7] which is well matched to the expected nano-porosity of amorphous ice. We have developed angular resolved VUV scattering capabilities to measure and characterize the porosity of amorphous solid water ice, making use of the VUV synchrotron beamline at the Advanced Light Source. We have measured the angular distribution of scattered ultraviolet light for ices formed with different structures and subjected to thermal processing. I will show that fitting these angular distributions to a simple theoretical model is providing new insight on the surface porosity of amorphous water ice structures, informing our understanding of the surface processes and reactions that can take place in interstellar ices.

References:

1. *Nature,* 319, 6051 (1986)
2. *J. Chem. Phys.,* 127*,* 20, (2007)
3. *J. Chem. Phys.,* 118, 1, (2003)
4. *A&A*, *573*, A16, (2015)
5. *J. Chem. Phys.,* 126, 24 (2007)
6. *Nature Photon*, *7*, 3, (2013)
7. *Review of Scientific Instruments*, *77,* 4, (2006)

Rotational spectroscopy of 1- and 5-cyanoacenaphthene and their astronomical search towards TMC-1

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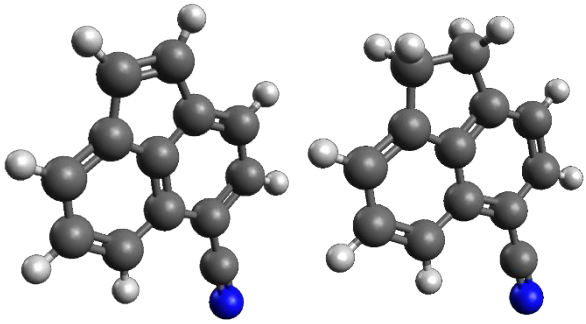
Most of the polycyclic aromatic hydrocarbons (PAHs) detected in TMC-1 are inherently unsaturated [1]. However, recent detection of the cyclic species cyclopentadiene [2], indene [3,4], phenalene [5,6] and 1H-cyclopent[cd]indene [7] toward TMC-1 and other sources contain a methylene (-CH_2-) group. This could suggest that limited hydrogenation and structural pertubations of the aromatic framework are chemically viable under cold cloud conditions. These findings motivated us to search for two isomers of the three-ring PAH cyanoacenaphthene, structurally similar to its dehydrogenated counterpart cyanoacenaphthylene (see Figure). We used chirped-pulse and Balle-Flygare-type Fourier-transform microwave spectroscopy in the 6.5 to 18 GHz frequency range to record and analyze the laboratory rotational spectra. A (non-)detection and constraints on their column densities relative to the cyanoacenaphthylenes detected in TMC-1 [8,9] would make these molecules sensitive probes of PAH hydrogenation and stability under cold cloud conditions. Here, we present the spectroscopic characterization and results of the astronomical search for both species.



References

[1] McCarthy & McGuire, Annu. Rev. Phys. Chem. 77.1, 345-369 (2026)
[2] Cernicharo et al., A&A 649, L15 (2021)
[3] Burkhardt et al., Astrophys. J. Lett. 913.2, L18 (2021)
[4] Agúndez et al., A&A (2023)
[5] Cabezas et al., Astron. Astrophys. 701, L8 (2025)
[6] Wenzel et al., ApJL 1006.2, L38 (2026)
[7] Fuentetaja et al., Astron. Astrophys. 706, L10 (2026)
[8] Cernicharo et al., Astron. Astrophys. 690, L13 (2024)
[9] Cernicharo et al., Astron. Astrophys. 705, L7 (2026)

Infrared Spectroscopy of the Cyanomethyl Anion CH_2CN^-

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Molecular anions are integral to astrochemistry, yet spectroscopic characterization remains limited. With JWST now enabling sensitive infrared searches for new molecular ions, laboratory reference spectra of candidate anions are critically needed[1]. The cyanomethyl anion CH_2CN^- is a long-proposed interstellar species and potential diffuse interstellar band carrier[2]. Although a photoelectron spectrum exists for this anion[3], there is no gas-phase vibrational spectrum recorded, yet. Here, we present our progress on infrared predissociation (IRPD) spectroscopy of CH_2CN^- using the FELion user station at HFML-FELIX[4,5].

The FELion user station combines a cryogenic 22-pole ion trap with the intense, tunable infrared radiation from the FELIX free-electron lasers, enabling vibrational spectroscopy of mass-selected ions at temperatures down to 4 K. This unique combination allows us to probe molecular anions that are challenging to study with conventional spectroscopic techniques[6]. For CH_2CN^-, ions are produced via dissociative electron attachment to CH_3CN and trapped at 10–30 K where collisions with cold H_2 buffer gas form weakly bound $CH_2CN^-\cdot H_2$ complexes. Vibrational spectra are obtained by monitoring H_2 loss upon resonant IR excitation across 400–3200 cm^{-1}, revealing all fundamental modes of the ionic core.

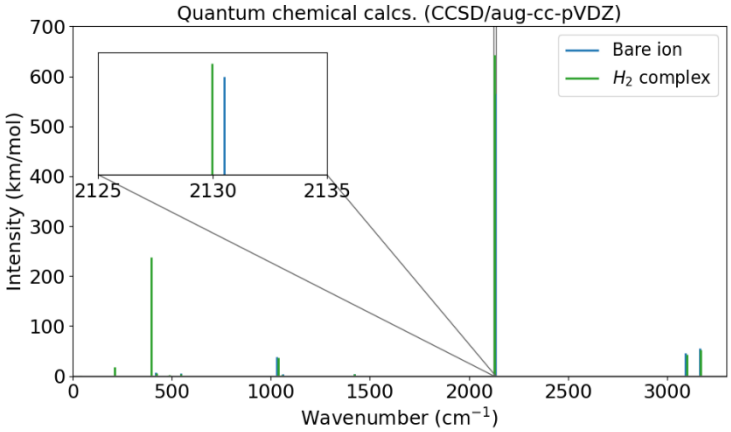

Figure 1: Simulated IR spectrum of CH_2CN^- with H_2 messenger species.

IRPD spectra are compared with high-level quantum chemical harmonic calculations at the CCSD/aug-cc-pVDZ level of theory (Fig. 1) to validate computational methods and quantify tag-induced frequency shifts. The measured spectrum could guide JWST searches in various environments where efficient electron attachment pathways may produce detectable CH_2CN^- abundances.

References:

1. O. Berné et al., *Nature*, 621, 56–59 (2023)
2. Fortenberry et al., *Astrophys. J.*, 762, 121 (2013)
3. Ashworth et. al., *Rev. Sci. Instrum.* 95, 075103 (2024)
4. Jusko et. al., *Faraday Discuss.*, 2019, 217, 172-202
5. https://www.hfml-felix.nl/en/
6. Melath et al., *Mol. Phys.*, e2564248 (2025).

Infrared Optical Constants of Astrochemical Ices for the JWST Era

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The interpretation of infrared ice features observed with the *James Webb Space Telescope* (JWST) relies critically on high-quality laboratory reference spectra that accurately reproduce interstellar ice conditions. In laboratory experiments, the growth of these ices depends on precise control of several parameters, including temperature, composition, and deposition rate. However, for practical reasons, laboratory ices are typically grown rapidly, on timescales of minutes, whereas the condensation of gaseous species onto dust grain surfaces in astrophysical environments occurs over orders of magnitude longer timescales.

This discrepancy raises the question of how deposition rate influences the physical properties of laboratory ice analogues. In particular, the growth rate may affect the density, porosity, and molecular structure of the resulting ice, with direct consequences for its infrared spectral signatures. Understanding these effects is therefore essential for reliably comparing laboratory spectra with astronomical observations.

We present ongoing work investigating the impact of deposition rate on the structure and spectroscopy of ices composed of the most abundant interstellar molecules. Using a highly controlled ultra-high vacuum chamber, we deposit ices over a wide range of growth rates, corresponding to timescales from seconds to several days. The resulting ices are characterized using infrared spectroscopy, while simultaneous laser interferometry measurements provide precise thickness determinations and enable the derivation of optical constants.

These measurements are specifically designed to produce high-quality laboratory reference data tailored to the sensitivity of JWST. By systematically probing deposition rate as a key experimental parameter, this work aims to bridge the gap between laboratory ice analogues and the conditions under which interstellar ices form.

References:
ARAA, 62,243-286,(2024) https://doi.org/10.1146/annurev-astro-071221-052732
MNRAS,486,4,(2019) https://doi.org/10.1093/mnras/stz1223
A&A,704,A56,(2025) https://doi.org/10.1051/0004-6361/202556786
A&A,699,A79,(2025) https://doi.org/10.1051/0004-6361/202555090

Laboratory rotational spectroscopy and interstellar detection of deuterated methyl formate

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Deuterium fractionation is an important astrophysical tool for tracing the evolution and inheritance of chemical material throughout the stages of star and planet formation.[a] Methyl formate has been well known in the interstellar medium (ISM) since its first detection in 1975 toward Sgr B2N[b] and its singly deuterated (CH_2DOCHO and CH_3OCDO) and doubly deuterated (CHD_2OCHO) isotopologues have been identified in the protostellar region IRAS16293-2422[c,d]. Until now, spectroscopic studies of multideuterated isotopologues of methyl formate were restricted to species with a doubly deuterated methyl group. Understanding the origin and chemical pathways leading to methyl formate, however, requires understanding the formation of all deuterated isotopologues. Our recent detection of CH_2DOCDO towards IRAS16293-2422 and its agreement with chemical models suggests that ice-phase chemistry in the pre-stellar phase is dominant. This detection was made possible by an extensive rotational spectroscopic investigation. In this talk, I will present our spectroscopic results of CH_2DOCDO and CHD_2OCDO both of which display internal rotation of their asymmetrical methyl rotor resulting in complex spectral patterns. I will also present the interstellar detection of, and search for, these isotopologues, and discuss the implications for understanding the chemistry of methyl formate and complex organic molecules in the ISM.

References

a. Ceccarelli *et al*., Protostars and Planets VI, 859 (2014)
b. Brown *et al*., ApJ, 197 (1975)
c. Jørgensen *et al*., A&A, 620 (2018)
d. Manigand *et al*., A&A, 623 (2019)

Band Strengths for O_2 and H_2 in Astrophysical Ices and Their Usefulness for Future JWST Campaigns

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To date, there have been no detections of solid phase O_2 or H_2 in interstellar space via their forbidden vibrational transitions at 6.447μm (~ 1551cm^{-1}) and 2.415μm (~ 4141cm^{-1}) respectively. With the new James Webb Space Telescope (JWST), detections of these two species and other homonuclear molecules (e.g. N_2) in the solid phase may be possible. To assist future observing efforts, we have measured the band strength of the O_2 absorption at 6.447μm [1] and the absorption of the two different nuclear spin states of H_2 (ortho and para) at 2.415μm (4141 cm^{-1}) and 2.420μm (4132cm^{-1}) in different astrophysical ice environments. Our experiments with O_2 focused on binary mixtures with H_2O, CO_2, and CO, while our experiments with H_2 focused on binary mixtures with H_2O. We chose the companion species to represent typical interstellar icy grain mantle compositions.

These new band strength values will be important for any future observing campaign of solid phase O_2 or H_2, as they will enable future observers to estimate time-on-target requirements for a detection. We have applied our measurements to the data acquired by van Dishoeck et al. 2025 [2] to provide updated observational estimates for O_2 along the line of sight towards the low mass protostar B1-c. In the event of a detection, these values will allow for the quantification of O_2 and H_2 in both its nuclear spin states. If not detected, they will allow scientists to place appropriate upper limits on their abundances.

References:

[1] Burris, W. A., Loeffler, M. J., Tegler, S. C., et al. 2025, Planetary Science Journal, In Review

[2] van Dishoeck, E. F., Tychoniec, Ł., Rocha, W. R. M., et al. 2025, Astronomy and Astrophysics, 699, A361,747

A CRYOGENIC ION TRAP BEAMLINE AT HFML-FELIX FOR ASTROCHEMICAL STUDIES

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Reactive molecular ions play a central role in the chemistry of planetary atmospheres and the interstellar medium. Laboratory astrophysics studies on the chemical reaction pathways under astronomically relevant conditions are crucial to interpret astronomical observations and as input for simulations in astrochemical networks. Of similar importance are spectroscopic studies of the often elusive, but essential, ionic reaction partners, intermediates and products that yield fundamental insights on their geometric and electronic structure, and provide spectroscopic signatures needed for their identification in space [1].

Cryogenic ion traps have proven to be ideal tools for studying ion-molecule reactions under controlled conditions and allow for sensitive spectroscopic studies of mass-selected, cold, and isolated molecular ions. Here, we will describe the combination of such a cryogenic 22-pole ion trap instrument (FELion) [2] with the widely tunable infrared free-electron lasers at HFML-FELIX [3]. It enables broadband infrared action spectroscopy of molecular ions such as hydrocarbons and interstellar complex organic molecules (iCOMs) ranging in size from comparatively small systems to polycyclic aromatic hydrocarbon (PAH) cations and anions. We will give a few examples of recent work on i) fundamental molecular physics studies, such as deciphering vibronic coupling effects [4,5], ii) in-situ spectroscopic probing of isomer-selective reaction kinetics involving PAHs and prebiotic species [6], iii) disentangling the isomeric composition of products in (dissociative) ionization processes [7].

References

[1] B.A. McGuire, O. Asvany, S. Brünken, S. Schlemmer, *Nat. Rev. Phys.* **2**, 402-410 (2020)
[2] P. Jusko, S. Brünken, O. Asvany, S. Thorwirth, A. Stoffels, L. van der Meer, G. Berden, B. Redlich, J. Oomens, S. Schlemmer, *Faraday Discuss*. **217**, 172-202 (2019)
[3] https://www.hfml-felix.nl/en/
[4] K. Steenbakkers, T.J.H.H van Boxtel, G.C. Groenenboom, O. Asvany, B. Redlich, S. Schlemmer, and S. Brünken, *Phys. Chem. Chem. Phys.* **26** 2692 (2024)
[5] K. Steenbakkers, P.B. Changala, W.G.D.P. Silva, J.F. Stanton, F. Lipparini, J. Gauss, O. Asvany, G.C. Groenenboom, B. Redlich, S. Schlemmer, and S. Brünken, *J. Phys. Chem. Lett.* **17** (2026) 4732-4740 (2026)
[6] D.B. Rap, J.G.M. Schrauwen, B. Redlich, and S. Brünken, *J. Am. Chem. Soc*. **146**, 23022-23033, (2024)
[7] H. Kaur, S. Petric, M. Gerlach, B. Redlich, and S. Brünken, *J. Phys. Chem. A* **130**, 433-445 (2026)

Development of an analytical pipeline to understand the molecular complexity generated in icy environments from laboratory astrophysics.

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Complex organic molecules are detected in the gaseous and solid phases of molecular clouds and protoplanetary disk. The origin of these molecules is still debated, but a large part is supposed to form on the surface of frozen grains. These icy grains, observable in dense molecular clouds, will be altered by highly energetic processes (VUV photons, ions, electrons) during the formation of planetary systems. These alterations allow the activation of molecules initially present in these ices, resulting in the development of a significant chemical reactivity. In certain environments such as the solar nebula, these grains can be heated, releasing in the gas phase a large part of the complex organic molecules initially formed on the surface or within the ice bulk. Some of these molecules can also react inside the ice forming nonvolatile molecules that remain on the grains leading to the formation of refractory organic residues. Part of the transformed grains can then agglomerate, resulting in interplanetary objects such as comets or asteroids. As a result, some of the organic matter present in solar system objects could come be inherited from ices found in dense molecular clouds.
On the basis of laboratory experiments, we develop an analytical strategy to study the chemistry generated by the processing of such ices during simulated solar system formation. We particularly demonstrated the richness of molecules formed in refractory organic residues [1]. We also investigated the composition of the gas phase depending of the initial composition of the ice [2,3] as well as the molecular composition of the refractory organic residues [4,5]. Finally, we demonstrated how this matter can evolve inside asteroids, parent bodies of meteorites in our solar system [6, 7]. Overall, our analyses show that this ice chemistry leads to the formation of all building blocks needed to start a prebiotic chemistry on telluric planets. All results obtained from these experiments suggest that ices of astrophysical objects are key environments to generate a rich molecular diversity, as it could be for our solar system, and question the role of this exogenous reservoir in the emergence of life on Earth..

References:
[1] GCO, 118, 184, (2013)
[2] AJ, 846, 124, (2017)
[3] ComChem, 8, 306, (2025)
[4] AJ, 2017, 837, 168, (2017)
[5] A&A, 667, A120, (2022)
[6] NatCom, 12, 3538 , (2021)
[7] ACS Earth and Space Chemistry, 8, 606, (2024)

Electronic Spectra of Doped Diamondoid Cations

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Pre-solar nanodiamonds grains have been found in significant abundance in primitive carbonaceous chondrites, suggesting a possible interstellar origin. Their presence raises the question of whether aliphatic (sp3-hybridized), diamond-like hydrocarbons can form and survive in the harsh conditions of the interstellar medium. Diamondoid cations represent compelling spectroscopic targets. Not only are diamondoids the smallest molecular units of bulk diamond, but their cations are relatively stable and have electronic transitions that lie in the visible range, making them potential candidates as carriers of the diffuse interstellar bands. While our previous work focused on bare and functionalized derivatives, we present our recently measured spectra of N-, O-, and S-doped (cage-modified) diamondoid cations, measured in the gas-phase using either a photoelectron spectrometer, a cryogenically cooled ion trap coupled to a tandem mass spectrometer, or both. These results are further supported by quantum chemical calculations and can provide critical reference data for astronomical searches in the pursuit of a broader understanding of the chemical inventory of the interstellar medium.

From Laser-Ablated Molecules to Mira Stars: Infrared Signatures of Refractory Species

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Refractory molecules play a significant role in the infrared spectra of late-type stars, yet their properties remain difficult to determine under astrophysical conditions. We present a laboratory-based approach that can be used to produce, characterize, and identify these species in stellar environments. Using laser ablation, molecules are generated in the gas phase and probed via infrared absorption spectroscopy. The resulting spectra are analyzed and used to develop models that allow for direct comparison with astronomical data. We apply this framework to infrared spectra of Mira variables obtained with the NASA Infrared Telescope Facility (IRTF), linking experimental results to observed molecular features and their variability over pulsation cycles. This approach establishes a direct link between controlled measurements and the analysis of infrared spectra from evolved stars.

UV-Vis spectroscopy of cold gas-phase benzonitrile in various charge states

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Following the detection of neutral benzonitrile in TMC-1 [1], the study of the molecular physics of gas-phase aromatic molecules has been revived. Experimental and computational studies have been conducted to better understand the spectroscopy and energetics of aromatic molecules. Depending on the astrophysical environment in which they are present, aromatic molecules are subject to different forms of radiation, such as UV light in planetary nebulae, dense PDRs, star-forming regions and diffuse clouds. Combining experimental evidence with theoretical calculations can help to better describe the photo-physical processes in the various environments.

Two experimental setups that can be exploited to study multiple charge states of gas-phase cyano-bearing aromatic molecules were used in this study of benzonitrile. One is equipped with a jet-cooled molecular beam, suitable for probing neutral molecules and singly-hydrogenated neutral radicals by exciting and ionising them. The second is a cryogenically cooled ion trap, allowing us to excite and photofragment ionic species, including protonated molecules [2] and radical cations. By investigating the photo-ionisation and photo-fragmentation of these molecules, we can probe their electronic and geometrical structures. Both of these experiments are done in environments where the molecules are vibrationally cold and both have this option of generating mass-selected aggregates with water [3]. Those configurations are ideal for studying the spectroscopy of aromatics, whether identifying and measuring individual, narrow vibronic transitions or measuring onsets for photo-detachment or fragmentation. Quantum chemical calculations performed using DFT at the CAM-B3LYP/aug-cc-pVDZ level are used to interpret the experiments.

Here, we will show various recent studies of different charge states of benzonitrile, measured between ~500 and 190 nm (2.5-6.5 eV) via the various available action spectroscopies, notably the neutral hydrogenated radical measured for the first time. Results from the combined study of neutral and ionic species show variations in their spectroscopy, ionisation energies and fragmentation dynamics. Our aim in comparing these results is to understand the stability of these species across diverse astrophysical environments and assess their observability.

References

[1] McGuire, B. A., et al *Science 359(6372), 202–205,* (2018), [2] Jacovella, U. et al *A&A, 657, A85, (2022).,* [3] Niedojadlo, A. et al *JMol Spec, 112078, (2026).*

Doubly-deuterated Ethanol - Spectroscopy and Interstellar Search

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Complex organic molecules (COMs) are widely detected in the Interstellar Medium (ISM). They are useful for source characterization and constitute the organic budget available for planets. Isotopic fractionation, particularly deuterium fractionation, traces the origin and inheritance of molecular complexity during star formation (Caselli & Ceccarelli 2012; Ceccarelli et al. 2014; Nomura et al. 2022). Observations of the protostellar core IRAS 16293-2422 reveal high COMs deuteration, including doubly-deuterated species with D_2/D ratios around 15–25%: methyl formate 22% (Manigand et al. 2019), dimethylether 15–20% (Richard et al. 2021), methanol 25% (Drozdovskaya et al. 2022), and acetaldehyde 20% (Ferrer Asensio et al. 2023). These high deuteration levels suggest formation during the pre-stellar core phase, though D_2/D ratios have been measured for few molecules due to limited spectroscopic data.

To explore whether this trend extends to other COMs, we focus on doubly deuterated ethanol (CH_3CD_2OH), an astrophysically relevant molecule and potential precursor to biologically important COMs, whose formation pathway is still uncertain. Its isotopologue has not yet been detected in the ISM due to the lack of accurate spectroscopic data. We investigate the rotational spectrum of CH_3CD_2OH (20–370 GHz) using two setups: SUMIRE (RIKEN) (Watanabe et al. 2021) for higher frequencies and the Toyama Microwave Atlas (Toyama University) for lower frequencies. This analysis will produce a precise spectroscopic catalogue, enabling the search for CH_3CD_2OH toward IRAS 16293-2422 in the ALMA Protostellar Interferometric Line Survey (PILS) (Jørgensen et al. 2016) and the derivation of its D_2/D ratio, shedding light on its origin and relation to other COMs.

References :
Caselli et al., Astron. Astrophys. Rev., 20, 56, (2012),
Ceccarelli et al., ApJL, 790, L1, (2014),
Drozdovskaya et al., A&A, 659, A69, 23, (2022),
Ferrer Asensio et al., A&A, 670, A177, 12, (2023),
Jørgensen et al., A&A, 595, A117, 41, (2016),
Manigand et al., A&A, 623, A69, (2019),
Nomura et al., PPVII, (2022),
Richard et al., A&A, 651, A120, (2021),
Watanabe et al., PASJ, 73, 2, 372-393 (2021)

Deciphering the IR Signatures of Circumstellar Envelopes using High-Resolution Spectroscopy

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Spectral High-resolution infrared spectra of stellar envelopes are difficult to interpret because, in addition to instrumental functions and telluric signatures, a wide variety of possible gas-phase species can be the sources of the spectral signatures, and these can also overlap closely. To gain an understanding of the observed spectra, the combined efforts of laboratory experiments, modeling, and observation are required. This contribution shows how this can be achieved using selected examples of circumstellar envelopes of hypergiants (e.g., VY CMa) and variable stars (e.g., chi Cyg and R Cas). Laboratory experiments will be presented, physical models of stellar envelopes will be discussed, and an analysis of stellar spectra will be explained. Example spectra of SiO, TiO, water, and ammonia will be shown.

Towards Isomer-Resolved Astrochemistry: REMPI and IR Spectroscopy of Complex Molecules in a Molecular Beam

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We present an experimental approach for investigating radiation-driven chemistry and molecular complexity under controlled gas-phase conditions, combining a pulsed supersonic molecular beam with an electrical discharge source and mass-selective spectroscopy. In discharge operation, a complex mixture of radicals, ions, and transient species is generated from simple hydrocarbon precursors, mimicking non-equilibrium processes in astrophysical environments. Time-of-flight mass spectrometry combined with resonance-enhanced multiphoton ionization (REMPI) reveals a broad distribution of products ranging from small fragments to larger carbonaceous species. Selected mass channels exhibit resonant UV features, while others act as fragmentation probes, providing insight into the underlying reaction pathways. To overcome the limitations of mass spectrometry, we combine REMPI with infrared (IR) depletion spectroscopy, enabling access to both electronic and vibrational fingerprints. This combined approach provides the basis for isomer-resolved identification of transient and stable species.

In addition to plasma-driven chemistry, the setup enables the investigation of stable molecules under isolated conditions. This is particularly relevant for chiral species, which have only recently been detected in the interstellar medium, such as propylene oxide. We have initiated spectroscopic studies of styrene oxide using REMPI in combination with infrared depletion spectroscopy (FELIX), providing access to both electronic and vibrational fingerprints. The combined REMPI and IR approach provides laboratory spectra that are directly relevant for astronomical observations. In particular, the infrared spectra of molecules in astrophysical environments, as observed by the James Webb Space Telescope (JWST), often exhibit ro-vibrational band structures that require laboratory benchmarks for reliable identification.

The present measurements contribute to such reference data, especially for transient and previously uncharacterized species. This work establishes a link between laboratory spectroscopy and astronomical observations, enabling the identification of complex and potentially chiral molecules in radiation-driven environments.

Soft X-ray absorption spectroscopy of interstellar ice analogs

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In the cold, dense environments where stars and solar systems form, icy dust grains represent the main reservoir of volatile material and host reactions leading to the emergence of interstellar chemical complexity.[1] In lab settings, interstellar ice analogs are commonly studied to characterize ice-phase chemical kinetics and spectroscopic features, using techniques like IR spectroscopy and mass spectrometry. We currently have a much poorer understanding of the structures and microphysics of interstellar-like ices, both in pure species and relevant mixtures.

X-ray absorption near edge fine structure spectroscopy (NEXAFS) is used to constrain the molecular orientation and binding behavior of materials, thin films, and aerosols, but little work has been done on ices with astrophysically relevant temperatures and amorphous structures.[2,3] We have developed a novel experiment at the Advanced Light Source at Lawrence Berkeley National Laboratory combining the cryogenic and vacuum techniques to form interstellar ice analogs, with the tunable soft X-ray source from the synchrotron. The total electron yield is measured as a function of X-ray photon energy at the Nitrogen, Carbon and Oxygen K-edges, providing insight into the local chemical environment and molecular ordering within the ice samples.

I will present our results on the microphysical behavior of guest molecules within water-dominated ice mixtures. Small volatiles like CO and N_2 are known to become trapped in the surrounding water matrix, remaining in the ice until temperatures far above their pure sublimation temperatures.[4] This phenomenon of entrapment is proposed to contribute to the formation chemistry of planets and their atmospheres, but the underlying microphysics remains poorly understood.[5] I will show how X-ray absorption spectroscopy can shed new light on the molecular-level interactions that lead to volatile entrapment. This will ultimately improve our understanding of the ice-phase processes that influence planet formation chemistry.

1 ARA&A, 53:541-581, (2015)
2 *J. Electron Spectrosc. Relat. Phenom.,* 151:105-120, (2006)
3 *Mol. Phys*., 120, 1-2, (2022)
4 *Mon. Not. R. Astron. Soc.* 354: 1141–1145, (2004)
5 *ApJ*, 955, 5, (2023)

Surface characterization of realistic cosmic dust grains analogues.

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Porous carbonaceous dust grains are among the key substrates for surface chemistry in astrophysical environments [1], yet their effective reactive surface area remains poorly constrained in astrochemical models, which typically assume a standard flat-surface monolayer density of 10^{15} sites/cm² [2]. Here we present results of the laboratory measurements aimed at quantifying the realistic ice-hosting capacity of porous analogues of carbonaceous cosmic dust, carried out with the FORMOLISM setup at LIRA.

Porous amorphous carbon layers (nanometer-scale thickness) were synthesised at the Friedrich Schiller University - Jena using the Jena Dust Machine via laser-ablation of a ^{13}C target, allowing isotopic discrimination between the sample and any ^{12}C surface contamination. To determine the effective reactive surface area, we performed a series of King-Wells During-Exposure Desorption (DED) experiments [3], exposing the porous ^{13}C samples and a flat metallic reference to an O_2 molecular beam. By comparing the integrated sticking coefficients on both surfaces kept at 26 K — a temperature at which only the first physisorbed O_2 monolayer is stable — we obtain the effective monolayer capacity of the porous sample relative to the flat reference.

Our measurements show that the effective reactive surface area of the porous grains is **24× larger** than the surface area of the flat substrate. We further investigated the effect of thermal annealing by repeating the King-Wells DED protocol after annealing the sample at 550K. Following this treatment, the effective reactive surface area was reduced to **4 times** the flat reference, demonstrating that prolonged exposure to high temperatures causes irreversible pore collapse.

These results could be a preliminary observation for grain evolution in protostellar envelopes and protoplanetary disks, where thermal processing is expected to modify grain microstructure over time. The temperature threshold at which pore collapse begins remains to be precisely determined and is the goal of our current research.

[1] Potapov A., et al. “Is Cosmic Dust Porous?” *The Astronomy and Astrophysics Review* 33, no. 1 (2025): 6. https://doi.org/10.1007/s00159-025-00164-5.

[2] Kimmel, G. A., et al., “Control of amorphous solid water morphology using molecular beams. I. Experimental results”, *Journal of Chemical Physics*, vol. 114, no. 12, AIP, pp. 5284–5294, 2001. doi:10.1063/1.1350580.

[3] King David A., and Michael G. Wells. “Molecular Beam Investigation of Adsorption Kinetics on Bulk Metal Targets: Nitrogen on Tungsten.” *Surface Science* 29, no. 2 (1972): 454–82. https://doi.org/10.1016/0039-6028(72)90232-4.

Precision X-ray absorption spectroscopy of metallic iron and its implication for the composition of Fe-bearing interstellar dust

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Iron (Fe) is primarily injected as a gas into the interstellar medium (ISM) by supernovae, where it swiftly condenses into unknown solid compounds. Bright galactic X-ray binaries can be used as back-lighters to study absorption by the intervening ISM, where Fe-bearing dust grains imprint Fe *L*-shell photoabsorption features at ∼700 eV. Recent observational studies have shown that the published Fe *L*-shell photoabsorption cross section data for Fe-bearing compounds need to be blue shifted by ∼1 to 2 eV to match the observations [1], possibly due to previously unrecognized systematic uncertainty in the laboratory energy-scale calibrations. But this energy difference is also similar to the spectral shift between metallic Fe, Fe oxides, and Fe silicates.

We have performed an experiment focusing on precision X-ray absorption spectroscopy of metallic Fe at the synchrotron light source PETRA III. We measured absolute cross sections for Fe *L*-shell photoabsorption of Au-coated, thin metallic Fe films. The samples were mounted in the Argus dynamic X-ray photoelectron spectroscopy setup, and the X-ray transmission vs. photon energy was measured using an intensity-calibrated photodiode. Au 4f photoelectron spectroscopy was used to monitor the photon energy. The photon energy was calibrated via resonant photoionization of F^{6+} ions measured in the simultaneously operated Photon-Ion merged-beams end station at PETRA III (PIPE). The transition energies for the $1s^2 2s \rightarrow 1s2s2p$ excitations in F^{6+} are known theoretically [2] and experimentally [3] to a precision of ∼3 meV. Taking into account these and other uncertainties, we have achieved an overall precision of 8 meV for the *L*-shell absorption feature of metallic Fe. In combination with our previous data for gas-phase Fe^+ [4], we have incorporated our results into astrophysical models and compared them to astronomical observations with the Chandra X-ray observatory. Our experimental results enable new insights for understanding the composition of Fe-bearing interstellar dust.

References:
[1] L. Corrales et al., Astrophys. J. **965**, 172 (2024).
[2] V. A. Yerokhin et al., Phys. Rev. A **96**, 042505 (2017).
[3] M. Togawa et al., Phys. Rev. A **110**, L030802 (2024).
[4] S. Schippers et al., Astrophys. J. **849**, 5 (2017).

Toward state-selective laser diagnostics of polyatomic ions inside the CSR: a multi-color laser spectroscopy scheme for highly excited H_3^+

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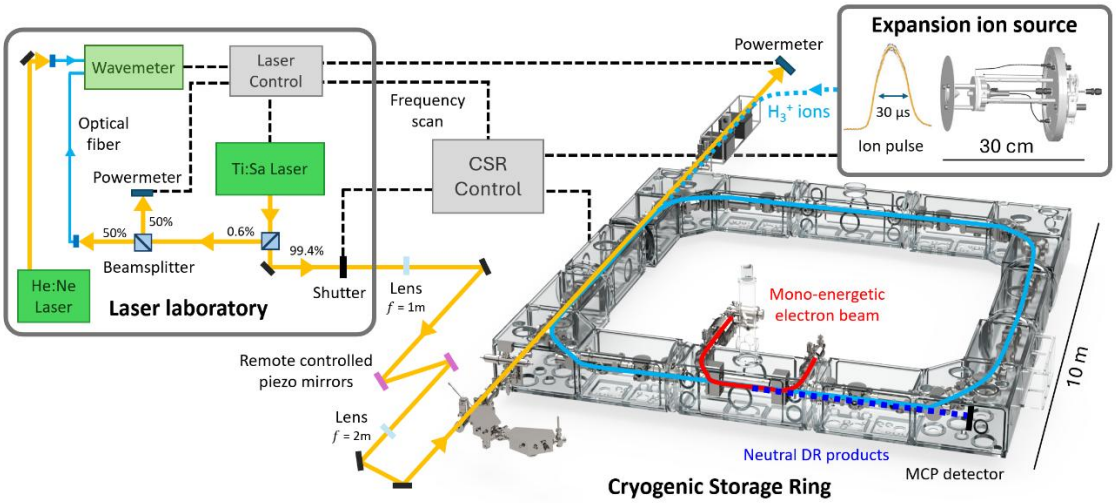
Small molecular ions with a substantial dipole moment cool to their lowest rotational quantum states within a few minutes of storage inside the Cryogenic Storage Ring (CSR). The cooling of polyatomic molecular ions is more complex to model and difficult to study experimentally. We are presently developing a versatile spectroscopy setup at the CSR, with initial measurements presented for H_3^+, the simplest polyatomic molecule. H_3^+ is one of the cornerstones of interstellar ion-neutral chemistry in the gas phase, and it serves as a benchmark of molecular theory for polyatomic ions. Despite being extensively studied in the past, the highly excited states of H_3^+ above 16 500 cm^{-1} remain largely unexplored, as they are experimentally challenging to access. As a step towards state-selective laser studies with polyatomic ions, we have proposed a multi-color action spectroscopy scheme to measure states above 20 000 cm^{-1} [1]. These measurements would allow for in situ monitoring of individual states during storage and they would bridge the large energetic gap to the unassigned pre-dissociation spectrum around 35 000 cm^{-1} [2]. In this approach, cold molecules stored in the CSR are excited in two steps from their ground state into the region of interest via a long-lived metastable state. The ions are then dissociated by a UV laser to measure the fragments using a single-particle detector. Since the recent successful demonstration of the first excitation step [3], a proof-of-principle study for the dissociation step was achieved, providing insight into cooling and photodissociation of highly excited HD^+ ions.



[1] J. Mol. Spectrosc. **378**, 111476 (2021),
[2] Acc. Chem. Res. **22**, 218-222 (1989),
[3] submitted to Phys. Rev. Res. (2026)

Photodesorption efficiency of O(^{3}P) from water ice surfaces in the visible region

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It is anticipated that many of the over 340 molecules detected in the interstellar medium (ISM) are formed on or in icy mantles on interstellar dust grains. The formation, evolution, and transport to the gas phase remain poorly constrained for these molecules on ice grains, as well as for the atoms and radicals assumed essential in their formation.

Recently, Miyazaki et al. (2020) found that OH radicals unexpectedly photodesorb in the visible region (532 nm). Sie et al. (2024) augmented this work by measuring the photodesorption efficiencies and cross sections for OH across a broader visible range (310–700 nm). Inspired by this work, we turned towards one of the most abundant atoms in the ISM: oxygen.

The ground-state triplet oxygen atom, O(^{3}P), is a product of the VUV photolysis of water. As a highly reactive and abundant species, involved in the formation of other abundant species in the ISM, such as H_2O and O_2, understanding its photodesorption behaviour is essential.

We used a combination of photostimulated desorption (PSD) and resonance-enhanced multiphoton ionisation (REMPI) techniques, known as the PSD-REMPI method, to selectively and sensitively monitor O(^{3}P) photodesorption from amorphous solid water in the visible range (410-700 nm). The O(^{3}P) was produced by irradiating H_2O ice (40 ML) with a VUV light source (deuterium lamp). The photodesorption efficiency depended strongly on both wavelength and temperature. Analysis of the photodesorption cross sections suggested desorption at different wavelengths may be occurring from different types of binding sites.

References:
Miyazaki, A. et al., *Phys Rev A*, **2020**, *102*, 052822,
Sie, N. et al., *CPL*, **2024**, *848*, 141384.

Dissociative recombination of internally cold H_2O^+ ions

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The transition from diffuse atomic to diffuse molecular clouds is an important early step in the star formation process in the interstellar medium (ISM) [1]. Tracing this transition directly is challenging because direct observation of H_2 is difficult [2]. Instead, observations of small molecular ions can be used to derive important information such as the fraction of molecular hydrogen f_{H_2} and the cosmic ray ionization rate of atomic hydrogen ζ_H, the latter of which is key to initiating astrochemical reactions and molecule formation in space. One of these astrophysically relevant small molecular ions is H_2O^+ [3]. In order to accurately model the interstellar conditions and infer f_{H_2} and ζ_H, the destruction rate of H_2O^+ due to dissociative recombination with free electrons has to be known under the conditions in the cold ISM, with temperatures of ~ 10 – 130 K. In these environments, the ions are mostly in their rovibrational ground states and electron-ion collisions occur predominantly at low collision energies.

We produced H_2O^+ ions and stored them for up to 1200 s in the Cryogenic Storage Ring **(**CSR) [4], located at the Max-Planck-Institut für Kernphysik in Heidelberg. The low black body radiation field of < 10 K in the cryogenic vacuum of the CSR enabled the stored water ions to radiatively relax to their lowest vibrational and rotational states, and more than 60 % of the population reached the ortho and para ground states. In the CSR electron cooler, the stored ion beam was overlapped with a beam of quasi mono-energetic electrons using the merged-beams technique. Here, we present first results from our measurement of dissociative recombination of internally cold H_2O^+ ions at electron-ion collision energies down to ~ 2 meV, corresponding to a temperature of ~ 20 K.

References:
[1] M. R. Krumholz, Phys. Rep. 539, 49 (2014)
[2] M. Gerin et al., Annu. Rev. Astron. Astrophys. 54, 181 (2016)
[3] N. Indriolo et al., Astrophys. J. 800, 40 (2015)
[4] R. von Hahn et al., Rev. Sci. Instrum. 87, 063115 (2016)

MOCCA - A 4k-Pixel Microcalorimeter for CSR

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More than 300 different molecules have been identified in interstellar clouds despite the low pressures and temperatures of only a few kelvins in these environments. The chemical pathways responsible for their formation, however, are still not fully understood. One of the key processes is dissociative recombination, in which a molecular ion captures an electron and subsequently dissociates into neutral fragments. To investigate reactions of cold molecular ions with a wide variety of different collision partners, the Cryogenic Storage Ring (CSR) [1] was built at the Max Planck Institute for Nuclear Physics (MPIK) in Heidelberg. In the CSR, extreme conditions similar to those in interstellar clouds can be reproduced in the laboratory and reactions such as dissociative recombination can be investigated. To reconstruct the complete reaction kinematics, position- and mass-sensitive coincident detection of all neutral reaction products is required [2]. For this purpose, the Molecule Camera Array (MOCCA) was developed in a collaboration between the Kirchhoff Institute for Physics at the University of Heidelberg and MPIK. MOCCA is based on metallic magnetic calorimeters operated at temperatures of only a few millikelvins. It has a sensitive area of about 45 mm × 45 mm consisting of 4094 pixels which can be read out with only 32 two-stage SQUID channels.

Before its installation into the CSR, the entire MOCCA setup, including its $^{3}He/^{4}He$ dilution refrigerator, is being tested, detecting neutral fragments from photon- and collision-induced ion fragmentation processes in a CSR-independent standalone setup. We present results from the first operation of this standalone setup.

References:
[1] R. von Hahn et al., Review of Scientific Instruments. 87, 063115 (2016)
[2] O. Novotný et al., Journal of Applied Physics. 118, 104503 (2015)

EFFECT OF REACTANT ABUNDANCES ON DIFFUSION-DRIVEN AMMONIUM CARBAMATE FORMATION IN CARBONACEOUS COSMIC DUST ANALOGUES

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In cold, dense regions of the interstellar medium, dust grains are coated and intermixed with molecular ices, creating dust–ice systems in which chemical evolution is governed by diffusion and surface reactions. Surface reactions on cosmic dust grains are key to the formation of complex molecules in interstellar and circumstellar environments. While reactions in mixed ices have been extensively studied, the role of diffusion through (across the surface of) porous dust aggregates, analogues of cosmic dust grains, is poorly explored.

We investigated diffusion-driven surface chemistry in a layered sample geometry, where reac-tants were initially spatially separated. Building on recent experimental evidence that porous silicate aggregates promote CO_2–NH_3 chemistry via diffusion (Potapov et al. 2025), we exam-ined this process in more detail also investigating another type of cosmic dust grain analogous. Thermal kinetic experiments carried out under high vacuum conditions, with CO_2 and NH_3 reactants isolated by porous layer of amorphous carbon dust, show that ammonium carbamate ($NH^+NH_2COO^-$) forms by pure thermal reaction when the dust layer is present between the species. Extending the previous silicate-based study to carbonaceous dust analogues, this result demonstrates that diffusion through the interconnected dust structure drives the reaction between initially separated species. We investigated the influence of the relative amounts of CO_2 and NH_3 on the reaction rate and yield. Moreover to produce a more realistic case, we investigated the influence of water ice mixed with dust aggregates on the reaction efficiency.

Our results highlight the role of porous carbonaceous aggregates not only as passive surfaces, but as active environments for molecular transport and reaction. They support scenarios in which dust-mediated diffusion contributes to chemical complexity in warm astrophysical environment, such as protostellar envelopes and protoplanetary disks.

References:

Potapov A., Pollok K., Langenhorst F., McCoustra M., Garrod R., “Cosmic dust as a prerequisite for the formation of complex organic molecules in space?”, The Astrophysical Journal, 2025, 993, 49, DOI: https://doi.org/10.3847/1538-4357/ae08ae

Measuring & Linking Mid-Infrared SiO_2 - Spectra to Dust Aggregate Growth in the GT4P Levitation Chamber – II. Experimental Setup

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The growth of µm-sized dust grains into larger aggregates is a key step in planet formation[1]. In protoplanetary disks, the 10 µm silicate feature is commonly used to trace dust processing and grain growth[2]. However, its spectral shape is not controlled by size alone, making controlled laboratory experiments essential for linking infrared spectra to aggregate evolution.

The GT4Pebbles experiment, “Ground Truth for Pebbles in Planet Formation”, is designed to investigate the growth of µm-sized dust grains into larger aggregates under controlled laboratory conditions. To achieve this, a large rotating levitation chamber will be equipped with several diagnostic units that monitor the evolving dust cloud non-invasively during the experiment. A central technical challenge is to combine optical information on aggregate morphology and size with infrared spectral information that is sensitive to structure and aggregate evolution.
One of the key diagnostic units is a filter-based infrared spectro-photometer focused on the mid-infrared SiO_2 feature around 10 µm. The system uses a custom-built blackbody source with a target temperature of up to approximately 2000 K. The emitted radiation is guided through a reflective chromium-plated tube toward a set of wavelength-selective filters. These filters allow measurements in selected spectral bands, initially covering the 7-13 µm region around the SiO_2 stretching feature, with the possibility to extend the diagnostic range toward 2-20 µm. After spectral selection, the radiation is guided through the levitation chamber by two Winston cones. A second reflective guide tube then transfers the transmitted radiation to the infrared photometer. Measurements are taken through and past the dust cloud to have a dynamic background measurement to determine extinction. This design allows time-resolved monitoring of the changing infrared extinction signal during dust aggregation.
The spectro-photometric data will be interpreted together with the Overview Observation System (OOS). The OOS observes the dust cloud through a window in the front of the levitation chamber and consists of four stationary cameras and four co-rotating illumination sources. The OOS therefore provides optical images of the dust cloud and enables measurements of cloud morphology, aggregate motion, spatial and apparent aggregate size distribution.
By combining both diagnostics, GT4P aims to connect changes in the infrared signal to independently observed changes in aggregate size and structure. The technical concept therefore provides a controlled laboratory link between infrared dust spectra and the physical evolution of growing planetary building blocks.

References:[1] Jürgen Blum, Dust agglomeration, Advances in Physics, 55:7-8, 881-947(2006)
[2] J. Varga, MINDS survey of silicates in T Tauri disks: Correlation between dust and gas, A&A, (2026)

Temperature Dependence of Interfacial CO_2 Formation via Electron Irradiation of H_2O Ice on Amorphous Carbon Dust Analogues

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Interstellar dust grains composed of silicate or carbonaceous material play a crucial role in the chemistry evolution of the interstellar medium. They provide a catalytic surface that allows gas-phase species to accrete, diffuse and react. Many groups have studied the surface interaction between carbonaceous dust analog and water ice, which is the most abundant ice species and with the highest frost line temperature to condense on the dust surface. Under various energetic sources, including X-ray, EUV, UV and ion bombardment, CO_2 formation is a common and prominent reaction. However, the underlying formation pathway remains a mystery. The CO formation is undetectable under Ar^+ ion bombardment in Raut et al. (2012)[1] and the formation cross section of CO is smaller than that of CO_2 under UV irradiation (Mennella et al. 2006[2]), X-ray irradiation (Chuang et al. 2023[3]) and EUV irradiation (Lee et al. 2026[4]). These findings imply that the CO_2 formation may proceed without passing through the intermediate CO phase.

In this study, we investigated the effects of energetic electron irradiation on thin H_2O ice layers deposited on isotopically labeled amorphous carbon (a-^{13}C) and hydrogenated amorphous carbon (a-^{13}C:H) dust analogues. To systematically examine whether CO acts as a necessary intermediate species, we performed a series of experiment across a temperature range of 13-90 K. If CO were a necessary intermediate product, CO_2 formation would be expected to decrease substantially above CO desorption temperature (~30 K). Via this method, we provide evidence that the formation of CO_2 at the ice–carbon interface does not require CO as an obligatory intermediate species. These results demonstrate that CO_2 formation can occur as long as H_2O ice covers the amorphous carbon substrate, revealing an alternative interfacial pathway for CO_2 ice production under relatively warm (>30 K) interstellar conditions where CO ice is thermally unstable.

References (Times New Roman 11):
[1]: Raut, U., Fulvio, D., Loeffler, M. J., & Baragiola, R. A., ApJ, 752, 159 (2012)
[2]: Mennella, V., Baratta, G. A., Palumbo, M. E., & Bergin, E. A., ApJ, 643, 923 (2006)
[3]: Chuang, K.-J., Jäger, C., Sie, N.-E., et al., ApJ, 956, 57 (2023)
[4]: Lee, C.-Y., Chuang K.-J., Hsu, Y.-Y., et al., ApJ, accepted, (2026)

Probing the Surface Chemistry Towards Interstellar Dust Grains: (Sub-)Millimeter-Wave Spectroscopic Characterization of NH_2Cl

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Under interstellar conditions, monochloramine (NH_2Cl) is believed to be formed by surface reactions between adsorbed nitrogen, hydrogen, and chlorine atoms. As such, it is considered an important probe for the mobility of nitrogen and a potential secondary reservoir of chlorine, along with HCl and CH_3Cl. Available laboratory data on this species do not cover the millimeter and submillimeter-wave domain [(sub-)millimeter, > 60 GHz] where the strongest transitions lie, even at low temperature, preventing interstellar searches.

In this context, a comprehensive pure rotational characterization of $NH_2{}^{35}Cl$ and $NH_2{}^{37}Cl$ has been carried out in this work. The experimental (sub-)millimeter wave spectra of both isotopologues have been recorded in the Doppler regime between 75 and 880 GHz with a broadband chirped-pulse Fourier transform microwave spectrometer and a source-frequency-modulated (sub-)millimeter wave spectrometer. In order to further improve the accuracy of the analysis, some lines have been recorded in sub-Doppler regime by exploiting the saturation spectroscopy technique known as Lamb Dip.
More than 2200 distinct frequencies belonging to $NH_2{}^{35}Cl$ and more than 1000 of the less abundant isotopologue $NH_2{}^{37}Cl$ have been assigned, determining with high accuracy the spectroscopic constants. Notably, the inversion splitting due to the amino inversion motion is experimentally determined for the first time.

An astronomical search of the main isotopologue ($NH_2{}^{35}Cl$) has been carried out in IRAS 16293-2422 young protostar through the high-resolution spectral survey COMPASS. No line could be unambiguously detected, but an upper limit on the column density has been derived and compared with predictions from our best model.

Effect of infrared irradiation in interstellar water ice analogues

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In the cold and dense part of the interstellar medium, dust grains are covered by icy mantles in which water plays a key role. Amorphous solid water (ASW) is the most dominant form of solid material present in these regions. Recent JWST observation by Noble et al. [1] revealed spectral features at 2.7 μm in the Chameleon I cloud, which are attributed to the dangling OH (dH) features from the water ice, confirming the presence of weakly bonded water molecules within the ice. Due to the porous and disordered nature, ASW can act as a substrate for interstellar chemistry. The surface of the ASW can accrete molecules such as CO, CO_2, N_2, CH_4 etc. leading to the formation of complex organic species.

A number of laboratory experiments and theoretical simulations are devoted to study the properties of water ice upon UV irradiation and photo-desorption [2-5]. However, only a very limited number of experiments have been dedicated to study the change in ice under infrared (IR) irradiation [6-8]. The aim of our experiment is to irradiate ice analogues using a continuous IR laser and to study the structural changes in ice.

I will present the results of our experimental approach to study the properties of water ice under the impact of infrared radiation. Water purified via multiple freeze pump thaw cycles is deposited on a copper substrate with the help of a dosing system. The substrate is held at the centre of an ultra-high vacuum chamber and is mounted to the head of a closed helium cryostat. The temperature of the substrate can be varied from 6-300K and the thickness of ice can also be adjusted. A continuous, high power, mid-IR laser, tunable over 1992-3060 nm wavelength range is employed for the ice irradiation experiments. The ice spectra before and after irradiation are analyzed in reflection-absorbance mode using an FTIR spectrometer coupled with an MCT detector. A quadrupole mass spectrometer is also deployed to monitor the desorption.

Current experiments focus on the deposition of porous ASW at 25K. Different surface modes of water ice namely doubly-coordinated dH (2.68 μm), triply-coordinated dH (2.7 μm), dangling oxygen dO (2.81μm) and tetra-coordinated at surface s4 (2.85 μm) were irradiated either separately or as a sequence. Hole-burning effects and restructuration of the ice were observed. Experiments were also performed as a function of irradiation time. Complementary experiments by varying the temperature of the substrate from 10-90 K were also performed to study the effect of thermal annealing. The decrease in the dangling modes and the shift in the bulk OH stretch towards red wing was observed. Overall, IR irradiation induced a restructuration of porous ASW. The photon flux in our experiments is typically on the orders of 10^{23} photons cm^{-2}, which is comparable to the total fluence in a dense cloud over its entire lifetime [9-10]. Hence the experimental data could be incorporated into the astrochemical models and could also serve as a preliminary data for the interpretation of observation from James Webb Space Telescope.
The results obtained so far will be presented and discussed.

References

[1] J.A. Noble et al., Nat. Astronomy, 8, 1169-1180 (2024).
[2] J. H. Fillion et al., ACS Earth Space Chem., 6, 100-115 (2022).
[3] S. Tachibana et al., Science Advances, 3, eaao 2538 (2017).
[4] M. Bulak et al., A&A 6799, A99 (2023).
[5] K. I. Oberg et al., Astrophys. J, 693, 1209-1218, (2009).
[6] S. Coussan et al., Phys. Chem. Chem. Phys. 17, 9429 (2015).
[7] J.A. Noble et al., Phys. Chem. Lett., 5, 826-829 (2014).
[8] J.A. Noble et al., J. Phys. Chem. C, 124, 20864-20873, (2020).
[9] L. Slumstrup et al., ACS Earth and Space Chem., 9(6), 1607-1621, (2025).
[10] J.S. Mathis et al., A&A, 128, 212-229, (1983).

How Molecular Size Regulates Efficient Volatile Delivery at the Water Snow Line

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Characterizing both the gas- and ice-phase reservoirs of a protoplanetary disk is important to understand how planets inherit their chemical building blocks. The most fundamental properties of these molecules, then, is the radial location at which the molecule is in the gas *vs.* the ice, *i.e.*, its snow line. Of these, the water (H_2O) snow line is of the most importance, as it is the most efficient location for planetesimal formation. Given that most stars host planetary systems and many exoplanets reside in the inner few au of the disk, characterizing the chemical inventory at the water snow line is essential for understanding the molecular composition inherited by protoplanets.

I will present laboratory experiments on the simplest sulfur-bearing complex organic molecule, methyl mercaptan (CH_3SH), with respect to its well-characterized and relatively abundant oxygen-bearing analogue, methanol (CH_3OH) [1]. Studying how these molecules sublimate allows us to determine each molecule's binding energy, which in turn, sets the snow line location, a critical parameter in disk models and planet formation at large. Notably, I discover molecular size to play a crucial role in enhancing the volatile abundance at the water snow line. Such a size effect in ices has never been seen before and has reshaped our understanding of how "simple" complex organics (including other O-/N-bearing species and hydrocarbons) commonly found in ice matrices can fundamentally change the distribution of volatiles across a protoplanetary disk. This effect persists in UV processed ices, demonstrating how microphysics at the angstrom level can influence processes on planetary scales, including how planets like Earth may get their volatiles.

References:
[1] Narayanan et al. 2025 ApJ 986 10

The Impact of Cluster Size on the DFT-Calculated Binding Energies of Interstellar Molecules on Ice Surfaces

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In the interstellar medium (ISM), dust grains covered by an icy mantle serve as cosmic reactors, catalyzing the formation of both simple molecules as H_2 as well as complex organic molecules. Accurately modeling the binding energies of chemical species on these ice surfaces is therefore vital for astrochemistry simulations. However, predicting these values remains a challenge. Computational studies using density functional theory (DFT) must balance the amorphous nature of interstellar ice and its diverse binding sites against high computational costs. Consequently, researchers often rely on small ice clusters (typically ~20 water molecules) or periodic crystalline structures, leaving the specific impact of cluster size poorly understood.

In this study, we systematically investigate the cluster size effect on calculated binding energies, using carbon monoxide (CO) and ammonia (NH_3) as a prototypical molecular probes. Utilizing the ωB97X-D4rev/TZVP level of theory, we isolated the electronic contributions to this size effect by performing single-point calculations on a series of pre-optimized ice clusters and CO/ice complexes. All binding energies were corrected for the basis set superposition error (BSSE), evaluating both flat and cavity-like binding sites. Our results reveal that the binding energies converge to the asymptotic value of a large 100-H_2O cluster at a threshold of just 30 to 40 water molecules. This study demonstrates that while overly truncated clusters fail to yield realistic binding energies, computationally manageable, slightly larger clusters are fully sufficient to capture accurate surface interactions for astrochemical modeling.

Experimental study of UV-induced sulfur chemistry in interstellar ice

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To date, more than 30 sulfur-bearing species have been securely identified in the interstellar medium (ISM), with the majority detected in the gas phase through rotational spectroscopy. However, the observed sulfur abundance in star-forming regions, particularly in dense molecular clouds, is significantly lower than the cosmic abundance ($S/H \sim 1 \times 10^{-5}$)[1], giving rise to the long-standing "missing sulfur" problem. It has been hypothesized that sulfur is efficiently depleted onto interstellar grains, where it may be either locked in refractory reservoirs or transformed into other sulfur-bearing species (allotropes or organosulfur) through energetic and non-energetic processing on dust grains.

Sulfur ice chemistry in star-forming regions is therefore crucial for understanding the overall chemical evolution of the ISM and its coupling to the astrochemistry of other abundant elements. Recent JWST observations have confirmed the presence of a few sulfur-bearing species in the interstellar ice mantles, including carbonyl sulfide (OCS) and sulfur dioxide (SO_2)[2], suggesting that sulfur actively participates in complex solid-state chemistry. However, the formation pathways of OCS and SO_2 in interstellar ices remain poorly constrained and require further investigation.

In this work, we experimentally investigate solid-state reactions involving CS and OH radicals upon the UV photolysis of CS_2:H_2O ice mixtures at ~20 K. The formation of sulfur-bearing photoproducts is systematically explored over a wide range of mixing ratios, spanning astronomically relevant H_2O-rich compositions to chemically optimized compositions. Several S-bearing products, including OCS, H_2S, SO_2, HS(O)OH, HC(S)SH, and H_2CS, have been identified in situ using IR spectroscopy. Their formation kinetics are monitored as a function of UV photon fluence to pinpoint the possible reaction pathways involving CS_2-derived species in interstellar ice mantles.

References

1. V. Wakelam, A. Castets, C. Ceccarelli, et al. *A&A*, 2004, 413, 60
2. K. McClure et al. Nat. Astron. 7.4 (2023): 431-443.

Spectral Signatures of Deuterated Formaldehyde in Astrophysical Ice Analogues

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Deuterated molecules are powerful tracers of the physical and chemical conditions prevailing during the earliest stages of star formation. In this work, we present a laboratory infrared spectroscopic study of deuterated formaldehyde (D_2CO) in astrophysical ice analogues, aimed at improving the identification and quantification of deuterated species in protostellar environments using observations from the James Webb Space Telescope.

We investigate the influence of abundant ice constituents, such as H_2O, CO_2, and CO, on the spectral signatures and band positions of D_2CO by analysing pure D_2CO ices, binary mixtures containing D_2CO:H_2O, D_2CO:CO_2, and D_2CO:CO, as well as ternary mixtures such as CO_2:H_2O:D_2CO and CO:CO_2:D_2CO. The experiments were performed in a high-vacuum chamber with a base pressure of $\simeq$ 10−6 mbar, where the samples were deposited onto a cryogenically cooled substrate at 10 K. Infrared spectra were acquired during deposition and throughout controlled thermal annealing, up to the complete desorption of the ices.

Our results show that the presence of H_2O, CO_2, and CO induces significant shifts, band broadening, and intensity variations in the IR features of deuterated formaldehyde, highlighting the strong matrix effects exerted by these dominant ice components. The spectral data obtained in this study contribute to the laboratory spectral libraries used in astrochemical models and simulations. By accounting for matrix-induced spectral shifts, this work enables a more accurate interpretation of JWST observations and improves constraints on the abundance and distribution of deuterated molecules in astrophysical ices in star-forming regions.

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References

[1] L. Chahine et al., Monthly Notices of the Royal Astronomical Society: Letters 2024, 534, L48–L57, DOI 10.1093/mnrasl/slae080.
[2] M. Faure et al., Astronomy & Astrophysics 2025, 693, A30, DOI 10.1051/0004-6361/202449937.
[3] L. Loinard et al., Planetary and Space Science 2002, 50, 1205–1213, DOI 10.1016/S0032-0633(02)00084-3.

From Micro-Scales to Megaparsecs: Forecasting relic yields for future observations

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Galaxy clusters sit at the top of the cosmic hierarchy, their deep gravitational potential wells retain nearly all the baryonic matter involved in their formation, including metals produced in stars and ejected from galaxies into surrounding gas (Mantz et al., 2017). The intracluster medium (ICM), the hot gas that fills a galaxy cluster, therefore preserves, on Mpc scales, a cumulative record of stellar and sub-galactic processes that originated within stars and galaxies. Elements forged in stars are expelled by supernovae and active galactic nucleus (AGN) winds and are then gradually mixed into the cluster as it grows (Werner et al., 2008; Böhringer & Werner, 2010). The TNG-Cluster simulations reproduce this, producing fairly smooth distributions of these elements throughout the gas (Nelson et al., 2024), while X-ray lines at 6.7–6.9 keV (Mernier et al., 2018), let us read this chemical history directly. Yet the ICM is an extreme fossil record (temperatures of 10^7–10^8 K and densities of $\sim 10^{-3}$ cm^{-3}), where no molecules or dust grains survive.

When clusters merge, the enriched ICM is crossed by Mpc scale collisionless shocks that (re-) accelerate cosmic ray electrons to relativistic energies via diffusive shock acceleration (DSA, Brunetti & Jones (2014)). This process is set by microphysics such as particle injection efficiencies and collisional ionization rates, which laboratory experiments help constrain. Spiraling in μG fields , these electrons radiate at MHz to GHz frequencies and appear as diffuse radio emission called *radio relics*, which are luminous, highly polarized arcs at cluster peripheries, that serve as a macro-scale imprints of microphysical shock processes (van Weeren et al., 2019).

To quantify how often such environments arise, we present a statistical framework for predicting radio relic yields in upcoming wide-area surveys. Building on Nuza et al. (2012) and calibrated against TNG-Cluster simulation results from Lee et al. (2024), we convolve the Tinker et al. (2008) halo mass function (HMF), (computed with `Colossus`) with a relic radio-power probability density function (PDF) to construct the radio relic luminosity function (RRLF). Integrating the RRLF over redshift and flux, weighted by a smooth detection probability for observational incompleteness, yields cumulative number counts ($N(> S_\nu)$).

The original Nuza et al. (2012) model treats all clusters of a given mass as equally likely to host a relic. We extend this assumption by introducing a *bimodal mixture PDF*, splitting the population into a faint component p_1 (relaxed clusters) and a bright component p_2 (merger-active clusters). The key idea is that more massive clusters are more likely to be undergoing active mergers, so the weight $w(\log M)$ shifts towards the bright component as mass increases. Calibrated to the relic occurrence rates of Lee et al. (2024), this concentrates detectable relics in the most massive systems without altering the intrinsic cluster physics, and bringing predictions closer to observed counts.

Calibrating against existing radio survey (NVSS, LoTSS DR2), we forecast relic yields for upcoming ones such as LoTSS DR3, MeerKLASS, and the SKA. The resulting census maps the large-scale environments where merger shocks sweep through metal-enriched plasma, marking the final stage of a journey that began in stellar interiors and ends in non-thermal afterglow of cluster mergers.

Keywords: radio relics, galaxy clusters, intracluster medium, diffusive shock acceleration, halo mass function, ICM metal enrichment, non-thermal emission, statistical astrophysics

References

Böhringer H., Werner N., 2010, Astron. Astrophys. Rev., 18, 127

Brunetti G., Jones T. W., 2014, Int. J. Mod. Phys. D, 23, 1430007

Lee W., Pillepich A., ZuHone J., Nelson D., Jee M. J., Nagai D., Finner K., 2024, , 686, A55

Mantz A. B., et al., 2017, , 472, 2877

Mernier F., Biffi V., Yamaguchi H., et al., 2018, Space Sci. Rev., 214, 129

Nelson D., Pillepich A., Ayromlou M., et al., 2024, , 686, A157

Nuza S. E., Hoeft M., van Weeren R. J., Gottlöber S., Yepes G., 2012, , 420, 2006

Tinker J., Kravtsov A. V., Klypin A., et al., 2008, , 688, 709

Werner N., Durret F., Ohashi T., Schindler S., Wiersma R. P. C., 2008, Space Sci. Rev., 134, 337

van Weeren R. J., de Gasperin F., Akamatsu H., Brüggen M., Feretti L., Kang H., Stroe A., Zandanel F., 2019, Space Sci. Rev., 215, 16

High-resolution laboratory study of the ν_2/ν_4 bending motion of CH_3^+ and the assignment of its astronomically observed lines

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The methyl cation, CH_3^+, is a peculiar cation that has been discovered through the detection of a 7 μm (1400 cm^{-1}) band observed in the d203-506 protoplanetary disk using the MIRI-MRS spectrometer onboard the JWST [1]. This feature has since been reported in numerous astronomical sources. The original discovery relied on simulations of the molecule's simultaneous and interacting bending modes (ν_2/ν_4), using both rough laboratory measurements and theoretical analyses. These results were then compared with astronomical data, which had an absolute wavelength calibration accurate to only a few cm^{-1}. Subsequent quantum-chemical calculations enabled the first spectroscopic assignment of the lines[2]. However, a comprehensive spectroscopic assignment of the astronomical features observed in the 7 μm range is awaiting high-resolution laboratory data. Here, we present a laboratory high-resolution study of the ν_2/ν_4 bending vibrations of CH_3^+ to provide accurate, calibrated data for the spectroscopic analysis of JWST detections of this species. The rovibrational structure of the ν_2/ν_4 bending vibrations of CH_3^+ is studied in a cryogenic 22-pole ion trap apparatus at 10 K. To detect vibrational excitation, the efficient leak-out spectroscopy method [3] is used in combination with a high-resolution quantum cascade laser operating at 7 μm. This is compared with MIRI-MRS data for d203-506, reduced with improved wavelength calibration. The measurement accuracy and precision of about 0.001 and 0.0007 cm^{-1}, respectively, allow spectroscopic constants and line predictions to be derived with high confidence, and thus permit accurate (Doppler velocity) diagnostics of CH_3^+ lines with JWST.

References :

[1] Berné, O., Martin-Drumel, M.-A., Schroetter, I., et al. 2023, Nature

[2] Changala, P. B., Chen, N. L., Le, H. L., et al. 2023, Astron. Astrophys., 680, A19

[3] Schmid, P. C., Asvany, O., Salomon, T., Thorwirth, S., Schlemmer, S. 2022, J. Phys. Chem. A, 126, 8111

An electrostatic ion beam trap setup for infrared spectroscopy with complex molecular ions

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Understanding the chemistry of complex organic molecules in interstellar space is at the forefront of molecular astrophysics [1]. Complex molecular ions, in particular, are promising carriers of features such as the diffuse interstellar bands (DIBs) and unidentified infrared emissions (UIE). However, laboratory spectroscopy of such species is particularly challenging, and no established technique for gas phase spectroscopy currently exists.
To address this challenge, we are developing an experimental setup to perform infrared spectroscopy of stored molecular ions using an electrostatic ion beam trap (EIBT) [2]. The molecular ions are injected into the EIBT and confined by reflections between two electrostatic mirrors. For future spectroscopy measurements a cryogenic EIBT will be installed and combined with a sensitive mid-infrared photon detector.
A characterization of the beamline and first results of the dynamics of trapped ions using a room-temperature EIBT (as seen in Figure 1) are presented in this poster.

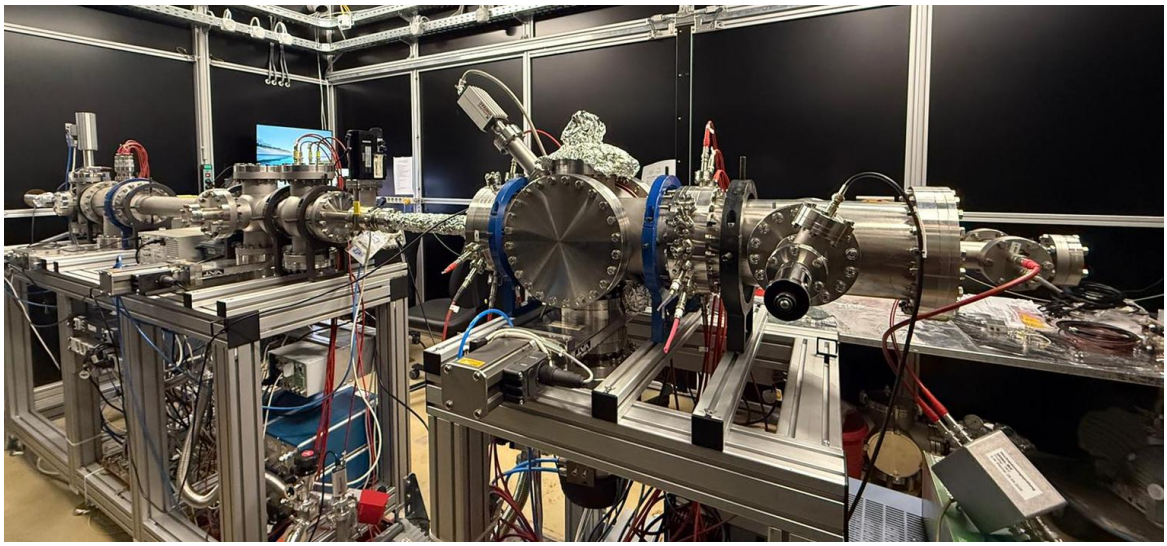

Figure 1: Current status of the laboratory facility: room-temperature electrostatic ion beam trap connected to the beamline

References:
[1] Herbst E, Vidali G, Ceccarelli C, ACS Earth Space Chem. 4, 488 (2020)
[2] Zajfman D et al., Phys. Rev. A 55, R1577 (1997)

A chemical census of ϱ Ophiuchus A: shocks and emission diversity across low-mass protostars

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The interplay of gravitational collapse, radiative feedback and mechanical energy input from embedded protostars shapes the chemical diversity observed across star-forming regions. ϱ Ophiuchus A (Oph A), the nearest embedded cluster-forming cloud at a distance of 138 pc, provides a unique laboratory in which to disentangle this complexity. It hosts an actively expanding HII region driven by the B-type star Oph-S1, which simultaneously irradiates and compresses the surrounding gas while multiple class 0 and I protostars drive energetic jets into the same material. Here we present spectral line maps of shock tracers (SO_2, SO), dense gas tracers (N_2H+, $H^{13}CO+$) and complex organic molecules (CH_3OH) observed with the APEX 12-m telescope towards nine embedded sources in Oph A, revealing strong chemical differentiation across the region. The SO_2 and SO emission peaks are towards GSS 30 and GY30 - class I protostars located at the eastern rim of the Oph-S1 bubble, with SO_2 detected at 99σ towards GSS 30 - while the VLA 1623 system, which drives the most energetic CO outflow in the region - shows no detectable emission in these shock tracers. The morphology of the SO_2 emission is further consistent with the shocked H_2 emission traced by JWST NIRCam F470N imaging, which traces the active outflow cavities associated with GSS 30. N_2H+ and $H^{13}CO+$ show the inverse trend, tracing the dense quiescent gas around VLA 1623 and SM1 being absent towards GSS 30, indicating a clear chemical dichotomy between shocked and quiescent environments. We perform non-LTE RADEX modelling of the detected species to constrain the physical conditions - gas temperature and column density towards each source, enabling a quantitative comparison of excitation conditions across the region. Our results suggest that feedback from Oph-S1 plays a key role in shaping the shock chemistry in Oph A, with GSS 30 emerging as the most chemically active protostellar source in the region.

Quantum-state-selective dissociative charge transfer collisions with stored molecular ions

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In atomic collisions, inelastic energy transfer among electronic, vibrational, and rotational states is essential for understanding molecular formation or destruction, ranging from atmospheric plasmas to cooled interstellar space. The destruction of state-prepared molecular ions via dissociative electron recombination sheds light on the high abundance of primordial molecules, such as HeH^+, in the early universe [1]. On the other hand, mutual neutralization between molecular cations and atomic anions unfolds the state-selective few-body dissociation dynamics [2]. The dissociative charge transfer (DCT) process is another spectroscopic imaging tool for investigating neutral molecular dissociation. Here, a molecular ion captures an electron from a neutral atomic or molecular target, populating a wide range of electronic states, including Rydberg and doubly excited states. The resulting electronic states either decay via direct dissociation (for repulsive states) or via predissociation and radiative decay, and the internal energy is converted into the kinetic energy of the neutral fragments. Combining a reaction microscope [3] with a neutral-fragment imaging detector enables high-resolution momentum-spectroscopic studies of such collisions [4]. The reaction microscope in the cryogenic storage ring CSR (the so-called CSR-ReMi) provides an excellent platform for studying the DCT process using state-prepared, cooled molecular ions [5,6]. Here, we report the DCT process in slow HeH^+-He collisions (and in HeH^+-H_2 collisions). The measured Q-value distributions (i.e., binding energy differences between the initial and final states) from recoil ions indicate the quantum yields for various final electronic states of neutral HeH molecules. On the other hand, scattering-angle differential cross-sections shed light on the state-selective charge-transfer dynamics that occur during the collisions. By taking advantage of kinematical complete measurements, the correlation between Q-value and neutral-fragment kinetic energy release unravels the various direct dissociation and pre-dissociation pathways.

References:

[1] O. Novotný *et al.* Science 365, 676-679 (2019).
[2] M. Poline *et al.* Nat. Commun. 16, 8528 (2025).
[3] J. Ullrich *et al.* Rep. Prog. Phys, 66, 1463 (2003).
[4] H. Schmidt-Böcking *et al.* Ann. Phys. (Berlin) 533, 2100134 (2021).
[5] F. Hermann *et al.* Phys. Rev. Research 7, L012082 (2025).
[6] R. von Hahn *et al.* Rev. Sci. Instrum. 87, 063115 (2016).

Quantifying NH_3 and CH_3OH Ice Features in Class 0 Protostars Observed with JWST

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Interstellar ices play a key role in the chemical evolution of protostellar environments, yet the identification and quantification of individual species remain challenging because of blended absorption features and strong matrix dependent effects. In particular, ammonia (NH_3) and methanol (CH_3OH) exhibit overlapping bands in the 8–11 μm region, complicating their interpretation in protostellar spectra.

We present a JWST/MIRI spectroscopic study of four Class 0 protostars observed as part of the CORINOS program (1): B335, IRAS 15398−3359, L483, and Ser-emb 7. The spectra are continuum corrected and compared directly with laboratory ice analogs, including pure ices and H_2O rich mixtures containing NH_3 and CH_3OH. Previous laboratory studies have shown that the spectral profiles of both species strongly depend on the surrounding ice matrix (2-4), motivating a systematic exploration of ice composition and mixing ratios.

We find that pure component laboratory spectra do not adequately reproduce the observed absorption profiles. Instead, significantly improved agreement is obtained using H_2O rich mixtures, highlighting the importance of matrix effects in shaping the NH_3 and CH_3OH features. From the best-fitting laboratory analogs, we derive NH_3 and CH_3OH column densities and estimate their abundance ratios across the four sources.

These results provide new constraints on the composition of interstellar ices in embedded protostars and demonstrate the importance of laboratory constrained spectral fitting.

References:
(1) ApJL,941,L13,(2022)
(2) ARA&A,53,541,(2015)
(3) ApJ,718,1110,(2010)
(4) ApJS,181,53,(2009)

Providing N_2O pressure-broadening coefficients for studies of exoplanetary atmospheres

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The James Webb Space Telescope (JWST), launched in 2021, together with upcoming facilities such as the Extremely Large Telescope (ELT), ARIEL, and GRAVITY+, is expected to deliver high-resolution spectroscopic data of exoplanetary atmospheres across the optical to mid-IR range. These observations will improve our understanding of atmospheric composition through the retrieval of molecular abundances, and provide new insights into planetary formation and evolution[1]. Interpretation of these spectra requires accurate line modeling based on laboratory spectroscopy data, including transition frequencies, line intensities, and temperature-dependent and pressure(P)-broadening coefficients. These parameters are compiled in databases such as HITRAN[2,3] and ExoMol[4].

While these catalogs contain molecular line lists for spectral modeling, laboratory measurements are limited for many molecular parameters required to accurately determine molecular abundances in exoplanet atmospheres. For example, N_2O is a biosignature gas with distinctive spectral features in the near- and mid-IR range[5,6]. However, current laboratory studies of P-broadening of N_2O-He[7,8] are insufficient for deriving a reliable model and are therefore supplemented with N_2O-CO_2 broadening coefficients in HITRAN[9]. In the case of N_2O-H_2 P-broadening, very limited experimental data are available[10,11], preventing reliable extraction of broadening parameters and consequently limiting their inclusion in HITRAN.

To address this, we present high-resolution gas-phase spectroscopy of N_2O broadened by He and H_2 using a Bruker IFS 120/5HR Fourier-transform infrared spectrometer. We report our latest experimental results for the ν_3 fundamental band, the overtone ($2\nu_1$), and the combination band ($\nu_1 + 2\nu_2$) of N_2O broadened by He and H_2 at room temperature and pressures up to 1 bar. This work aims to provide laboratory data that support the inclusion of N_2O-H_2 and N_2O-He P-broadening parameters in HITRAN, enhance existing spectroscopic databases, and enable more accurate characterization of exoplanetary atmospheres.

References

1. Exp. Astron., **46**, 135-209 (2018)
2. J. Quant. Spectrosc. Radiat. Transf., **353**, 109807 (2026)
3. Astrophys. J. Suppl. Ser., **262**, 40 (2022)
4. J. Quant. Spectrosc. Radiat. Transf., **326**, 109083 (2024)
5. Planet. Space Sci., **98**, 66-76 (2014)
6. Astrophys. J., **937**, 109 (2022)
7. J. Chem. Phys., **132**, 16 (2010)
8. Chem. Phys., **334**, 196-203 (2007)
9. Phys. Chem. Chem. Phys., **8**, 364-368 (2006)
10. J. Mol. Spectrosc., **27**, 218-224 (1968)
11. J. Opt. Soc. Am., **63**, 859-863 (1973)

CO ice structure on HOPG: how binding energy and diffusion drive bilayer growth

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The interstellar medium (ISM) is a dynamic environment in which various atoms and molecules freeze onto dust grains and react together to form increasingly complex species, enriching its chemical composition. The accretion of gaseous species depends on both the nature of the substrate and that of the ice itself. Until now, the accretion of ice has been understood as a simple model where molecules freeze out on dust grains one layer at a time. However, recent work has suggested that this process may be more complex than previously understood.

To study this, a series of studies were conducted to characterize the growth of CO ice on a flat, carbonaceous surface using low-temperature scanning tunnelling microscopy (LT-STM). This was investigated by adding CO to the surface in a setup imitating interstellar conditions, using a succession of small doses. This study was done in parallel with molecular dynamics (MD) simulations driven by a MLIP trained on dispersion-corrected DFT data. The STM measurements provide direct atomic-scale imaging of the ice morphology as a function of coverage, while the simulations reproduce the experimental ice morphologies and reveal the microscopic mechanisms underlying nucleation of both the first and the second CO ice layer. Together, these complementary approaches provide an atomically-resolved picture of CO ice formation on carbonaceous surfaces under conditions directly relevant to dense interstellar clouds.

The study has shown that CO ice grows in a series of subtle steps rather than layer-by-layer. These steps depend on the surface features, the density of the ice, the temperature of the system, amongst other parameters. These results have further implications in the study and analysis of interstellar chemistry, providing more insight on the structure and mechanics of CO ice freezing, opening a door towards the structural accretion of other ices on more realistic dust grain analogues.

Publication in preparation

Radiative stabilization of the first aromatic rings

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Aromaticity is ubiquitous in the universe, as indicated by the widespread detection of polycyclic aromatic hydrocarbons (PAHs) in a variety of astrophysical environments [1]. However, their formation in space is poorly understood. Crucially, the formation of the first aromatic ring, benzene, which is considered a bottleneck in PAH formation, remains poorly characterized. Most astrochemical models use the dissociative recombination of $C_6H_7^+$, formed through H_2 addition to phenylium ($C_6H_5^+$), as the primary route to benzene formation, highlighting the central role that $C_6H_5^+$ plays in its production. However, the formation of phenylium itself through radiative association pathways has recently been questioned [2]. Furthermore, while this sequence of reactions has been validated in warmer environments such as the protoplanetary nebula CRL 618 [1a], it underestimates the observed abundances in colder environments such as TMC-1 [1b]. Thus, it is timely to experimentally constrain the formation routes of phenylium, which ultimately affect the formation of benzene and, by extension, PAHs.

Here, we investigate the radiative stabilization of phenylium and benzene monocations using experiments carried out at one of the cryogenic ion-beam storage rings at DESIREE. The cryogenic ultra-high-vacuum conditions allow ions to be stored in isolation for time periods longer than those accessible in traditional mass spectrometers, enabling measurements under conditions directly comparable to astrophysical environments. We measured the time-dependent dissociation rates of vibrationally hot cations, which were used as benchmarks for modeled dissociation and radiative cooling rates. The critical energies below which the cations can be radiatively stabilized against dissociation were found to be 5.03 and 4.14 eV for phenylium and benzene monocations, respectively, constraining both the exothermicity and the maximum collision energy possible in potential radiative association reactions. These results have important implications for both the formation and survival of benzene across a wide range of astrophysical environments.

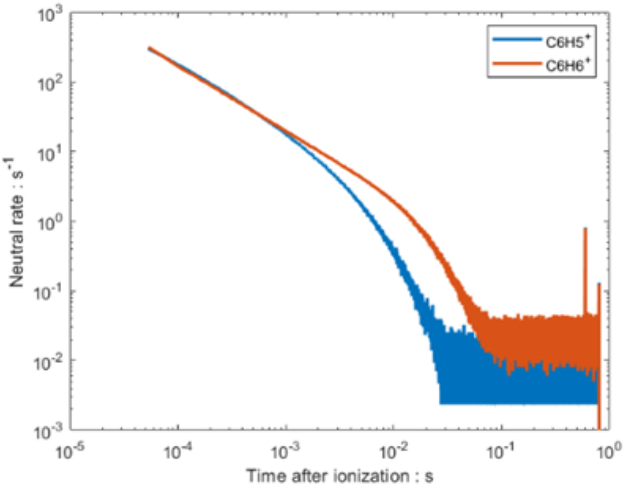

Figure 1: Absolute dissociation rates of $C_6H_5^+$ and $C_6H_6^+$ depicting the former is stabilised approximately four times faster than the latter.

References :
[1] (a) Cernicharo, José, et al. *ApJL* 546.2 (2001). (b) McGuire, Brett A., et al *Science* 359.6372 (2018)
[2]Kocheril, G.S., et al *Nat Astron* **9**, 685–691 (2025).

Infrared spectroscopic studies of complex organic molecular ions, COMIs

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Vinyl cyanide (C_2H_3CN) and ethyl cyanide (C_2H_5CN) are among the most abundant complex organic molecules (COMs) observed in the interstellar medium and have also been studied extensively by spectroscopy in the laboratory. In contrast, much less is known about their isoelectronic and charged relatives, such as the protonated variants, $C_2H_3CNH^+$ and $C_2H_5CNH^+$,[1,2] or the corresponding oxygen-containing species, $C_2H_3CO^+$ (propenoyl or acryloyl cation) and $C_2H_5CO^+$ (propanoyl cation).

Here, we report recent infrared spectroscopic studies of $C_2H_3CO^+$ and $C_2H_5CO^+$ using infrared photodissociation (IRPD) spectroscopy of their weakly bound Ne complexes and the FELion 22-pole cryogenic ion-trap apparatus connected to the Free Electron Laser for Infrared eXperiments (FELIX) at Radboud University (Nijmegen, The Netherlands). The study of $C_2H_3CO^+$ significantly extends an earlier IRPD investigation employing CO tagging [3], while $C_2H_5CO^+$ has been studied spectroscopically here for the first time. In addition, the first high-resolution infrared spectra of $C_2H_3CNH^+$ have been obtained using leak-out spectroscopy[4] in Cologne. The spectroscopic analysis was supported by coupled-cluster calculations performed at the CCSD(T) level of theory.

[1] Martinez Jr. et al., J. Chem. Phys., 138, 094316 (2013)
[2] Thorwirth et al., J. Mol. Spectrosc. 386, 111615 (2022)
[3] Li et al., Sci. Sin. Chim. 48, 218 (2018)
[4] Schmid et al., J. Phys. Chem. A, 126, 8111 (2022)

IR-induced photodesorption of volatile species from interstellar ice surfaces

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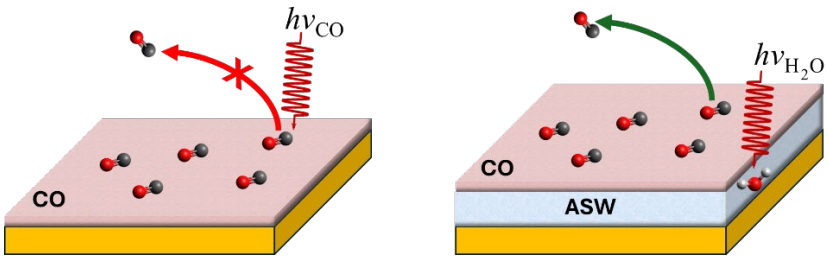
Surface processes play a key role in dense, molecular clouds in the interstellar medium, where dust grain temperatures are as low as 10 K. Under these conditions, carbon monoxide (CO) freezes out as a non-polar layer on top of a layer of amorphous solid water (ASW), reactively formed in situ on the grain. H-atom addition to CO has been shown to initiate the formation of a variety of complex organic molecules (COMS) starting with methanol (CH_3OH) [1]. In addition to atomic species, interstellar ices are exposed to photons and charged particles that can drive both chemical reactions and physical processes such as the desorption of species. In the coldest regions of the ISM, thermal desorption is inefficient and photodesorption can provide an important route by which condensed phase species are returned to the gas phase.

Previous investigations employing microwave discharge lamps [2] and synchrotron light sources [3] have revealed that UV photons can drive the desorption of CO from interstellar ice analogues. However, within dense clouds, the external UV radiation field is strongly attenuated, and such regions can be considered to be dominated by IR radiation [4]. The role of IR photons in the processing of interstellar ices remains less well understood.

We have used the FELIX IR Free Electron Laser (FEL) FEL-2 to investigate the IR induced photodesorption from model interstellar ices consisting of a few layers of CO deposited on top of either an ASW [5] or hydrogenated PAH film [6]. IR induced changes in the ice film were monitored through reflection-absorption infrared spectroscopy, while photodesorbing species were detected directly with a quadrupole mass spectrometer. The tunability of the FEL light source allowed us to selectively excite different IR bands of the individual species. Our results demonstrate that photon absorption by the underlying layer results, following energy transfer, in the efficient photodesorption of CO, while direct excitation of the CO stretching mode is inefficient in driving desorption. These results indicate that IR induced processes should be included in astrochemical models.



[1] Fuchs, G. W. *et al*. (2009), *Astron. Astrophys*., **505**, 629-639.
[2] Öberg, K. I. *et al*. (2009), *Astron. Astrophys*., **496**, 281-293.
[3] Fayolle, E. *et al*. (2011), *Astrophys. J. Lett.*, **739**, 1-5.
[4] Mathis, J. S. *et al.* (1983), *Astron. Astrophys*., **128**, 212-229.
[5] Slumstrup, L. *et al.* (2025), *ACS Earth Space Chem*., **9**, 1607-1621.
[6] Slumstrup, L. *et al.* (2025), *Astron. Astrophys.*, **704**, A74.

Structural characterization and restructuring effects of thick interstellar water ice analogues

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Astrochemical models show that gas-grain interactions strongly influence the abundance ratios of H_2 nuclear spin isomers in molecular clouds, with important consequences for interstellar chemistry.[1,2] The structure and morphology of interstellar water ices impact processes such as H_2 adsorption and desorption in cold astrophysical environments, which in turn play a role in H_2 nuclear spin isomer abundances both on grains and in the gas phase. [3]

In this study, we investigate the physical properties of amorphous solid water (ASW) ices deposited at temperatures ranging from 10 K to 150 K under ultra-high vacuum using the COSPINU2 setup. We characterized ASW films grown via background and doser-assisted deposition with thickness ranging from 0 to 10 µm, for different deposition rates. Their thickness, refractive index, density, and macroscopic topology were characterized through a combination of near- and mid-infrared FTIR spectroscopy, He-Ne laser interferometry, optical imaging (Hg vapor lamp and white light), and mass spectroscopy.

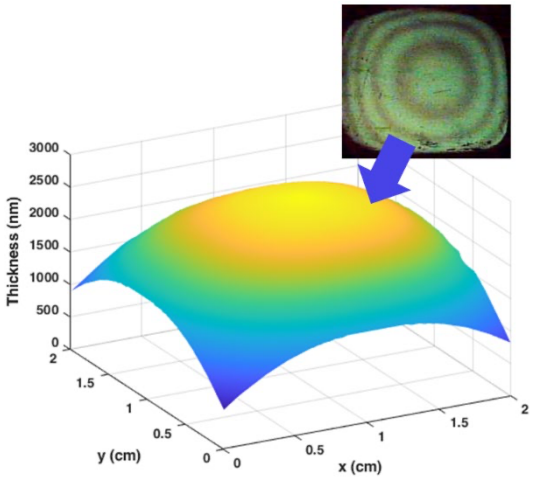

Figure 1 - Thickness profile retrieved from interference patterns on the ice

The measurements show that the refractive index increases with deposition temperature and decreases with higher deposition flux, consistent with a transition from highly porous to more compact ice structures. For localized deposition through a dosing tube, localized interference patterns in green light reveal dome-shaped ice profiles, allowing a three-dimensional reconstruction of the deposited films. A key result is the observation of sudden restructuring events in thick, porous, low-temperature ices under strong molecular flux. We observed an abrupt decrease in specular reflectance and increased diffuse scattering, associated to a sudden decrease in dangling-OH spectral signatures. These events suggest a partial collapse or reorganization of the porous network, highlighting the fragility of amorphous water ice.[4] These results provide a reliable laboratory framework for understanding how porous icy grain mantles control molecular adsorption, diffusion, and gas trapping in cold astrophysical environments and more specifically for future investigation of H_2 nuclear spin conversion mechanisms.

References

(1) Le Petit, F.; Nehme, C.; Le Bourlot, J.; Roueff, E. A Model for Atomic and Molecular Interstellar Gas: The Meudon PDR Code. *Astrophys. J. Suppl. Ser.* **2006**, *164* (2), 506–529. https://doi.org/10.1086/503252.

(2) Bron, E.; Le Petit, F.; Le Bourlot, J. Efficient Ortho-Para Conversion of H_2 on Interstellar Grain Surfaces. *Astron. Astrophys.* **2016**, *588*, A27. https://doi.org/10.1051/0004-6361/201527879.

(3) Sugimoto, T.; Fukutani, K. Electric-Field-Induced Nuclear-Spin Flips Mediated by Enhanced Spin–Orbit Coupling. *Nat. Phys.* **2011**, *7* (4), 307–310. https://doi.org/10.1038/nphys1883.

(4) Bu, C.; Dukes, C. A.; Baragiola, R. A. Spontaneous Cracking of Amorphous Solid Water Films and the Dependence on Microporous Structure. **2016**. https://doi.org/10.1063/1.4967789.

Formation of N_2H^+ and N_2D^+ in Collisions of N_2 with H_3^+ Isotopologues

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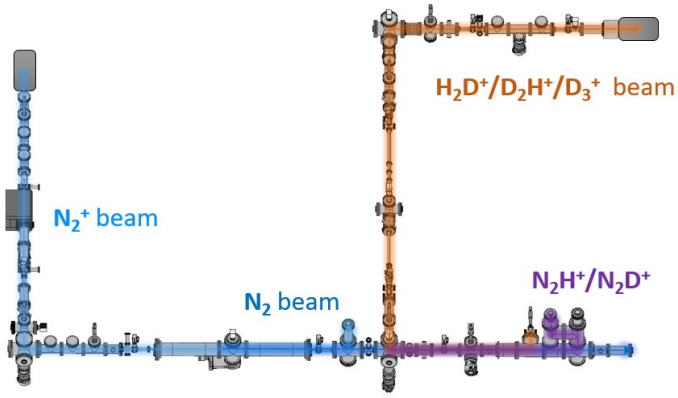
The properties of prestellar cores and the outer midplane of protoplanetary discs can be inferred using observations of deuterated molecules.[3,4] In particular, the N_2D^+-to-N_2H^+ abundance ratio is a commonly used diagnostic, the accuracy of which requires an understanding of the underlying chemical processes forming these ions. For that purpose, we used a dual-source, ion-neutral, merged-fast-beams apparatus[1,2] to investigate reactions of N_2 with H_3^+ isotopologues leading to the formation of N_2H^+ and N_2D^+. The schematic of our instrument along with the six reactions studied are presented below.



$$N_2 + H_3^+ \rightarrow N_2H^+ + H_2 \quad (1)$$
$$N_2 + H_2D^+ \rightarrow N_2H^+ + HD \quad (2)$$
$$N_2 + H_2D^+ \rightarrow N_2D^+ + H_2 \quad (3)$$
$$N_2 + D_2H^+ \rightarrow N_2H^+ + D_2 \quad (4)$$
$$N_2 + D_2H^+ \rightarrow N_2D^+ + HD \quad (5)$$
$$N_2 + D_3^+ \rightarrow N_2D^+ + D_2 \quad (6)$$

Fast ion beams of N_2^+ and H_3^+ isotopologues were produced in duoplasmatron sources. The N_2^+ ions were neutralized to the $X^1\Sigma^+_g$ ground electronic state by electron capture from N_2 in a gas cell at room temperature. The H_3^+ isotopologue ions were then merged onto the neutral beam. The N_2H^+ and N_2D^+ daughter products were detected using an electrostatic energy analyzer. This procedure allowed us to measure the integral cross section for the ion-molecular reaction and determine thermal rate coefficients, both to an accuracy of ~ 20%. These results can be used in astrochemical models to describe the processes taking place at dense cold regions found in prestellar cores and protoplanetary disks.

This work was supported, in part, by a grant from the U.S. National Science Foundation Division of Astronomical Sciences Astronomy and Astrophysics Grants Program. XU acknowledges support from the Fonds de la Recherche Scientifique – FNRS.

[1] O'Connor A *et al.* Reaction studies of neutral atomic C with H_3^+ using a merged-beams apparatus. *Astrophys. J. Suppl. Ser.* 219, 6 (2015)
[2] Hillenbrand P-M. *et al.* Experimental and theoretical studies of the isotope exchange reaction D + H_3^+ → H_2D^+ + H. *Astrophys. J.* 877, 38 (2019)
[3] Aikawa, Y. *et al.* Multiple paths of deuterium fractionation in protoplanetary disks. *Astrophys. J.* 855, 119 (2018)
[4] Sipilä, O. and Caselli, P. Hydrodynamics with gas–grain chemistry and radiative transfer: comparing dynamical and static models. *Astron. Astrophys.* 615, A15 (2018)

Experiments to constrain the properties of macromolecular organics in the outer Solar System

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The surface composition of trans-Neptunian objects (TNOs) provides a window into the chemical complexity of the protoplanetary disk (Pinilla-Alonso et al. 2025). However, characterizing the macromolecular organic components on these outer bodies remains challenging due to subtle spectral features in the visible and near-infrared. We performed a laboratory study on organic refractory residues (ORRs) produced through the energetic processing of TNO ice analogues (Baratta et al. 2019, Urso et al. 2020), with the aim of constraining the physical and chemical properties of macromolecular complex organics in the outer Solar System. Volatile mixtures containing including CO, CH_4, CH_3OH, N_2, NH_3, also in presence of H_2O, were deposited under ultra-high vacuum at 18 K and exposed to 200 keV ion bombardment, simulating the cosmic ray and solar particle exposure of icy surfaces in space. After irradiation, samples were gently warmed up to room temperature, allowing the formation of ORRs. These samples were further processed at high temperature (up to 973 K) and in vacuum. In the experiments, we observe the formation of features attributed to CN-bearing complex organics. These species were recently revealed in TNO spectra acquired by the JWST (Cryan et al. 2025). Complementary Raman spectroscopy was performed on processed samples, allowing us to detect the D and G bands of amorphous carbon. We retrieve the structural properties of the amorphous carbon, revealing a dependence on the ice's irradiation and thermal history. Laboratory data are used to interpret JWST observations of CN-bearing TNOs and of N-rich particles expected to originate in the outer Solar System.

References

Baratta, G. A., Accolla, M., Chaput, D. et al. 2019, Astrobiology, 19, 8
Urso, R. G., Vuitton, V., Danger, G., et al. 2020, A&A, 644, A115
Cryan, S., Brunetto, R., Guilbert-Lepoutre, A., et al. 2025, ApJ, 993, 188
Pinilla-Alonso, N., Brunetto, R., De Prá, M. N., et al. 2025, Nature Astronomy, 9, 230

Diffusion of CH_4 in amorphous D_2O ice using confocal Raman spectroscopy

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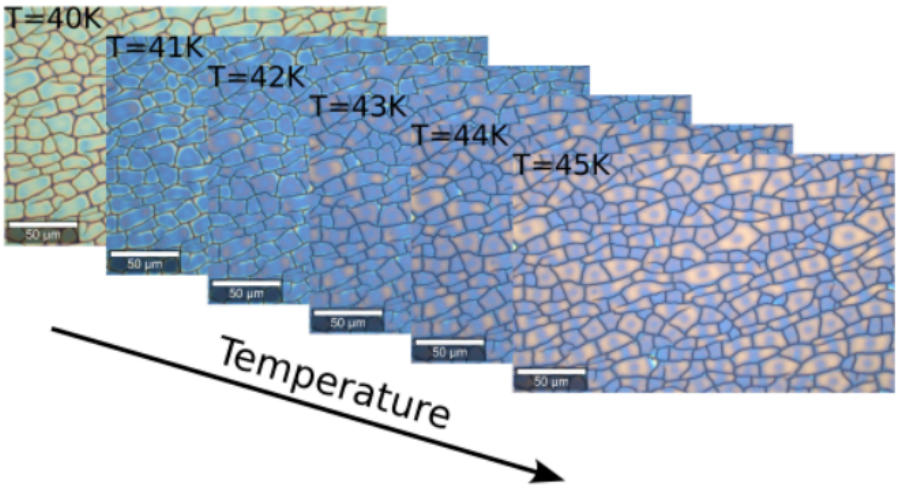
Molecular diffusion through amorphous water ice governs how volatile species are redistributed, trapped, and released from interstellar ice mantles, and is a key ingredient in astrochemical models of star- and planet-forming regions. In our laboratory we grow analogues of these ice mantles under cryogenic, high-vacuum conditions, and use them to study their spectroscopic and physical properties. Laboratory constraints on diffusion coefficients remain limited and rely almost exclusively on indirect infrared measurements.

We present a new experimental approach based on depth-resolved confocal Raman spectroscopy, which directly images the spatial redistribution of a volatile species through a water-ice film. Bilayer D_2O/CH_4 ices are deposited at 10 K onto a silicon substrate, and the evolution of the CH_4 distribution is tracked through successive depth scans during isothermal annealing. Upon warming to 30 K, rapid CH_4 redistribution into the porous D_2O layer is observed, while control experiments on compact D_2O show no transport, confirming that pore diffusion is the dominant mechanism. Isothermal measurements at 26–28 K yield diffusion coefficients of 10^{-14}–10^{-13} cm² s^{-1}. Complementary lateral Raman mapping reveals an inhomogeneous diffusion front, reflecting the underlying morphology of the water-ice layer.



Bu et al. 2016, ApL 109, 201902 | He et al. 2018, ApJ 863, 156 | Maté et al. 2020, A&A 643, A55 | Mispelaer et al. 2013, A&A 555, A13

Similarity of molecular abundances in laboratory-irradiated ice with those of telescope observations of abundances in icy bodies

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The relative abundances of molecules synthesized from organic ices samples (CHON composition) after irradiation by cosmic ray analogues (H, He, and heavier ions) were compiled from experimental data reported in the literature (1, 2, 3, 4, 5). These molecular abundances (H_2O, CO, CO_2, CH_3OH, NH_3, CH_4, etc.) were compared with those observed in cometary tails (6), the icy mantles of interstellar medium grains and circumstellar regions (7, 8). All molecular abundances reveal significant similarity, suggesting that they follow a similar evolutionary process. The relative abundances of unobserved molecules are also predicted. Additionally, a cosmic ray absorbed dose was estimated as a time function to reach the maximum chemical abundance of synthesized species as reported in previous works (1, 2, 3).

References

(1) A. L. F. de Barros, et al. Chemical and physical effects induced by heavy cosmic ray analogues on frozen methanol and water ice mixtures, MNRAS 2014, Volume 443, Issue 3, 21, 2733–2745.

(2) Mejía, C., et al. Radiolysis of Ices by Cosmic-Rays: CH4 and H2O Ices Mixtures Irradiated by 40 MeV 58Ni11+ Ions. ApJ 2020, 894(2), 132.

(3) Bordalo, V., et al. Chemical processing of pure ammonia and ammonia-water ices induced by heavy ions. ApJ 2013, 774 (2), 105.

(4) A L F de Barros, et al. Chemical reactions in H2O:CO interstellar ice analogues promoted by energetic heavy-ion irradiation, MNRAS 2022, Volume 511, Issue 2, 2491–2504.

(5) Mejía, C., et al. Modifications of astrophysical ices induced by cosmic rays-I. Water, carbon monoxide, and methanol mixtures. A&A 2024, 687, A227.

(6) Michael J. Mumma, Steven B. Charnley. The Chemical Composition of Comets-Emerging Taxonomies and Natal Heritage. Annual Review A&A 2011. 49:471-524.

(7) A.C. Adwin Boogert, et al. Observations of the Icy Universe. Annual Review A&A 2015. 53:541-581.

(8) McClure, M.K., et al. An Ice Age JWST inventory of dense molecular cloud ices. Nat Astron 2023, 7, 431–443.

Cosmic rays' doses absorbed by nucleobases in thick samples

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Nucleobases have been found in meteorites, revealing that these molecules can withstand radiation [1]. Although the molecules are protected by the meteorite's outer layers (< 1 m), ionizing radiation can penetrate to a depth of several meters. In this study, the dose absorbed by molecules after energetic ion impact is calculated down to a depth of ten meters.

The ionizing energetic particles observed in the galactic cosmic ray distribution (GCR) are used to estimate inelastic interactions with nucleobases [2]. The relation of chemical modification with the transferred energy by inelastic interaction was used to measure the absorbed dose by the nucleobase molecules [3].

The results show that the total dose is constant for depth less 10^{-4} m, after that depth the dose decreases as a function of the intensity form parameter (E_o) of the GCR [2]. In this calculation a depth function is found proportional to E_o^n. Additionally, the ionization rate and the half lifetime are shown for each nucleobase as function of the radiation penetration depth.

References

[1] Koga T. et al. A complete set of canonical nucleobases in the carbonaceous asteroid (162173) Ryugu. Nature Astronomy, p. 1-9, 2026.

[2] Shen et al. Cosmic ray induced explosive chemical desorption in dense clouds. A&A, 415(1), 203–215, 2004.

[3] Mejía C. et al. Swift heavy ion irradiation of thymine cryogenic temperature. NIMP-B, 534, 11–15, 2022.

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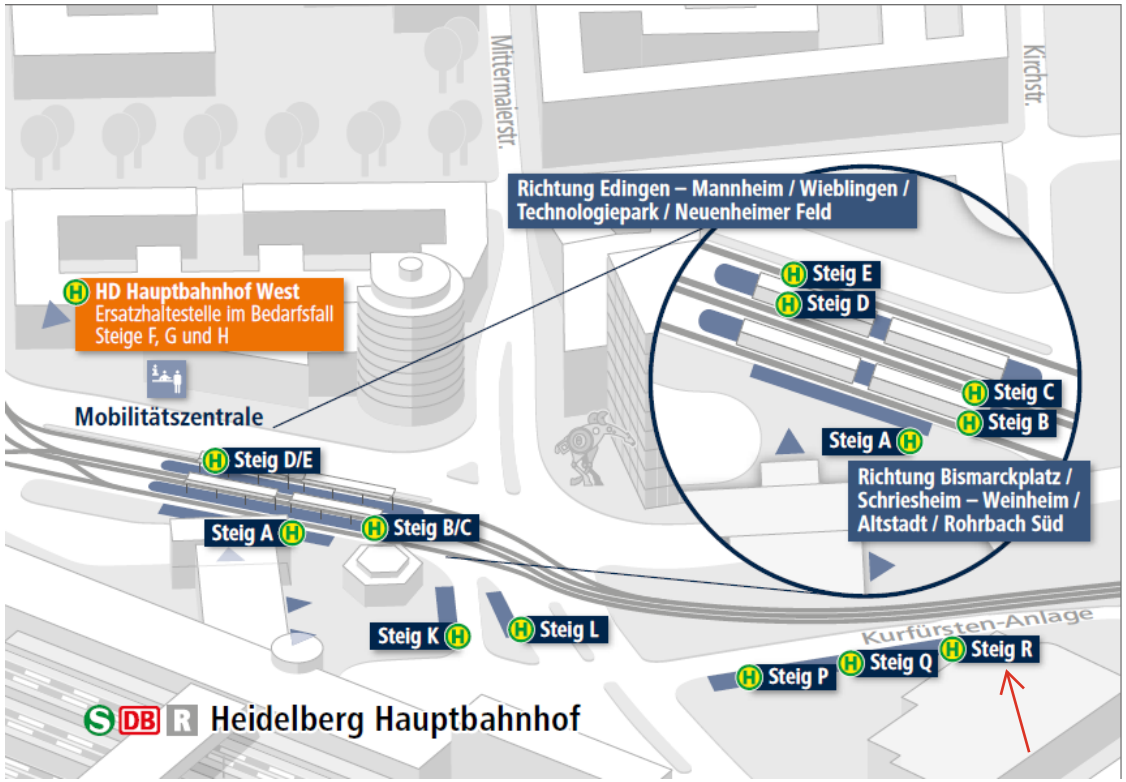
Transportation



Heidelberg main station "Steig R"

Alois Link platz

Shuttle bus timetable

HD main station → MPIK	**Monday**	**Tuesday - Friday**	
Heidelberg main station	8:30	8:45	
Alois-Link-Platz	8:35	8:50	
MPIK	8:45	9:00	
MPIK → HD main station	**Monday**	**Tuesday & Thursday**	**Friday**
MPIK	18:15	19:15	13:00
Alois-Link-Platz	18:25	19:25	13:10
Heidelberg main station	18:30	19:30	13:15

Please note: The shuttle bus stops at "**Steig R"** shown with red arrow Someone holding an ECLA sign will be there to assist you. Please be on time as the shuttle leaves promptly and cannot wait

MPIK → Molkenkur (conference dinner)	**Wednesday**
MPIK	17:15
Molkenkur	17:30
Molkenkur → HD main station	
Molkenkur	21:00
Heidelberg main station	21:20

Public transport goes via Alois Link Platz

Line 28:
Heidelberg main station (Steig C)→ Bierhelderhof/Ehrenfriedhof (not MPIK!): departures at 8:38 and 8:58, then hourly from 9:18 (also at 11:48 and 12:48)
Bierhelderhof/Ehrenfriedhof → Heidelberg main station: departures in the afternoon from 14:01, then every 20 minutes until 19:21, then every 40 minutes, last bus at 21:31

From **Bierhelderhof/Ehrenfriedhof, one can walk to MPIK entrance within 5 mins**
Line 39:
Bismarckplatz (Steig G, not shown in the map on the left)→ MPIK: departures at 8:43, then 9:00 and then once per hour (one additional bus at 11:30)
MPIK → Bismarckplatz: from 6:44 to 20:44 once per hour