AstroChemical Newsletter #115

July & August 2025

You can access the full abstracts by clicking the paper titles. Submit your abstracts before the 25th of each month for inclusion in the following newsletter.

Abstracts

Recent observational studies on carbon-chain species with current facilities and future prospects with ALMA & JWST

Kotomi Taniguchi, Ryan M. Lau, Masao Saito

Carbon-chain species have been widely found in star-forming regions and are considered to form via a bottom-up mechanism in which ionic and atomic carbon (C+ and C) play essential roles. Recent deep line survey observations toward the Cyanpolyyne Peak in Taurus Molecular Cloud-1 (hereafter TMC-1 CP) have achieved the discovery of new carbon-bearing species; e.g., large hydrocarbon rings and species including benzene rings such as cyanobenzene, cyanonaphthalene, and cyanopyrene. The bottom-up mechanism cannot explain their presence and now we need to revisit the carbon chemistry in the interstellar medium (ISM). One possible approach is to explore the carbon chemistry from evolved stars where carbon is ejected into the ISM through the diffuse ISM to the next-generation star-forming regions, or molecular clouds. Combining ALMA and JWST, we will be able to explore carbon chemistry including top-down mechanisms.

Accepted by Life Sciences in Space Research
DOI: 10.1016/j.lssr.2025.05.002
Full-text URL: https://www.sciencedirect.com/science/article/abs/pii/S2214552425000616

Formation of hydroxy, cyano and ethynyl derivatives of C4H4 isomers in the interstellar medium

M. Largo, M. Sanz-Novo, and P. Redondo

The study of cyclic hydrocarbons is of utmost relevance in current astrochemical research, as they are considered to be among the most significant reservoirs of carbon in the interstellar medium. However, while unsaturated cyclic hydrocarbons with three, five, and six carbon atoms have been widelyinvestigated, the highly strained antiaromatic cyclobutadiene (c-C4H4) still remains uncharted. Here, we employed high-level CCSD(T)-F12/cc-pVTZ-F12//B2PLYPD3/aug-cc-pVTZ theoretical calculations to analyze whether the cyano (CN), ethynyl (CCH), and hydroxy (OH) derivatives of c-C4H4 and its structural isomers butatriene (H2CCCCH2) and vinylacetylene (H2CCHCCH) can readily form via the gas phase reaction: C4H4 + X - C4H3X + H (where X = CN, CCH, and OH). For each system, we thoroughly explored the corresponding potential energy surfaces, identifying their critical points to enable a detailed analysis of the thermochemistry. Hence, we found various exothermic pathways for the formation of CN and CCH derivatives of butatriene and vinylacetylene, with no net activation barriers, while the formation of the OH derivatives is in general less favorable. Prior to the mechanistic study, we also analyzed the complete conformational panorama and stability of all the derivatives at the CCSD(T)-F12/cc-pVTZ-F12 level. Overall, c-C4H3CN and c-C4H3CCH emerge as particularly promising candidates for interstellar detection, provided that the parental c-C4H4 is present in the gas phase. These findings highlight the potential for detecting polar derivatives of c-C4H4 as indirect evidence of its presence in the ISM, as it appears to be ‘‘invisible’’ to radioastronomical observations. Also, this study underscores the need for future laboratory and theoretical efforts to characterize the spectroscopic properties of the proposed derivatives, paving the way for their eventual identification in space.

Phys. Chem. Chem. Phys., 2025, 27, 11413
DOI: 10.1039/d5cp00781j
Full-text URL: https://arxiv.org/abs/2505.03321

Hydroxylated Mg-rich amorphous silicates as catalysts for molecular hydrogen formation in the interstellar medium

Mennella. V, Suhasaria. T, Kerkeni, B and Ouerfelli, G

We present results from an experimental study on the interaction of atomic deuterium with Mg-rich amorphous enstatite and forsterite type silicates. Infrared spectroscopy was used to examine the process. During D atom exposure, deuteroxyl group formation was observed. The cross section for OD group formation, estimated from the OD stretching band intensity with D atom fluence, is σf,OD = 4.2e-18 cm2 for both silicates. HD (D2) molecules form via D atom abstraction of chemisorbed H (D) atoms from OH (OD) groups, with a cross section of σf,D2 = 7.0e-18 cm2. Quantum chemical calculations on enstatite and forsterite amorphous nano-clusters were used to analyze chemisorption and abstraction energies of H atoms. The formation of OH groups on forsterite is barrierless, while enstatite has a small energy barrier. H2 abstraction from hydroxyl groups is barrierless in both silicates. The results support our interpretation of IR spectral changes during D atom exposure as addition and exchange reactions, with catalytic molecular deuterium formation. These findings, obtained at 300 K, are relevant to astrophysical environments like photodissociation regions and interstellar clouds at lower temperatures.

Amorphous silicates, like carbon grains, undergo hydrogenation in the diffuse interstellar medium due to interactions with atomic hydrogen and UV photons. The detection of these components on comet 67P/Churyumov Gerasimenko connects primitive solar system objects to interstellar dust, offering new insights into their evolution.

Accepted in The Astrophysical Journal
DOI: 10.3847/1538-4357/ade2d3
Full-text URL: https://arxiv.org/abs/2506.11596

PRODIGE – envelope to disk with NOEMA: V. Low 12C/13C ratios for CH3OH and CH3CN in hot corinos

Laura A. Busch, J. E. Pineda, O. Sipilä, D. M. Segura-Cox, P. Caselli, M. J. Maureira, C. Gieser, T.-H. Hsieh, M. T. Valdivia-Mena, L. Bouscasse, Th. Henning, D. Semenov, A. Fuente, M. Tafalla, J. J. Miranzo-Pastor, L. Colzi, Y.-R. Chou, and S. Guilloteau

The 12C/13C isotope ratio has been derived towards numerous cold clouds (20-50 K) and a couple protoplanetary disks and exoplanet atmospheres. However, direct measurements of this ratio in the warm gas (>100 K) around young low-mass protostars remain scarce, but are required to study its evolution during star and planet formation. We derived 12C/13C ratios from the isotopologues of the complex organic molecules (COMs) CH3OH and CH3CN in the warm gas towards seven Class 0/I protostellar systems to improve our understanding of the evolution of the 12C/13C ratios during star and planet formation. We used the data that were taken as part of the PRODIGE large program with the NOEMA at 1mm. The emission of CH3OH and CH3CN is spatially unresolved in the PRODIGE data (300au scale). Derived rotational temperatures exceed 100K, telling us that they trace the gas of the hot corino, where CH3CN probes hotter regions than CH3OH on average (290 K versus 180 K). The column density ratios between the 12C and 13C isotopologues, derived from LTE analysis, range from 4 to 30, thus, are significantly lower than the expected local ISM isotope ratio of about 68. Assuming that CH3CN and CH3OH may inherit the 12C/13C ratio from their precursor species, astrochemical models were conducted for the latter and compared with our observational results. We conclude that an enrichment in 13C in COMs at the earliest protostellar stages is likely inherited from the COMs' precursor species, whose 12C/13C ratios are set during the prestellar stage via isotopic exchange reactions. This also implies that low 12C/13C ratios observed at later evolutionary stages could at least partially be inherited. A final conclusion on 12C/13C ratios in protostellar environments requires improved observations to tackle current observational limitations and additional modelling efforts.

Accepted in A&A
DOI: 10.1051/0004-6361/202554104
Full-text URL: https://arxiv.org/abs/2505.21307

Exploring the formation and alteration of organics in ice: experimental insights for astrochemistry and space missions

Florence Hofmann, Nariste Asanova, Riccardo Giovanni Urso, Andreas Elsaesser

The formation and alteration of organic molecules within the Solar System and beyond is closely related to the life cycle of ice in space. While energetic photons, charged particles, and thermal processing drive the formation of complex organic compounds within ices in cold molecular clouds in the interstellar medium, their accretion into comets and asteroids would allow their delivery on planetary surfaces. Further, complex organics are also present on the icy moons of giant planets which are key targets in both NASA’s and ESA’s space exploration programs. In this paper, we present a new experimental setup, built to study the formation and alteration of complex organic molecules of astrobiological-relevance in cryogenic environments. Possible sample configurations allow us the combination of inorganic and organic molecules, such as minerals, PAHs and amino acid mixtures in contact with various ice mixtures (e.g. H2O, NH3, CO, CO2, CH3OH). These samples can be exposed to UV photons, electron bombardment and undergo thermal processing while being continuously monitoring by FT-IR transmission spectroscopy during the ice deposition, irradiation, and warm-up to room temperature. Here, we present calibration measurements of pure H2O, NH3 and CH3OH ices deposited at 15 K and show spectral changes induced by heating and electron bombardment. Furthermore, we show the formation of new molecular species within NH3:CH3OH and NH3:CH3OH:H2O ice mixtures under electron bombardment. We outline the experimental design, which has recently been used to investigated the photochemistry of amino acids under simulated cryo-volcanic regions of Titan (Gonçalves D. et al, ACS Earth and Space Chemistry 2025 9 (3), 715-728, DOI: 10.1021/acsearthspacechem.4c00376) and envision to provide spectral information on astrobiologically-relevant molecules, such as organic species fundamental for living organisms and potential biosignatures, in contact with ices of relevance for astrophysics and planetary science.

Earth, Planets Space 77, 70 (2025)
DOI: 10.1186/s40623-025-02207-8
Full-text URL: https://earth-planets-space.springeropen.com/articles/10.1186/s40623-025-02207-8

Photoionization of small neutral polycyclic aromatic hydrocarbons: Testing photoelectric models of interstellar dust

H. R. Hrodmarsson, L. Verstraete, E. Dartois, J. Fréreux, O. Lacinbala, L. Nahon, G. A. Garcia, T. Pino, and P. Bréchignac

In the interstellar medium (ISM) and circumstellar environments, photoionization, or the photoelectric effect, emerges as a prevalent phenomenon. In regions exposed to UV photons, either stellar or secondary photons induced by cosmic rays, polycyclic aromatic hydrocarbons (PAHs) liberate electrons through the photoelectric effect, efficiently contributing to the heating budget of the gas. In contrast to shielded areas, neutral and cationic PAHs can scavenge electrons and retain a significant portion of the cloud's electronic charge. This dual behavior of PAHs not only influences the gas thermal and dynamical behavior but also plays a pivotal role in shaping the chemistry of the environments. Our aim was to measure the photoelectron kinetic energy distribution (KED) of PAHs of varying sizes, symmetries, and C:H ratios to describe the photoelectron KED with a law that can be implemented in astrophysical photoelectric models that describe gas heating. We used a double-imaging photoelectron photoion coincidence spectrometer coupled with the DESIRS VUV beamline at the SOLEIL synchrotron to record the gas-phase spectra of a series of sublimated PAHs with different sizes and structures in the 13–20 C atom range. We then compared our data to current astrophysical dust photoelectric models used to describe the PAH charge and gas photoelectric heating in the ISM. In particular, we extended the Kimura 2016, (MNRAS, 459, 2751) model (eK16) to take into account the KED of the photoelectron and its interaction with the grain. We show that although subtle differences between the molecules in our dataset arise from individual electronic structures, the photoelectron KED of PAHs of different sizes and symmetry display remarkable similarities. A general law can thus be implemented in sophisticated ISM astrochemical models to describe their photoelectron KED behavior. We find that the eK16 photoelectric model closely reproduces the present photoionization cross sections of neutral, small PAHs as well as literature data obtained on cationic PAHs. It is noteworthy that the eK16 model, unlike former models, matches the absolute scale of the measured photoionization cross sections. We show that the eK16 model predicts a maximum photoelectric efficiency significantly lower than the previous models, implying a lower interstellar gas temperature and less emission.

A&A, 698, A202 (2025)
DOI: 10.1051/0004-6361/202554245
Full-text URL: https://hal.science/hal-05116244/

Rotational equilibrium of C2 in diffuse interstellar clouds. II. Formation-excitation at work?

J. Le Bourlot, E. Roueff, S. R. Federman, A. M. Ritchey, and D. L. Lambert

Context. Recent spectroscopic measurements have revealed absorption from higher rotational levels in C2 than previous observations. These improvements are accompanied by the availability of updated radiative and collisional data. Aims. We revisit the density and radiation field intensity diagnostics provided by the observations of many rotational levels of interstellar C2 and extensive molecular information. Methods. We built an excitation model of C2 without spatial structure, including levels up to J = 34 where updated radiative and collisional excitation data are introduced as well as excitation by chemical formation. Results. We confirm the importance of the recent collisional excitation rate coefficients of C2 by molecular H2. We show that the new higher level observations cannot be explained by the standard balance between collisional excitation and radiative transitions. We propose that chemical excitation at formation provides a plausible mechanism to explain the observed high excitation of C2. In addition, it allows us to lift the degeneracy of the density over radiation field strength parameter in the excitation model. Conclusions. A 0D model remains limited and it is highly desirable to use a full Photon Dominated Region (PDR) model, which includes all excitation processes introduced here and full chemical and thermal balance.

Accepted in Astronomy & Astrophysics
DOI: 10.1051/0004-6361/202554760
Full-text URL: https://arxiv.org/abs/2505.21273

Deuterated water abundance in the young hot core RCW 120 S2

Kirsanova M. S., Farafontova A. A.

Since the emission of water molecules cannot be observed from Earth, less abundant isotopologues, such as H182O and HDO, are used to trace water in star-forming regions. The main aim of this study is to determine HDO abundance in the hot core RCW 120 S2. We performed observations of the hot core in the 200-255~GHz range using the nFLASH230 receiver on the APEX telescope. Two HDO lines were detected toward RCW 120 S2. Their intensities are described by excitation temperature approx 300~K and gas number density higher than 1e9 cm-3. The emission originates from the hot core rather than the warm dense envelope surrounding a central young stellar object. The HDO column density ranges from (3.9−7.9)e13 cm-3 with a most probable value 5.6e13 cm-3. The HDO abundance relative to hydrogen nuclei is 1.5e-9. This HDO abundance value is among the lowest reported for hot cores. Combined with the non-detection of the H218O line, we conclude that protostellar heating in RCW 120 S2 is still in its early stages.

Accepted by Astronomy Letters
Full-text URL: https://arxiv.org/abs/2505.21945

Metallic species in interstellar medium: Astrochemical modeling

Ankan Das, Milan Sil, and Paola Caselli

Metal-bearing species in diffuse or molecular clouds are often overlooked in astrochemical modeling except for the charge exchange process. However, catalytic cycles involving these metals can affect the abundance of other compounds. We prepared a comprehensive chemical network for Na, Mg, Al, Fe, K, and Si-containing species. Assuming water as the major constituent of interstellar ice in dark clouds, quantum chemical calculations were carried out to estimate the binding energy

of important metallic species, considering amorphous solid water as substrate. Significantly lower binding energies (approximately 5 to 6 times) were observed for Na and Mg, while the value for Fe was roughly 4 times higher than what was used previously. Here, we calculated binding energy values for Al and K, for which no prior guesses were available. The total dipole moments and enthalpies of formation for several newly included species are unknown. Furthermore, the assessment of reaction enthalpies is necessary to evaluate the feasibility of the new reactions under interstellar conditions. These parameters were estimated and subsequently integrated into models. Some additional species that were not included in the UMIST/KIDA database have been introduced. The addition of these new species, along with their corresponding reactions, appears to significantly affect the abundances of related species. Some key reactions that significantly influence general metal-related chemistry include: M+ + H2 -> MH2+ + h nu, MH + O -> MO + H (M = Fe, Na, Mg, Al, K), and M_1+ + M_2H -> M_1H + M_2+ (where M_1 not equal to M_2, M_1, M_2 = Na, Mg, Al, K, Fe). Significant changes were observed in magnesium and sodium-bearing cyanides, isocyanides, and aluminum fluoride when additional reaction pathways were considered.

Accepted for publication in Astronomy and Astrophysics
DOI: 10.1051/0004-6361/202452044
Full-text URL: http://arxiv.org/abs/2506.19463

CO2 infrared spectra on silicate dust grain analogs: Implications for JWST observations

Tushar Suhasaria, Vanessa Leuschner, Cornelia Jäger, Caroline Gieser, and Thomas Henning

Carbon dioxide is one of the three most abundant species within the ice mantles around dust grains inside molecular clouds. Since a substantial amount of interstellar grains is made of siliceous materials, we have studied the infrared profile of CO2 deposited on top of a bare and ice-coated amorphous silicate (MgFeSiO4) film using reflection absorption infrared spectroscopy (RAIRS). In contrast to a metal surface, the CO2 IR profile shows a relaxation of the metal surface selection rule in the presence of the bare MgFeSiO4 dust grain analog, which brings the IR profile closer to the observational spectra while maintaining the sensitivity of RAIRS. Experiments with the underlying CO and CH4 ices show that their presence facilitates structural changes toward crystalline ice for the deposited CO2 at much lower temperatures than on the polar ice layers. Warming-up experiments of CO2 showed that it tends to stay on the silicate surface for much longer than on the gold surface without the silicate layer. We noticed for the first time a split in the 13CO2 IR feature on the pure or ice covered silicate grain as a marker for the onset of diffusion. The laboratory 13CO2 profile then closely resembles recent JWST observations of this feature around young and embedded protostars, suggesting that it can be linked to the observed feature.

accepted in The Astrophysical Journal Letters
DOI: 10.3847/2041-8213/ade993
Full-text URL: https://arxiv.org/abs/2507.00836

Investigating Formation Pathways and the Spectroscopic Constants of Aluminum Nitrides from AlH and NH3

C. Zachary Palmer, Jacob A. Johns, and Ryan C. Fortenberry

Reactions of AlH and NH3 are shown to produce Al–N containing species that could potentially contribute to the composition of dust grains, like the Murchison CM2 chondritic meteorite. The present computational study couples explicitly correlated coupled cluster theory and density functional theory to produce a gas-phase chemical formation pathway from AlH and NH3 to Al4N4H8, a stable, cubic structure with the proper Al/N ratio expected for larger aluminum nitride species. Rovibrational spectroscopic analyses of HAlNH3, AlNH2, Al2N2H4, and Al4N4H8 reveal consistently intense vibrational transitions and large absorption cross sections of modes associated with spectral features typically associated with dust grain formation in circumstellar media. The ν5 wagging frequency for Al4N4H8 at 748.8 cm–1 (13.35 μm) exhibits a vibrational transition intensity of 428 km mol–1, more than 5× larger than the antisymmetric stretch in water. Hence, the present formation pathway and rovibrational analysis should assist in the potential detection of a class of inorganic molecules that may contribute to the nucleation and formation of dust in protoplanetary disks and stellar outflows of AGB stars.

J. Phys. Chem. A 2025, 129, 28, 6404–6413
DOI: 10.1021/acs.jpca.5c01490
Full-text URL: https://pubs.acs.org/doi/10.1021/acs.jpca.5c01490

Announcements

Training Workshop for Meudon PDR Code Users (3-4 December)

A dedicated training session on the Meudon PDR code will be held at the Paris Observatory on December 3–4, 2025.

This workshop will introduce participants to the Meudon PDR code (https://ism.obspm.fr/), covering how to run simulations, analyze the results, and make use of the ISMDB database of precomputed models, along with its associated tools for observational data analysis.

The course is designed for both new users and those already familiar with the code who wish to deepen their understanding

and enhance their practical skills.

To register, please contact: emeric.bron@obspm.fr
Some travel funding is available if needed.

About the Meudon PDR Code:

The Meudon PDR code is a state-of-the-art numerical model describing the physics and chemistry of UV-irradiated neutral interstellar gas (coupling chemistry, radiative transfer, thermal balance, statistical equilibrium in the quantum levels), and predicting both the spatial profiles (as a function of depth in the cloud) of the chemical densities and physical variables, and the observable line intensities and column densities.
The code can be used to interpret both emission and absorption observations across a wide range of galactic and extragalactic environments — including diffuse clouds, photo-dissociation regions (PDRs) in star-forming regions, protoplanetary disks, damped Lyman-alpha systems, and regions with enhanced cosmic-ray fluxes such as the Galactic Center. It can be used to interpret observations in neutral gas from many instruments (JWST, IRAM, ALMA, SOFIA, visible and UV telescopes, …).
Preliminary Program:
- Overview of the new version of the code and its underlying physics
- Installing and running the code; understanding and editing configuration files
- Exploring model outputs with dedicated tools (IDAT, Chemistry Analyzer) to study the physics and chemistry of neutral gas
- Introduction to ISMDB, the online database of precomputed models, and its tools for analyzing observations, both via the web interface and through local Jupyter notebooks using pyismtools

The training will be primarily hands-on, featuring practical tutorials and several application examples — such as fitting observational data and exploring the effects of specific physical or chemical processes.

COST Action CA22133 PLANETS - WG1 meeting 23 - 25 September 2025, High Tatras, Slovakia

The COST Action, The Birth of Solar Systems (PLANETS), is delighted to announce a meeting of Working Group 1 - “Planet formation: Laboratory Perspectives”. □□
Join us from September 23rd (Tuesday) to 25th (Thursday) 2025, in the beautiful High Tatras mountain region of Slovakia, in the Hotel Panorama (www.hotelpanorama.sk/en) located in picturesque Štrbske Pleso. This meeting will be held in person only to facilitate face-to-face discussions on the role of laboratory experiments and theory in the study of planet formation. Special emphasis will be put on the measurement of physical and chemical data and its inclusion in models of protoplanetary disks, planet formation and exoplanets.
Hotel Panorama will offer a special rate for conference participants.□□
Preliminary information is now available on the meeting website: https://sites.google.com/view/laboratory-planet-formation/home
Registration is open now at the following link:
https://docs.google.com/forms/d/e/1FAIpQLSc1_euF4n2m8VFQp7did30M7NoWDN-R8ou9d1JVobc91bvP5A/viewform
Please note that places are limited, so we encourage you to apply as soon as possible should you wish to attend the workshop. We will keep the application form open until spaces fill up.
For more information, please contact the working group leaders Jenny Noble (jennifer.noble at univ-amu.fr) and Zuzana Kanuchova (pipovci at gmail.com).

Registration open for “Astrochemistry: From Quantum to Cosmos” at Radboud University, Nijmegen, The Netherlands, October 21-24, 2025

This meeting will bring together the extended Dutch Astrochemistry Network (DAN) community with members of the German Laboratory Astrophysics groups and guests from Europe and abroad.
The meeting’s webpage including a list of invited speakers can be found at: https://indico.imapp.ru.nl/event/330/overview
Registration is now open!
Registration deadline is 15 August 2025, with the deadline for submission of abstracts for oral or poster contributions at 31 August 2025.
The registration fee is €200 and covers all lunches and drinks, plus the conference dinner. Information to book accommodation is provided on the website.
We will update the meeting website with a detailed program and add additional information as we approach the workshop.
Selected topics are:
• Gas-phase experiments and spectroscopy, fundamental processes
• From PAHs to dust grains
• Prebiotic chemistry in the gas phase and interstellar ices
• New developments and discoveries in observational astronomy (JWST, ALMA, ...)
• Data needs for astrochemistry
• Large scale research infrastructure for astrochemistry
• Computational astrochemistry
• New frontiers in astrochemistry

The meeting is supported by the Dutch Research Council (NWO) and the national research institute HFML-FELIX.

We look forward to a very lively meeting with lots of discussions.

On behalf of the organizers,
Sandra Brünken
Thanja Lamberts
Jos Oomens
Silvia Spezzano
Guido Fuchs
Oskar Asvany