AstroChemical Newsletter #127

September 2026

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

The fundamental vibrational frequencies of methanetetrol and their role in the infrared spectrum of the complete methane alcohol family

N. K. Carlson, R. C. Fortenberry

Methanetetrol showcases notable intensity in the range of 1060 cm−1 for both of its conformers as provided by quantum chemical methods known to be highly accurate in the prediction of fundamental vibrational frequencies. This C−O stretch intensity is in line with the other methane alcohols in this family such as methanediol and methanetriol. Though the increasing instability of the higher alcohols implies a lower abundance in most astronomical environments, higher intensities still provide an opportunity for detection. As such, these complementary factors may still allow the geminal orthoacids to be observed astronomically since they have been successfully produced in the laboratory under simulated interstellar conditions.

J. Molec. Spectrosc. 2026, 420(112127)
DOI: 10.1016/j.jms.2026.112127
Full-text URL: https://www.sciencedirect.com/science/article/abs/pii/S0022285226000597

Testing various assumptions for radiolysis, non-diffusive chemistry, and chemical desorption in cold cores

V. Wakelam and T. Tu

Context. To study interstellar gas and grain chemistry, gas-phase astrochemical models have been developed since the early 1980s and gas-grain models since the 1990s. Each published model includes various assumptions mainly for surface processes. Aims. In this paper, we compare recently added mechanisms for grain surface chemistry, namely, non-diffusive chemistry, radiolysis, and chemical desorption. Methods. Several formalisms for these processes have been added to our astrochemical model Nautilus, and we tested them, compar- ing the predicted gas-phase and ice abundances. Our predictions are also compared to gas and ice observed compositions. Results. Our main findings are that radiolysis itself does not influence the results. Non-diffusive chemistry can have an impact on the gas-phase and ice species, but it depends on the adopted formalism. In particular, the one of Shingledecker & Herbst (2018) changes the main reservoirs of the species in the ices, impacting the species in the gas-phase as well. The adopted formalism for chemical desorption can produce differences in the gas-phase by up to a factor of ten. Last, our standard model, without non-diffusive chemistry and with the chemical desorption from Fredon et al. (2021), produces the best results in relation to observed gas-phase abundances, while the ice observed agreement is unchanged. Conclusions. The formalism for some grain surface processes are important even for gas-phase abundances. More experiments are needed to constrain their efficiency, however. For the chemical desorption, each formalism relies on an uncertain parameter, which is the fraction of the energy actually delivered to the products, that can be adjusted to reproduce the experiments.

Accepted for publication in A&A
Full-text URL: https://arxiv.org/abs/2607.15747

A tale of two isotopes: Spatial variation in HCN fractionation toward young cores

Sigurd S. Jensen, Silvia Spezzano, Olli Sipilä, Paola Caselli, Laura Colzi, Elena Redaelli

Isotopic fractionation can serve as a powerful tracer of the chemical evolution during star and planet formation. To accurately interpret observations, it is crucial to identify the dominant pathways of nitrogen and carbon fractionation at different evolutionary stages. We aim to study nitrogen and carbon fractionation in a sample of young cores at the onset of star formation. Methods. We map H13CN and HC15N around one starless and three pre-stellar cores. We compute the N(H13CN)/N(HC15N) column density ratio across the cores and compare the distribution with N(H2) maps from Herschel/SPIRE. In addition, we calculate 14N/15N maps using the double isotope method for comparison with earlier studies. The results are compared with astrochemical modeling of carbon and nitrogen fractionation for a one-dimensional pre-stellar core model. Results. The computed N(H13CN)/N(HC15N) ratio exhibit clear spatial variation across the maps. This variation is correlated with N(H2) in three out of four cores. Our analysis reveals a correlation between the H13CN/HC15N ratios and the N(H2) maps. According to the astrochemical model, the correlation is mainly due to variations in the 12C/13C ratio. Consequently, the results caution against applying the double-isotope method to derive 14N/15N ratios without independently assessing possible spatial variations in the 12C/13C ratio. Furthermore, the leading cause of the isotopic variation in the model is not isotope-selective photodissociation, but rather more efficient fractionation through exchange reactions at lower temperatures in the denser regions of the cores.

Accepted in A&A.
Full-text URL: https://arxiv.org/abs/2607.26187

Chemical modelling of interstellar MgS

M. Rey-Montejo, I. Jimenez-Serra, T. Millar, R.C. Fortenberry, S. Viti, J. Garcia de la Concepcion, G. Vermarien, M. Sanz-Novo, L. Colzi, S. Zeng, V.M. Rivilla

The detection of magnesium sulphide (MgS) and sodium sulphide (NaS) towards the Galactic Center molecular cloud G+0.693 constitutes the first detection of metal sulphides in the interstellar medium (ISM). However, there is scarce information about the key reactions (either in the gas phase or on grains) involved in their formation. In this paper, we model the chemistry of MgS simulating the passage of a low-velocity shock to recover the abundances recently measured towards G+0.693. Through this chemical modelling, we analyse the dominant reactions involved in the formation and destruction of this molecule, their associated chemical time-scales, and the depletion factor needed to recover the observed abundances. We build the initial chemical network of MgS by using SiS as a proxy for this metal sulphide, and we investigate the exothermicity of these and additional, uniquely proposed reactions through quantum chemical computations. We run a three-phase model (initial translucent cloud, cloud collapse phase and shock interaction stage) that mimics the evolution and physical conditions of G+0.693. Our results show that a depletion factor of 1000 is required for elemental Mg to recover the observed abundances of MgS. This implies that potentially more than 99.9% of Mg is locked in dust grains. The dominant reaction leading to the formation of MgS is the neutral-neutral reaction between MgH and S in the gas phase. This work represents the first analysis of the chemistry of the metal-sulphide MgS and suggests that Mg is largely incorporated into dust grains, most likely in the form of silicates. However, additional laboratory and/or theoretical studies of the key MgS formation reactions are essential to obtain more reliable constraints. Future missions, such as PRIMA, will provide insights into the amount of metal-sulphides locked into interstellar dust grains.

Accepted in A&A
DOI: 10.1051/0004-6361/202661161
Full-text URL: https://arxiv.org/abs/2607.25758

Influence of through-space and through-bond interactions on the ionization behavior of pyridyl and diazinyl radicals: A computational study

M. Saraswat

Understanding the structure and properties of heterocyclic radicals and their cations is essential for elucidating reaction mechanisms, as these species act as versatile reactive intermediates in fields ranging from synthetic organic chemistry to atmospheric, combustion and interstellar chemistry. In this work, we investigated the role of orbital interactions, namely through-space (TS) and through-bond (TB) interactions, between the nitrogen lone pair and the radical electron in the ionization of pyridyl radicals and diazinyl radicals, as well as in the formation of the corresponding pyridyl cations and diazinyl cations. The photoelectron spectra of six dehydrodiazine radicals (2a-c, 3a-b and 4a) were simulated through the calculation of Franck-Condon (FC) factors using density functional theory (DFT) at the B3LYP/aug-cc-pVQZ level of theory. Additionally, the adiabatic ionization energies (AIEs) of all three pyridyl radicals and six diazinyl radicals leading to their singlet and triplet cations were computed using DFT as well as the G4, CBS-QB3 and W1BD composite methods. Our investigation revealed that the presence of strong TS and TB interactions in the radicals leads to lower adiabatic ionization energies because the corresponding cations are also strongly stabilized through these interactions. In contrast, higher AIE values are observed for radicals in which TS and TB interactions are minimal, resulting in cations that are not effectively stabilized by orbital interactions. Interestingly, the singlet-triplet energy gap (ΔES-T) of the resulting pyridyl and diazinyl cations depends directly on the extent of TS interaction, where stronger TS interaction in the radical leads to larger ΔES-T gaps.

Journal of Molecular Spectroscopy 420–421 (2026) 112128
DOI: 10.1016/j.jms.2026.112128
Full-text URL: https://www.sciencedirect.com/science/article/pii/S0022285226000603

Raman analysis of organic refractory materials after energetic processing: Evidence for amorphous carbon on TNOs and comets

Germanà, M., Vyjidak, A., Baratta, G.A., Giuliano, B.M., Urso, R.G., Scirè, C., Fulvio, D., Grassi, T., Jusko, P., Caselli, P. and Palumbo, M.E.

Amorphous carbon (αC) is found in various extraterrestrial particles, including those thought to originate from the outer Solar System. αC can form through two main processes involving C-rich materials: exposure to energetic charged particles and thermal processing. Laboratory analyses can constrain the origin of αC in space, as it is not easily detectable through remote sensing. We here investigate the formation of αC on the icy surface of Trans-neptunian objects and Oort cloud comets throughout their exposure to energetic ions. We use organic refractory residues (ORRs), which are laboratory simulants of refractory organics in space, obtained from the irradiation (200 keV ions) of various icy mixtures (N2, CO, CH4, CH3OH). As formed ORRs were further irradiated at room temperature (αC-ORRs) and analyzed by Raman spectroscopy. Our as formed ORRs do not exhibit αC that is in turn detected in αC-ORRs. The carbonaceous structure of αC-ORRs shows high disorder and dependence on the initial icy composition. Nitrogen-bearing αC-ORRs exhibit structural properties similar

to some extraterrestrial particles likely originating from icy outer bodies, whereas annealed αC-ORRs mimic materials that underwent different degrees of metamorphism. Our findings highlight how Raman characterization of αC in extraterrestrial samples serves as a strong analysis tool in providing insights into the evolution of different Solar System objects.

2026, Meteorititics and Planetary Science, 61: 1994-2015
DOI: 10.1111/maps.70190
Full-text URL: https://onlinelibrary.wiley.com/doi/10.1111/maps.70190

Theoretical Determination of the Binding Energies of Methanol and Related Species onto Amorphous Solid Water Ice

Aneesa Ahmad, Catherine Walsh, Stefan Vogt-Geisse, Gabriela Silva-Vera, and Felix Sainsbury-Martinez

The formation and survival of complex organic molecules (COMs) in cold interstellar environments depends on their interactions with icy dust grain surfaces. Methanol, a key COM detected in cold cores and protoplanetary disks, is believed to form on amorphous solid water (ASW) through surface reactions and reside there until it is desorbed into the gas phase. We present a theoretical study of the binding energies (BEs) of methanol and its photolysis-derived species on ASW clusters by means of dispersion-corrected density functional theory using a refined protocol implemented in the Binding Energy Evaluation Platform. Molecules capable of hydrogen bonding, such as H2O, CH3OH, HCOOH, and OH, exhibit high BEs and broad BE distributions that reflect the structural heterogeneity of the ASW surface. In contrast, weakly interacting volatiles including CO, CO2, CH4, and CH3 display narrower distributions dominated by dispersion interactions. Open-shell radicals such as CH2OH and OH bind more strongly than HCO and CH3 due to their ability to form directional hydrogen bonds. Incorporation of our BEs into an astrochemical model, in conjunction with a recalculation of the pre-exponential factor using transition state theory, demonstrates the sensitivity of model results to the method of calculation of the grain-surface reaction rates. The new approach generally predicts a higher abundance of radicals on the ice that are key reactants for the formation of COMs when surface diffusion is assumed to be efficient. These findings emphasize the importance of incorporating BEs that have been determined in a self-consistent manner into astrochemical models, and provide reliable theoretical benchmarks for species with limited experimental data.

ApJ, 1006, 225 (2026)
DOI: 10.3847/1538-4357/ae84bb
Full-text URL: https://arxiv.org/abs/2606.26833

Bottom-Up Formation of the Simplest Geminal Thiol─Methanedithiol (CH2(SH)2)─and the Methyl Hydrodisulfide (H3CSSH) Isomer in Interstellar Analogue Ices

Jia Wang, Ashanie Herath, Andrew M. Turner, Mason McAnally, Ryan C. Fortenberry, André K. Eckhardt, Ralf I. Kaiser

Geminal dithiols─organic molecules bearing two thiol groups on the same carbon atom─are versatile synthons in organic and atmospheric chemistry, exhibiting significantly greater stability than their oxygen analogues. Here, we report the first formation of the smallest geminal dithiol, methanedithiol (CH2(SH)2), and its structural isomer, methyl hydrodisulfide (CH3SSH), in low-temperature model interstellar ices composed of methane and hydrogen sulfide via energetic electron irradiation, simulating secondary electrons generated by galactic cosmic rays. Both isomers were identified in the gas phase using isomer-selective vacuum ultraviolet (VUV) photoionization reflectron time-of-flight mass spectrometry (PI-ReToF-MS), guided by quantum chemically computed adiabatic ionization energies, and confirmed through isotopic labeling and ultraviolet photolysis studies. These results not only demonstrate that methanedithiol and methyl hydrodisulfide can form on ice-coated interstellar nanoparticles and represent promising candidates for future astronomical detection, but they also provide fundamental insights into the nonequilibrium synthesis of geminal dithiols in extraterrestrial environments.

J. Phys. Chem. Lett. (2026) 17 (28): 8090–8097
DOI: 10.1021/acs.jpclett.6c01781
Full-text URL: https://pubs.acs.org/jpclcd/article-abstract/17/28/8090/5177548/Bottom-Up-Formation-of-the-Simplest-Geminal-Thiol

First detection of C2H+ in the interstellar medium

Jacob, Arshia M. ; Menten, Karl M. ; Brünken, Sandra ; Belloche, Arnaud ; Wyrowski, Friedrich ; Silva, Weslley G. D. P. ; Asvany, Oskar ; Khan, Sarwar ; Kabanovic, Slawa ; Steenbakkers, Kim ; Groenenboom, Gerrit C. ; Redlich, Britta ; Schlemmer, Stephan

Despite the detection of nearly 350 molecules in the interstellar medium, almost half of which are carbon chains, the pathways that build molecular complexity remain poorly understood. Observed abundances of carbon-chain and aromatic species are difficult to reconcile with existing top-down or bottom-up formation scenarios, due in part to limited observational constraints and incomplete theoretical understanding. In particular, small intermediary ions, key drivers of ion-molecule reactions capable of seeding larger hydrocarbons and aromatic rings, could provide critical support for the bottom-up formation scenario. Constraining the abundance and chemistry of these ions is therefore essential to test whether bottom-up growth can operate efficiently under interstellar conditions. Here, we report the first detection of the small hydrocarbon cation ethynylium, C2H+, toward the Orion Bar, based on observations with the APEX 12m sub-mm telescope of its lowest-lying J=3-2 rotational transition near 211GHz, which exhibits a unique spectroscopic fingerprint through resolved Lambda-

doubling and hyperfine splitting components, as recently measured in the laboratory. Meudon PDR models successfully reproduce these values, placing C2H+ formation at the outer edges of PDR fronts. Our results link C2H+ production to CH+ and CH3+ within a network of ion-molecule reactions driven by vibrationally excited H2, a scenario now further supported by recent detections of these species in PDRs like the Orion Bar with JWST observations. The importance of C2H+ lies in its role as a key intermediate: it produces C2H2+ and subsequently C2H3+, effectively channelling small C2 building blocks toward larger hydrocarbons and facilitating bottom-up growth at the PDR surface. Targeted searches for C2H+ in other regions promise to provide a potentially decisive probe of ion-driven bottom-up chemistry in the ISM.

A&A, Forthcoming
DOI: 10.1051/0004-6361/202661924
Full-text URL: https://arxiv.org/abs/2608.08014

Searching for the elusive CH2+ with the James Webb Space Telescope. Another carbocation to constrain astrochemical networks.

M. Zannese, L. H. Coudert, E. Dartois, P. Dell'Ova, O. Roncero, P. del Mazo-Sevillano, U. Jacovella, B. Gans, J. R. Goicoechea, D. Van De Putte, C. Boersma, E. Habart, E. Peeters, J. Cami, R. Chown, I. Schroetter and O. Kannavou

Carbocations are key species in interstellar chemistry, providing entry points for building larger hydrocarbons. CH+, and more recently, CH3+, have been detected. Other carbocations await detection to provide a comprehensive view of the astrochemical network that is at work in the interstellar medium. We search for CH2+ in objects in which CH3+ was detected and evaluate the most favorable conditions for detecting the elusive CH2+ reactive cation. We calculated the CH2+ rotational and rovibrational transitions expected to contribute in the mid- to far-infrared, focusing on the lower-energy rovibrational levels. We then calculated CH2+ infrared emission spectra at different excitation temperatures and compared them to JWST spectra of the externally irradiated disk d203-506 in Orion, where CH+ and CH3+ have already been detected. We used thermochemical models to predict the abundance and spatial morphology of CH2+ to better understand its nondetection. The comparison to JWST spectra allowed us to provide excitation-temperature-dependent upper limits to the excited column density. These are several times lower than those detected for CH+ and CH3+ in their excited states. Based on model calculations for photodissociation regions and assuming similar excitation temperatures, the upper limit derived from observations and CH2+ model spectrum is either slightly above or below the column density expected from models of photodissociation regions. We provide a list of tabulated transitions to allow the community to search for this carbocation in future observations as CH2+ is key in providing observational constraints on astrochemical models.

A&A, 712, A98 (2026)
DOI: 10.1051/0004-6361/202660602
Full-text URL: https://arxiv.org/abs/2607.01155

Stability and IR Spectra of Functionalized, Cyclic Hexamers of Cyclopropenylidene, C18Xy (X=C, O, S; y = 0 . . . 6)

Charles T. Earl, Andrew J. Stoda, and Ryan C. Fortenberry

The astronomically abundant molecule cyclopropenylidene (c-C3H2) can form sta- ble hexamer rings. Additionally, the related carbene cyclopropenylidene (c-C3H2C) can do the same, and this work explores the continuum of molecules from C18 to C24. The stability and IR features of each molecule are quantum chemically computed show- casing a surprising stability in C23 and C24. The latter is actually more stable than even C18 itself. Regardless, each molecule in the class exhibits notable IR features, in- cluding a high intensity C=C stretch, which may be observable from the James Webb Space Telescope (JWST). This feature falls in the vicinity of 1600 cm−1 (6.2 μm), a region typically associated with polycyclic aromatic hydrocarbon cations. Addition- ally, each apical carbon on the carbene cyclopropenylidene hexamer is further replaced by an oxygen and sulfur to create a hexamer ring of each molecule, but the stability patterns for these substitutions are not favorable for higher substitutions, reducing the likelihood that C18 functionalized with O or S could contribute to any observable, naturally-produced IR features.

J. Phys. Chem. A (2026) 130 (32): 6400–6408.
DOI: 10.1021/acs.jpca.6c03811
Full-text URL: https://pubs.acs.org/jpcafh/article-abstract/130/32/6400/5237667/Stability-and-IR-Spectra-of-Functionalized-Cyclic

Molecule-specific diffusion and desorption of interstellar ices on carbonaceous dust

C. Yi-Hsuan, S. Tushar, J. Cornelia, L. Chun-Yi, C. Ko-Ju, H. Thomas, and C. Yu-Jung

Interstellar ices form on dust grains in the coldest regions of molecular clouds and preserve key volatile reservoirs that could be incorporated into protoplanetary disks during star and planet formation. However, the effect of the dust surface composition on the ice structure and spectroscopic behavior remains poorly constrained. We present a comparative laboratory study of astrophysically relevant ices (CO, CO2, and H2O) deposited on inert calcium fluoride (CaF2) substrate and carbonaceous dust analogs under interstellar conditions. Infrared spectroscopy and temperature-programmed desorption reveal pronounced molecule-specific infrared spectral responses to the amorphous carbonaceous surface. CO and CO2 both exhibit broadened absorption bands, redshifted band positions, and delayed desorption, arising from thermally activated diffusion into the porous dust matrix and indicating strong molecule-surface interactions. By contrast,

H2O varies only very little spectrally and thermally, indicating weak wetting and limited coupling to the substrate. These results provide direct laboratory evidence that dust-ice interfaces can affect the ice structure and desorption kinetics of interstellar ices even in thick ice layers. These findings offer new constraints for interpreting infrared absorption bands in astronomical observations and highlight the importance of surface effects in models of interstellar ice chemistry.

A&A, 712, L16 (2026)
DOI: 10.1051/0004-6361/202661379
Full-text URL: https://arxiv.org/abs/2608.11729

Detection of a four-carbon sugar in interstellar space

Izaskun Jimenez-Serra, Juan Garcia de la Concepcion, Herma M. Cuppen, Marta Rey-Montejo, Miguel Sanz-Novo, Victor M. Rivilla, Jesus Martin-Pintado, Andres Megias, Carlos Briones, David San Andres, Laura Colzi, Shaoshan Zeng, Sergio Martin, Joseph Salaris, Antonio Martínez-Henares, Alvaro Lopez-Gallifa, Miguel Requena-Torres, Belen Tercero, Pablo de Vicente, Aran Insausti, Elena R. Alonso, Emilio J. Cocinero

Sugars are essential biomolecules, serving as metabolic fuels, nucleic acid backbone components, and structural or energy-storage polymers. A central question in origin-of-life research is how monosaccharides formed on the primitive Earth, as laboratory experiments under prebiotic conditions yield insufficient concentrations. The detection of ribose, glucose and other monosaccharides in asteroids and meteorites suggests an exogenous origin, possibly in the interstellar medium (ISM) prior to meteoritic parent-body formation. However, no sugar has been observed in the ISM so far. We report the discovery of erythrulose, a chiral four-carbon ketose, in the ISM. The detection has been achieved thanks to ultrasensitive, broadband spectral surveys toward the Galactic Center molecular cloud G+0.693-0.027 using the Yebes 40m and IRAM 30m telescopes. Erythrulose appears to be at least eight times more abundant than analogous three-carbon sugars, which remain undetected in our ultrasensitive observations. Quantum chemical and astrochemical models indicate that erythrulose forms efficiently on interstellar dust grains from simpler two-carbon aldehydes and alcohols. As ketoses readily isomerize into aldoses in aqueous conditions, interstellar erythrulose could have contributed to the sugar inventory available for early metabolic and replication processes.

Published in Nature Astronomy
DOI: 10.1038/s41550-026-02905-7
Full-text URL: https://arxiv.org/abs/2606.03313

Cycloalkanes and Aromatics on a Model Astrophysical Surface: Wetting, Dewetting and Thermal Desorption

Rushdi Senevirathne, Martin R. S. McCoustra

The interaction of small aromatic molecules (benzene and naphthalene), and of small cycloalkanes (cyclohexane and decalin), with an amorphous silica (aSiO2) surface as a model of interstellar silicate grain materials has been explored. Experimental studies of the interaction of cycloalkanes with the aSiO2 surface, employing temperature-programmed desorption to explore directly the binding of the adsorbates to the surface, are combined with data derived from previously published studies of the small aromatics. This reveals that, in the monolayer, the aromatic species wet the aSiO2 surface while the cycloalkanes tend to dewet. The results of a simple computational comparison of the two reported herein suggest that this behavior results from the donation of charge from the extended π electron structure on the aromatic molecule to Lewis acid Si sites on the aSiO2 surface forming a dative interaction and making these Si atoms hypervalent. Such behavior is not possible with the cycloalkanes and their interaction with the aSiO2 surface is dominated by weak van der Waals interactions. Reduction of the binding energy of the cycloalkanes compared to the aromatic sees the surface residence time of the former significantly reduced compared to the latter. We speculate as to the possible impact of the role of Lewis acid–base behavior in weakening the bonding in the aromatics consequently reducing the activation energy for their surface hydrogenation in a catalytic fashion.

2026, ACS Earth Space Chem.,ASAP
DOI: 10.1021/acsearthspacechem.6c00174
Full-text URL: https://pubs.acs.org/aesccq/article/doi/10.1021/acsearthspacechem.6c00174/5285249/Cycloalkanes-and-Aromatics-on-a-Model

A quantum chemical investigation of electro-optical properties and spectroscopic features of propargylimine

Pravi Mishra, Parmanand Pandey, Rachana Singh, Manisha Yadav, Shivani, Aftab Ahamad, Alka Misra, Poonam Tandon and Amritanshu Shukla

Propargylimine (HC≡CH–CH=NH), detected toward the Galactic Center molecular cloud G+0.693–0.027, is a potential a nitrogen-bearing 3C-atom species in prebiotic chemistry. In this study, we present a comprehensive computational investigation of its thermodynamics, reaction mechanism, electro-optical properties, global reactivity descriptors, and vibrational spectroscopic signatures. The formation of Z and E conformers of propargylimine was explored through radical–radical association pathway in the gas phase using density functional theory (DFT) (M06-2X/aug-cc-pVTZ), and benchmarked with CCSD(T)/aug-cc-pVTZ single-point calculations. Thermodynamic parameters, electro-optical properties, global reactivity descriptors, and molecular electrostatic potential surfaces were evaluated to assess its chemical stability

and detectability. The simulated infrared spectrum provides characteristic vibrational markers, particularly the C=N stretch at 1691.9 cm−1 and N–H stretching bands (∼3430–3447 cm−1), which may facilitate astronomical identification. UV absorption features and the electronic absorption properties of propargylimine were investigated using time-dependent (TD)-DFT. This work offers a theoretical framework for understanding its formation and spectroscopic features, reinforcing its role as a chemically robust molecule in the nitrogen-bearing chemistry and molecular complexity in Galactic Center molecular clouds.

Canadian Journal of Chemistry
DOI: 10.1139/cjc-2025-0198
Full-text URL: https://doi.org/10.1139/cjc-2025-0198

Ammonium salt formation and abundance in protoplanetary disks

Ruaud M., Loison J.-C., Gorti U.

Ammonium salts may represent an important reservoir of volatile species in Solar system primitive bodies, but the question of how and when these salts can form during the star formation process remains unknown. In this paper, we use thermo-chemical models to study the formation of ammonium salts during the protoplanetary disk stage. We show that ammonium salts form efficiently in the inner disk midplane (i.e. r <~ 50 au), inside the comet forming region. In this region, our model predicts that almost all the available nitrogen is in the form of salts (i.e. mainly in ammonium cyanate) at the surface of grains after evolving for 10 Myrs. For sulfur, we show that almost all the available S is in the form of ammonium hydrosulfide in the inner disk midplane. We show that inside r~ 30 au, ammonium salt formation is enhanced by a cosmic-ray-driven sink effect that progressively converts gas-phase CO and N2 into carbon dioxide and salts, respectively, at the surface of grains on a timescale >~ 1 Myr. This impacts the location of the CO and N2 radial snowlines which both shift closer to the star as a function of time.

Accepted for publication in ApJ
Full-text URL: https://arxiv.org/abs/2608.02173

A Chemical Inventory of the Disk around the Class 0 Protostar L1527 IRS with ALMA

Merel L.R. van 't Hoff, Łukasz Tychoniec, John J. Tobin, Daniel Harsono

Planet formation starts in disks that are still embedded within their natal envelopes. Here, we compile an extensive inventory of the chemical composition of the disk and envelope (< 3500 au) around the Class 0 protostar L1527 IRS. Using all publicly available ALMA (Atacama Large Millimeter/submillimeter Array) data, we report the detection of 39 molecules, including isotopologues. Of these, 22 are different molecular species and 28 are reported here for the first time toward L1527 in ALMA observations. CH3OH is the only complex organic molecule detected, while the hydrocarbon CH3CCH is the largest molecule detected. Overall, only a few programs are sensitive enough to detect emission unambiguously originating from the disk based on the kinematics. Nitrogen-bearing molecules are predominantly detected on more extended scales, while hydrocarbons show a distinct tail roughly along the southeastern outflow cavity wall, probably due to a stronger UV field in the eastern outflow lobe. The L1527 IRS protostellar system is not rich in sulfur-bearing molecules, with only strong emission observed for CS and SO. Overall, the envelope appears dominated by a carbon-rich chemistry, which seems to transition into an oxygen-rich chemistry in the disk. We calculate column densities of all detected species, providing a starting point to quantify the chemical diversity among young disks and the chemical evolution of the planet-forming material.

Accepted by Frontiers in Astronomy and Space Sciences. Special Issue: Birthplaces of Planets in Their Earliest Stages: Towards Characterization of Young Protostellar Disks
Full-text URL: https://arxiv.org/abs/2608.09627

Chemistry of Dark Molecular Clouds

Yuri Aikawa, Izaskun Jimenez-Serra, Paola Caselli

Recent molecular line surveys, particularly toward the starless core TMC-1 CP, have greatly expanded the inventory of interstellar molecules, revealing numerous isomers and even aromatic species. Their diverse formation pathways — from ion-molecule reactions to the possible fragmentation of carbonaceous grains — remain under debate, linking chemistry to the life cycle of the interstellar medium. Simple tracers such as carbon chains and deuterated ions are used to probe the physical conditions and evolutionary state of nearby filaments and cores, as well as in massive infrared dark clouds. Ice chemistry has also entered a new era with JWST: spatial distributions of ices indicate a connection between catastrophic freeze-out, established in the prestellar core L1544, and formation of complex organic molecules. Overall, TMC-1 CP and L1544 are not outliers but representative laboratories of molecular cloud physics and chemistry. Extending these findings across diverse environments, from the Central Molecular Zone to low-metallicity galaxies, is essential for a unified picture of how interstellar chemistry regulates the path from clouds to stars and planets.

Annual Review of Astronomy and Astrophysics 2026. 64:673-716
DOI: 10.1146/annurev-astro-051024-031607
Full-text URL: https://arxiv.org/abs/2607.25515

Announcements

4 Postdoctoral positions at INAF-Osservatorio Astrofisico di Arcetri within iSEEDs

Applications are now open for 4 postdoctoral positions (Incarico Post-Doc, fascia 2) at INAF - Arcetri Astrophysical Observatory (Florence, Italy) within the framework of the project “iSEEDs: Astrochemical Study of Early Embedded Disks” (FIS 2 Call - Ministerial Decree No. 1236 of 1 August 2023, grant FIS-2023-00170).
For further details about the project, please visit www.iseeds.inaf.it.

The four renewable, one-year positions are titled “From protostars to the Solar System and exoplanets: synergy between observations, chemistry, and data science”.

The full official announcement and details are available at the following links:
http://www.inaf.it/it/lavora-con-noi/incarichi-post-doc/2026inafincpos-oaa-fis2iseeds-006
https://www.inpa.gov.it/bandi-e-avvisi/dettaglio-bando-avviso/?concorso_id=85629b16128446fcba06bf8242f6850f

The application deadline is September 20, 2026.

The research activities will focus on:
- Characterising the physical and chemical properties of young disks with the ultimate goal of determining the initial conditions for planet formation.
- Exploiting the synergy between multi-wavelength observations, physical and astrochemical models, computational chemistry, and data science techniques to constrain fundamental disk properties and connect them to the formation of the Solar System and exoplanets.

Previous experience in star and planet formation and/or astrochemistry is preferred but not required, and a background in data science and machine learning techniques is also welcome.

For further details please contact eleonora.bianchi@inaf.it
[via Eleonora Bianchi]

Biennial European Astrobiology Conference (BEACON) 2027

The Biennial European Astrobiology Conference, BEACON 2027, will take place in Tartu, Estonia from 25-30 May 2027.

The last BEACON in Iceland (July2025) was a great success: With around 350 participants and over 400 submitted abstracts it was the largest astrobiology event in Europe for a very long time. A video of the Iceland conference can be watched at: https://youtu.be/sI6hlAquCHk.

There will be about 1 day devoted to astrochemistry-related talks, so there will be plenty of possibilities to present oral and poster contributions.

The conference will be organised in the modern Vanemuise Conference and Concert Hall in central Tartu. We will also organise conference excursions to geologically interesting sites (impact craters, ice age features, sandstone caves) and cultural monuments. We will also organise an after-conference outing to the very interesting islands of Saaremaa and Hiumaa as well as public engagement activities. Tartu is a charming university town and everything (venue, hotels, restaurants, old city) See https://www.visittartu.ee.

The conference hotel (Hotel Dorpat) has a direct (every 30 minutes) connection with modern and comfortable buses to the well-organised and modern Tallinn airport from which direct flights operate to many European cities.

Please mark the dates in your calendar. For other information see the preliminary website of the event:
https://europeanastrobiology.eu/beacon-2027-landing/

[via Wolf Geppert]

PhD position in astrochemistry and machine learning at University College Dublin

We invite applications for a PhD position in astrochemistry and machine learning at the School of Physics at University College Dublin, Ireland. You will work with Dr Marie Van de Sande on the ERC Starting Grant ASHES on dust formation in the outflows of asymptotic giant branch (AGB) stars.

Project background:
Stars like our Sun will go through an AGB phase near the end of their lives, losing their outer layers by means of a stellar outflow and enriching the interstellar medium with the building blocks for the next generation of stars and planets. To study how the chemistry is affected by the dynamics of the outflow, 3D hydrochemical models are essential. Machine learning is crucial to make this possible: by emulating, rather than calculating the chemistry, an on-the-fly hydrochemical model can finally be built.

What you will do:
You will optimise the proof-of-concept emulator MACE by postprocessing Phantom SPH models of AGB binary interactions. While generating the training dataset using snapshot models, you will already be able to determine how different binaries affect the outflow’s chemistry. Coupling the emulator to Phantom, your on-the-fly hydrochemical model will then

demonstrate how chemistry is affected by the dynamics. In the next stage, you will train the emulator on a novel chemical reaction network that includes dust formation. This will give us the first 3D and time-dependent overview of how dust formation is affected by AGB stars and their companions.

As part of ASHES, you will interact with all aspects of astrochemistry: chemistry, computational modelling, and astronomical observations. You will start alongside another PhD student, with two postdocs joining the group later. There are ample opportunities for attending conferences, workshops, and research stays.

Who we are looking for:
The project is suitable for a student with a degree in physics or astronomy and a genuine interest in building skills in coding (Python and Fortran), machine learning, data analysis, and visualisation. Prior experience in chemical modelling or hydrodynamical modelling is a strong advantage, but not a strict requirement.

Application instructions:
Applications should include a CV (including personal data, education, skills, and expertise), a one-page motivation letter, and the names and contact details of two references. Please send the documents to marie.vandesande@ucd.ie before 1 October 2026.

More information: https://marievds.github.io/jobs.html

[via Marie Van de Sande]

Two PhD positions in experimental astrochemistry at Aarhus University, Denmark

PhD #1 in Astrochemistry:
Laboratory Studies of Radiation-Driven Chemistry and Desorption in Interstellar Ices
We invite applications for a PhD position in experimental astrochemistry at the Department of Physics and Astronomy at Aarhus University, Denmark. You will work with Associate Professor Sergio Ioppolo on the DFF-Research Project 2 BRIDGE: From Laboratory Ices to Astronomical Observations, investigating how radiation and thermal processing shape the chemistry of interstellar ices and the molecules released from them. The project is carried out in close collaboration with Professor Jes Kristian Jørgensen at the University of Copenhagen and will connect laboratory measurements directly with JWST and ALMA observations.

Position details
• Fully funded PhD position
• Based at Aarhus University, Denmark
• Earliest start date: February 2027
• Applications open: 1 September 2026
• Application deadline: 1 November 2026

Project background
Interstellar dust grains are coated by icy mantles that act as tiny chemical laboratories in the coldest regions of space. Atoms and simple molecules accrete onto these grains, react and form increasingly complex species that can later be released into the gas as stars and planets form. JWST now provides unprecedented information on the composition and structure of interstellar ices, while ALMA maps related gas-phase molecules at high spatial and spectral resolution. Connecting these observations, however, requires laboratory measurements of how realistic interstellar ices respond to radiation and heating. The BRIDGE project will establish this connection by combining laboratory astrochemistry at Aarhus University with irradiation experiments at international facilities and JWST and ALMA observations at the University of Copenhagen.

What you will do
You will investigate the formation, processing and desorption of interstellar-ice analogues under astrophysically relevant conditions using the Red Chamber, an ultrahigh-vacuum cryogenic setup at Aarhus University. You will prepare pure, layered and mixed molecular ices at temperatures of approximately 10-20 K, beginning with benchmark species such as H2O, CO, CO2 and CH3OH and progressing to selected complex organic molecules and N- and S-bearing species. You will combine FTIR spectroscopy, cryogenic quartz-crystal microbalance measurements, optical interferometry and time-resolved quadrupole mass spectrometry to determine ice spectra, optical properties, densities and thermal and non-thermal desorption behaviour. Experiments at Aarhus University and the ASTRID2 synchrotron will investigate UV- and electron-driven processing, while short experimental campaigns at HUN-REN Atomki in Hungary will extend the project to keV–MeV ion irradiation as laboratory analogues of solar particles and cosmic rays.

Together with Professor Jes Jørgensen and the BRIDGE observational PhD student at the University of Copenhagen, you will connect the laboratory spectral and desorption measurements with JWST and ALMA observations. The project will ultimately produce open spectral and desorption libraries and investigate whether the chemical diversity observed around forming stars originates directly from processed interstellar ices or requires additional gas-phase chemistry. As part of BRIDGE, you will work at the interface of chemistry, physics and astronomy and interact closely with both laboratory and observational astrochemists. There will be opportunities for international experimental campaigns, research visits, conferences, workshops and summer schools, as well as close collaboration between Aarhus University, the University of Copenhagen and HUN-REN Atomki.

Who we are looking for
The project is suitable for applicants with a background in physics, chemistry, astronomy, nanoscience or a related field and a strong interest in experimental astrochemistry. Applicants should have a relevant Master's degree or meet the alternative GSNS admission requirements for applicants who have completed at least one year of a Master's programme. Experience with ultrahigh vacuum, cryogenic experiments, FTIR spectroscopy, mass spectrometry, surface science, laboratory astrochemistry, optical analysis or scientific programming is an advantage, but is not a strict requirement. Training will be provided. We are particularly looking for a candidate who enjoys experimental design, careful data acquisition, quantitative analysis and interdisciplinary collaboration.

Application instructions
Applications must be submitted through the Graduate School of Natural Sciences (GSNS), Aarhus University, under the November 2026 specific call for Physics and Astronomy. The application portal opens on 1 September 2026, and the deadline is 1 November 2026 at 23:59 CET. Applications should include the documentation required by GSNS, including a CV, academic transcripts and diplomas, grade-point-average information, at least one reference and a motivation statement. For this specific project, applicants should use the PhD announcement as their project description. For more information see link here: https://phd.nat.au.dk/for-applicants.

Inquiries
For questions about the project, please contact Associate Professor Sergio Ioppolo at s.ioppolo@phys.au.dk.

PhD #2 in Astrochemistry:
Infrared-Driven Energy Dissipation and Structural Change in Complex Interstellar Ices We invite applications for a PhD position in experimental astrochemistry at the Department of Physics and Astronomy and the Center for Interstellar Catalysis (InterCat) at Aarhus University, Denmark. You will work with Associate Professor Sergio Ioppolo and Professor Herma Cuppen on infrared-driven energy dissipation and structural change in complex interstellar ices, as part of the second funding period of the Center of Excellence for Interstellar Catalysis (InterCat2).

Position details
• Funded PhD position
• Based at Aarhus University, Denmark
• Research stays at HFML-FELIX in Nijmegen, the Netherlands
• Earliest start date: February 2027
• Applications open: 1 September 2026
• Application deadline: 1 November 2026

Project background
Interstellar dust grains are coated by molecular ices that evolve as material moves from cold molecular clouds toward star- and planet-forming regions. These ices are chemically and structurally complex: abundant species such as H2O, CO and CO2 coexist with complex organic molecules, aromatic species, carbon chains and potentially molecular building blocks of life. Infrared radiation can deposit vibrational energy into these icy grains, but we still do not understand how this energy moves through chemically complex ices, how the local molecular environment controls energy dissipation, or under which conditions infrared excitation causes restructuring, segregation or molecular desorption. Understanding these processes is increasingly important for interpreting observations from the James Webb Space Telescope (JWST), which is revealing the composition and structure of interstellar ices in unprecedented detail.

What you will do
You will experimentally investigate how infrared radiation interacts with astrophysically relevant molecular ices under ultrahigh-vacuum and cryogenic conditions. You will prepare mixed interstellar-ice analogues containing major ice components such as H2O, CO and CO2 together with minority species including methanol, aromatic and carbon-chain molecules, and selected amino acids. Using infrared spectroscopy and mass spectrometry, you will determine how ice composition, molecular environment and excitation wavelength influence vibrational energy dissipation, structural rearrangement, segregation and molecular desorption. A central part of the project will involve targeted experimental campaigns at the LISA end station of HFML-FELIX in Nijmegen, the Netherlands, where intense and wavelength-selective infrared radiation will be used to excite individual vibrational modes in the ice. Complementary experiments, sample preparation and data analysis will be performed at Aarhus University.

You will work closely with Professor Herma Cuppen and collaborators developing molecular-dynamics and machine-learning models of complex interstellar ices. The combination of experiment and theory will provide a molecular-level interpretation of how absorbed infrared energy is redistributed through realistic icy environments. The resulting laboratory spectra will also support the interpretation of JWST observations of interstellar ices, and validated spectral data will be contributed to the Leiden Ice Database for Astrochemistry (LIDA) or equivalent open databases. As part of InterCat2, you will join an interdisciplinary and international research environment bringing together laboratory astrochemistry, surface science, computational chemistry, machine learning and astronomical observations. InterCat collaborators work across Aarhus University, the University of Copenhagen, Leiden University and several international facilities. The project therefore offers opportunities for international research stays, experimental campaigns, conferences, workshops and close interaction with both experimental and theoretical astrochemists.

Who we are looking for
The project is suitable for applicants with a background in physics, chemistry, astronomy, nanoscience or a related field and a strong interest in experimental astrochemistry. Applicants should have a relevant Master's degree or meet the alternative GSNS admission requirements for applicants who have completed at least one year of a Master's programme. Experience with ultrahigh vacuum, cryogenic experiments, infrared spectroscopy, mass spectrometry, surface science, laboratory astrochemistry or scientific programming is an advantage, but is not a strict requirement. Training will be provided. We are particularly looking for a candidate who enjoys careful experimental work, quantitative data analysis and collaboration across disciplines. The project requires short research stays at HFML-FELIX in Nijmegen, the Netherlands.

Application instructions
Applications must be submitted through the Graduate School of Natural Sciences (GSNS), Aarhus University, under the November 2026 specific call for Physics and Astronomy. The application portal opens on 1 September 2026, and the application deadline is 1 November 2026 at 23:59. For this specific project, applicants should use the PhD announcement as their project description and submit the remaining documentation required by GSNS. For more information see link here: https://phd.nat.au.dk/for-applicants.

Inquiries
For questions about the project, please contact Associate Professor Sergio Ioppolo at s.ioppolo@phys.au.dk.

[via Sergio Ioppolo]