AstroChemical Newsletter #111

March 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

Redistribution of ices between grain populations in protostellar envelopes. Only the coldest grains get ices

J. Kalvans

Context. Matter that falls onto a protoplanetary disk (PPD) from a protostellar envelope is heated before it cools again. This induces sublimation and subsequent re-adsorption of ices that accumulated during the prestellar phase. Aims. We explore the fate of ices on multiple-sized dust grains in a parcel of infalling matter. Methods. A comprehensive kinetic chemical model using five grain-size bins with different temperatures was applied for an infalling parcel. The parcel was heated to 150 K and then cooled over a total timescale of 20 kyr. Effects on ice loss and re-accumulation by the changed gas density, the maximum temperature, the irradiation intensity, the size-dependent grain temperature trend, and the distribution of the ice mass among the grain-size bins were investigated. Results. A massive selective redistribution of ices exclusively onto the surface of the coldest grain-size bin occurs in all models. The redistribution starts already during the heating stage, where ices that are sublimated from warmer grains re-adsorb onto colder grains before complete sublimation. During the cooling stage, the sublimated molecules re-freeze again onto the coldest grains. In the case of full sublimation, this re-adsorption is delayed and occurs at lower temperatures because a bare grain surface has lower molecular desorption energies in our model. Conclusions. Most protostellar envelope grains enter the PPD ice poor (bare). Ices are carried by a single coldest grain-size bin, here representing 12 % of the total grain surface area. This bare ice-grain dualism can affect the rate of the grain coagulation. The ice components are stratified on the grains according to their sublimation temperatures.

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DOI: 10.1051/0004-6361/202452526
Full-text URL: https://arxiv.org/abs/2501.15609

Effects of the grain temperature distribution on the organic chemistry of protostellar envelopes

Juris Kalvāns, Juris Freimanis

Context. Dust grains in circumstellar envelopes are likely to have a spread-out temperature distribution. Aims. We investigate how trends in the temperature distribution between small and large grains affect the hot-corino chemistry of complex organic molecules (COMs) and warm carbon-chain chemistry (WCCC). Methods. A multi-grain multi-layer astrochemical code with an advanced treatment of the surface chemistry was used with three grain-temperature trends: a grain temperature proportional to the grain radius to the power -1/6 (Model M-1/6), to 0 (M0), and to 1/6 (M1/6). The cases of hot-corino chemistry and WCCC were investigated for a total of six models. The essence of these changes is that the main ice reservoir (small grains) has a higher (M-1/6) or lower (M1/6) temperature than the surrounding gas. Results. The chemistry of COMs agrees better with observations in models M-1/6 and M1/6 than in Model M0. Model M-1/6 agrees best for WCCC because earlier mass-evaporation of methane ice from small grains induces the WCCC phenomenon at lower temperatures. Conclusions. Models considering several grain populations with different temperatures reproduce the circumstellar chemistry more precisely.

Astronomy & Astrophysics, Volume 692, id.A261
DOI: 10.1051/0004-6361/202451858
Full-text URL: https://arxiv.org/abs/2410.02346

Detection of thioacetaldehyde (CH3CHS) in TMC-1: sulfur-oxygen differentiation along the hydrogenation sequence

M. Agundez, G. Molpeceres, C. Cabezas, N. Marcelino, B. Tercero, R. Fuentetaja, P. de Vicente, J. Cernicharo

In recent years the chemistry of sulfur in the interstellar medium has experienced a renewed interest due to the detection of a large variety of molecules containing sulfur. Here we report the first identification in space of a new S-bearing molecule, thioacetaldehyde (CH3CHS), which is the sulfur counterpart of acetaldehyde (CH3CHO). The astronomical observations are part of QUIJOTE, a Yebes 40m Q band line survey of the cold dense cloud TMC-1. We detected seven individual lines corresponding to A and E components of the four most favorable rotational transitions of CH3CHS covered in the Q band (31.0-50.3 GHz). Assuming a rotational temperature of 9 K, we derive a column density of 9.8e10 cm-2 for CH3CHS, which implies that it is 36 times less abundant than its oxygen counterpart CH3CHO. By comparing the column densities of the O- and S-bearing molecules detected in TMC-1, we find that as molecules increase their degree of hydrogenation, sulfur-bearing molecules become less abundant compared to their oxygen analog. That is, hydrogenation seems to be less favored for S-bearing molecules than for O-bearing ones in cold sources like TMC-1. We explored potential formation pathways to CH3CHS and implemented them into a chemical model, which however underestimates by several orders of magnitude the observed abundance of thioacetaldehyde. Quantum chemical calculations carried out for one of the potential formation pathways, the S + C2H5 reaction, indicate that formation of CH3CHS is only a minor channel in this reaction.

A&A, 693, L20
DOI: 10.1051/0004-6361/202453459
Full-text URL: https://arxiv.org/abs/2501.05125v1

Identification of the interstellar 1-cyano propargyl radical (HCCCHCN) in TMC-1

C. Cabezas, M. Agúndez, N. Marcelino, C.H. Chang, R. Fuentetaja, B. Tercero, M. Nakajima, Y. Endo, P. de Vicente, J. Cernicharo

We report the first detection in interstellar medium of the 1-cyano propargyl radical, HC3HCN. This species is an isomer of the 3-cyano propargyl radical (CH2C3N), which was recently discovered in TMC-1. The 1-cyano propargyl radical was observed in the cold dark cloud TMC-1 using data from the ongoing QUIJOTE line survey, which is being carried out with the Yebes 40m telescope. A total of seven rotational transitions with multiple hyperfine components were detected in the 31.0-50.4 GHz range. We derived a column density of (2.2±0.2)e11 cm-2 and a rotational temperature of 7±1K. The abundance ratio between HC3HCN and CH2C3N is 1.4. The almost equal abundance of these isomers indicates that the two species may be produced in the same reaction with a similar efficiency, probably in the reaction C + CH2CHCN and perhaps also in the reaction C2 + CH3CN and the dissociative recombination with electrons of CH2C3NH+.

A&A, 693, L14
DOI: 10.1051/0004-6361/202453419
Full-text URL: https://arxiv.org/abs/2501.01938

Correlation between formaldehyde and methanol in prestellar cores

A. F. Punanova, K. Borshcheva, G. S. Fedoseev, P. Caselli, D. S. Wiebe, A. I. Vasyunin

Formaldehyde is a key precursor in the formation routes of many complex organic molecules (COMs) in space. It is also an intermediate step in CO hydrogenation sequence that leads to methanol formation on the surface of interstellar grains in cold dense prestellar cores where pristine ices are formed. Various chemical models successfully reproduce the COMs abundances in cold cores, however, they consistently overpredict the abundance of formaldehyde by an order of magnitude. This results in an inverse H2CO:CH3OH abundance ratios obtained in the astrochemical simulations as compared to the observed values. In this work, we present a homogeneous data set of formaldehyde observational maps obtained towards seven dense cores in the L1495 filament with the IRAM 30 m telescope. Resolving the spatial distribution of the molecules is essential to test the chemical models. We carefully estimate the formaldehyde column densities and abundances to put reliable observational constraints on the chemical models of cold cores. Through numerous tests, we aim to constrain the updated chemical model MONACO to better align with the observed formaldehyde abundance and its ratio to methanol. In particular, we elaborate on the branching ratio of the CH3 + O reaction at low temperatures. The revised MONACO model reproduces abundances of both methanol and formaldehyde within an order of magnitude. However the model tends to overproduce formaldehyde and underpredict methanol. Consequently, the model systematically overestimates the H2CO:CH3OH ratio, although it remains within an order of magnitude of the values derived from observations.

Accepted for publication in MNRAS
DOI: 10.1093/mnras/staf214
Full-text URL: https://arxiv.org/abs/2502.00538

On the abiotic origin of dimethyl sulfide: discovery of DMS in the Interstellar Medium

M. Sanz-Novo, V. M. Rivilla, C. P. Endres, V. Lattanzi, I. Jiménez-Serra, L. Colzi, S. Zeng, A. López-Gallifa, A. Megías, A. Martínez-Henares, D. San Andrés, B. Tercero, P. de Vicente, S. Martín, M.A. Requena-Torres, P. Caselli and J. Martín-Pintado

Following the discovery of dimethyl sulfide (CH3SCH3, DMS) signatures in comet 67P/Churyumov-Gerasimenko, we report the first detection of this organosulfur species in the interstellar medium, during the exploration of an ultradeep molecular line survey performed toward the Galactic Center molecular cloud G+0.693-0.027 with the Yebes 40m and IRAM 30m telescopes. We derive a molecular column density of N = (2.6 ± 0.3)×1e13 cm−2, yielding a fractional abundance relative to H2 of ∼1.9e−10. This implies that DMS is a factor of ∼1.6 times less abundant than its structural isomer CH3CH2SH and ∼30 times less abundant than its O-analogue dimethyl ether (CH3OCH3) toward this cloud, in excellent agreement with previous results on various O/S pairs. Furthermore, we find a remarkable resemblance between the relative abundance of DMS/CH3OH in G+0.693-0.027 (∼1.7e−3) and in the comet (∼1.3e−3). Although the chemistry of DMS beyond Earth is yet to be fully disclosed, this discovery provides conclusive observational evidence on its efficient abiotic production in the interstellar medium, casting doubts about using DMS as a reliable biomarker in exoplanet science.

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DOI: 10.3847/2041-8213/adafa7
Full-text URL: https://arxiv.org/abs/2501.08892

Reevaluation of ALMA detection of circumstellar PH3 in the AGB envelope IRC+10216: evidence

for misidentification with HCN

M. Agundez, L. Velilla-Prieto, J. P. Fonfria, J. Cernicharo

The article "Confirmation of interstellar phosphine towards asymptotic giant branch star IRC+10216" by A. Manna and S. Pal uses ALMA data of the C-star envelope IRC+10216 to claim a confirmation of the detection of PH3 in this source. The article however incorrectly assign an emission feature observed in the ALMA spectrum of IRC+10216 to PH3, while we find that it arises from a highly vibrationally excited state of HCN. Concretely the feature can be confidently assigned to the J=3-2 l=0 transition of HCN in the v1+4v2 vibrational state based on the observation of the l=+2 and l=-2 components of the same rotational transition, J=3-2, with the observed relative intensities in agreement with the relative line strengths. The detection of PH3 in IRC+10216 remains confirmed based on the observation of the J=1-0 and J=2-1 lines with the single-dish telescopes IRAM-30m, ARO SMT-10m, and Herschel (Agundez et al. 2008, 2014; Tenenbaum et al. 2008).

Response to the article published by A. Manna and S. Pal entitled "Confirmation of interstellar phosphine towards asymptotic giant branch star IRC+10216". Accepted for publication in Journal Of Astrophysics and Astronomy
Full-text URL: https://arxiv.org/abs/2502.02276

ALMA reveals thermal and non-thermal desorption of methanol ice in the HD 100546 protoplanetary disk

L. Evans, A. S. Booth, C. Walsh, J. D. Ilee, L. Keyte, C. J. Law, M. Leemker, S. Notsu, K. Öberg, M. Temmink, N. van der Marel

Methanol (CH3OH) and formaldehyde (H2CO) are chemically coupled organic molecules proposed to act as an intermediate step between simple molecules and more complex prebiotic compounds. Their abundance distributions across disks regulate the prebiotic potential of material at different disk radii. We present observations of multiple methanol and formaldehyde transitions toward the Herbig Ae disk HD 100546 obtained with ALMA, building upon the previous serendipitous detection of methanol in this source. We find that methanol has a higher rotational temperature (Trot) than formaldehyde towards both the centrally concentrated emission component in the inner disk (0-110 au) and a radially separate dust ring farther out in the disk (180-260 au). Trot decreases for methanol and formaldehyde from the inner (152(+35)(-27) K and 76(+9)(-8) K) to the outer disk (52(+8)(-6) K and 31(+2)(-2) K), suggesting that we are tracing two different chemical environments. Trot for both species in the inner disk is consistent with thermal desorption as the origin, while the outer disk reservoir is driven by non-thermal desorption. The CH3OH/H2CO column density ratio decreases from 14.6(+5.2)(-4.6) in the inner disk to 1.3(+0.3)(-0.2) in the outer disk, consistent with modelling predictions. The CH3OH/H2CO column density ratio for the inner disk is consistent with the median value in the range of column density ratios compiled from Solar System comets which would have formed at a similar distance. This supports the notion that interstellar ice is inherited and preserved by protoplanetary disks around solar-mass and intermediate-mass stars as we are seeing 'fresh' ice sublimation, as well as providing more evidence for the presence of prebiotic precursor molecules in planet-forming regions.

Accepted in The Astrophysical Journal
Full-text URL: https://arxiv.org/abs/2502.04957

Ly-α processing of solid-state Ethanolamine: Potential Precursors to Sugar and Peptide Derivatives

T. Suhasaria, S. M. Wee, R. Basalgete, S. Krasnokutski, C. Jaeger, K. Schwarz, and Th. Henning

Ethanolamine (EA), a key component of phospholipids, has recently been detected in the interstellar medium within molecular clouds. To understand this observation, laboratory studies of its formation and destruction are essential and should be complemented by astrochemical models. This study investigates the photostability of EA ice under Lyman (Ly)-α (10.2 eV) irradiation at 10 K, and explores its potential role in the formation of simple and complex organic molecules in molecular clouds. The UV destruction cross section of EA was estimated to be (4.7 ± 0.3) × 1e-18 cm-2, providing insight into its half-life of 6.5e7 yr in dense interstellar clouds. Fourier transform infrared spectroscopy and quadrupole mass spectrometry were used to identify various photoproducts, with their formation pathways discussed. Ethylene glycol and serine were tentatively detected during the warming up process following irradiation, suggesting that EA could contribute to the formation of prebiotic molecules such as sugars, peptides and their derivatives. High mass signals detected in the mass spectrometer suggest the presence of several complex organic molecules, and further analysis of residues at room temperature is planned for future work. The results suggest that EA could contribute to the formation of prebiotic molecules in space, with implications for the origin of life.

Accepted in The Astrophysical Journal
Full-text URL: https://arxiv.org/abs/2502.07970

Modelling methanol and hydride formation in the JWST Ice Age era

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(Abridged) JWST observations have measured the ice composition toward two highly-extinguished field stars in the

Chamaeleon I cloud. The observed extinction excess on the long-wavelength side of the H2O ice band at 3 micron has been attributed to a mixture of CH3OH with ammonia hydrates, which suggests that CH3OH ice could have formed in a water-rich environment with little CO depletion. Laboratory experiments and quantum chemical calculations suggest that CH3OH could form via the grain surface reactions CH3+OH and/or C+H2O in water-rich ices. However, no dedicated chemical modelling has been carried out thus far to test their efficiency and dependence on the astrochemical code employed. We model the ice chemistry in the Chamaeleon I cloud using a set of astrochemical codes (MAGICKAL, MONACO, Nautilus, UCLCHEM, and KMC simulations) to test the effects of the different code architectures and of the assumed ice chemistry. Our models show that the JWST ice observations are better reproduced for gas densities >1e5 cm-3 and collapse times >1e5 yr. CH3OH ice forms predominantly (>99%) via CO hydrogenation. The contribution of reactions CH3+OH and C+H2O, is negligible. The CO2 ice may form either via CO+OH or CO+O depending on the code. However, KMC simulations reveal that both mechanisms are efficient despite the low rate constant of the CO+O surface reaction. CH4 is largely underproduced for all codes except for UCLCHEM, for which a higher amount of atomic C is available during the initial translucent cloud phase. Large differences in the ice abundances are found at Tdust<12 K between diffusive and non-diffusive chemistry codes. This is due to the fact that non-diffusive chemistry takes over diffusive chemistry at such low Tdust. This could explain the rather constant ice chemical composition found in Chamaeleon I and other dense cores despite the different visual extinctions probed.

Accepted in A&A
Full-text URL: https://arxiv.org/abs/2502.10123

Predicting the detectability of sulphur-bearing molecules in the solid phase with simulated spectra of JWST instruments

A. Taillard, R. Martín-Doménech, H. Carrascosa, J.A. Noble, G.M. Muñoz Caro, E. Dartois, D. Navarro-Almaida, B. Escribano, A. Sanchez-Monge, A. Fuente

(Abridged) To date, gas phase observations of sulphur in dense interstellar environments have only constrained the molecular carriers of 1% of its predicted cosmic abundance. An additional 5% is known to be locked up in molecular solids in dense clouds, leaving the main reservoir of depleted sulphur in the solid phase unknown. The spectral resolution and sensitivity of the JWST could make a substantial difference in detecting part of this missing sulphur, with its wavelength coverage that includes vibrational absorption features of the S-carriers H2S, OCS, SO2, CS2, SO, CS, and S8. The aim of this study is to determine whether these molecules may be viable candidates for detection. We carried out new laboratory measurements of the IR absorption spectra of CS2 and S8 to update the IR band strength of the most intense CS2 absorption feature at 6.8 {\mu}m, as well as to determine that of S8 at 20.3 {\mu}m for the first time. These data, along with values previously reported in the literature, allow us to evaluate which S-bearing species could be potentially detected with JWST in interstellar ices. Taking the literature abundances of the major ice species determined by previous IR observations towards starless cores, LYSOs and MYSOs, we generated simulated IR spectra using the characteristics of the instruments on the JWST. Thus, we have been able to establish a case study for three stages of the star formation process. We conclude that the detection of S-bearing molecules remains challenging. Despite these obstacles, the detection of H2S and potentially SO2 should be possible in regions with favourable physical and chemical conditions. In contrast, S8 would remain undetected. Although the sensitivity of JWST is insufficient to determine the sulphur budget in the solid state, the detection of an additional icy sulphur compound (H2S, SO2) would enable us to elevate our knowledge of sulphur chemistry.

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DOI: 10.1051/0004-6361/202452900
Full-text URL: https://arxiv.org/abs/2502.09384

Announcements

Association of Radiation Research Conference 2025 - Keswick, June 9-11

When? 9 - 11 June 2025
Where ? Lodore Falls Hotel & Spa, Keswick

https://uobevents.eventsair.com/arr-2025/

We are very pleased to invite you to the Association for Radiation Research (ARR) meeting for 2025 near Keswick, Cumbria. The meeting will cover a whole breadth of topics related to radiation research and will provide a fantastic platform for interdisciplinary learning and development of collaborations with the radiation research community in the UK. We will have exciting talks from experts in their field, as well as opportunities for early career researchers to present through talks and posters. There will be great opportunities to network between junior and senior researchers, and to provide an inclusive interdisciplinary environment enabling the exchange of results and new ideas through social events, including the conference dinner.
Topics to be covered during the conference:

- Medical Isotopes
- Radiotherapy
- Clinical/Translational
- Space
- Radiation protection

- Nuclear/Radiation Chemistry & Physics
- Radiation Biology/DNA Damage Repair

Key Dates
- Abstract Submission Deadline - 16th March 2025
- Abstract Notification - 20th March 2025
- Early Bird Registration Deadline - 31st March 2025
- Standard Registration Deadline - 21st May 2025

Scientific Committee
- Dr Ruth Edge (Chair, Dalton Cumbrian Facility, The University of Manchester)
- Professor Fred Currell (Dalton Cumbrian Facility, The University of Manchester)
- Dr Alex Baidak (Dalton Cumbrian Facility, The University of Manchester)
- Professor Jason Parsons (University of Birmingham)
- Professor Jonathan Coulter (Queen’s University Belfast)

Postdoctoral Position Available at HUN-REN ATOMKI

A two-year postdoctoral position in experimental astrochemistry is available in the Space Chemistry Group at the HUN-REN Atommagkutató Intézet (ATOMKI), under the direction of PI Prof. Nigel J. Mason.

You will join an active and growing team of researchers having expertise in various aspects of molecular astrophysics, who are developing and making use of a suite of experimental systems to study ion and electron collision-induced molecular destruction, synthesis, and sputtering in astrophysical ice analogues. Some examples of our group’s recent research interests include investigating the role of sulphur ions in the surface chemistry of the Galilean moons of Jupiter, and the energetic synthesis of biomolecules from simple precursors; thereby coupling astrochemistry with planetary science and astrobiology.

Your research project will investigate key questions in experimental astrochemistry; particularly:
(1) How does the morphology of ice depend on the conditions under which it is formed? How is this morphology changed by temperature cycling?
(2) How does the morphology of the ice influence its radiation-induced destruction and the associated formation of new molecules?

These experiments will be combined with simulations of such processes to test the validity of laboratory experiments with actual astrophysical conditions.

The work forms part of a wider astrochemistry and planetary science programme involving collaborations across Europe and beyond. You will, therefore, also participate in joint projects with visitors to ATOMKI and conduct experiments in partner laboratories.

The ideal candidate will have a PhD degree (or equivalent) in physics, chemistry, materials science, engineering, or a related discipline. Previous experience with ultrahigh-vacuum chambers and spectroscopic techniques (e.g., FTIR, UV-vis, Raman) is necessary. Previous knowledge of astrochemistry, planetary science, and / or astrobiology is highly desirable. Previous publications in the field are not necessary but are advantageous. The candidate must be fluent in spoken and written English, although knowledge of Hungarian is not expected. The successful candidate will be offered support and encouragement to pursue further postdoctoral fellowships and funding schemes.

Interested candidates are kindly invited to apply for the position by contacting Prof. Nigel J. Mason directly (n.j.mason@atomki.hu) with a CV (resume) and a short cover letter. Applicants should also cc Dr Zoltán Juhász (zjuhasz@atomki.hu), Dr Béla Sulik (sulik@atomki.hu), and Dr Duncan V. Mifsud (mifsud.duncan@atomki.hu) in their initial email. Applications will be accepted until Friday, 4th April 2025 at 17:00 CET. Shortlisted candidates will be invited to an online interview that will take place in mid-April, with the successful candidate being notified shortly thereafter.

ATOMKI is located in Debrecen, Hungary’s second-largest city. The Institute was founded in 1954 by Sándor Szalay; a pioneer in the field of nuclear physics. Today, ATOMKI is Hungary’s national accelerator centre and has an international reputation for excellence in the fields of particle, nuclear, atomic, and molecular physics; as well as ion beam analytics, environmental science, and cultural heritage science. The Institute hosts a suite of accelerators that can be used as a Solar Wind Simulator, since they are able to provide a wide selection of ions having energies analogous to the solar wind and galactic cosmic rays (300 eV – 30 MeV).