AstroChemical Newsletter #118

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Abstracts

Pristine ices in a planet-forming disk revealed by heavy water

Margot Leemker, John J. Tobin, Stefano Facchini, Pietro Curone, Alice S. Booth, Kenji Furuya, Merel L. R. van 't Hoff

Water is essential to our understanding of the planet-formation process and habitability on Earth. Although trace amounts of water are seen across all phases of star and planet formation, the bulk of the water reservoir often goes undetected, hiding crucial parts of its journey from giant molecular clouds to planets. This raises the question of whether water molecules in comets and (exo-)planets is largely inherited from the interstellar medium or if the water molecules are destroyed and then reformed in the disk. Water isotopologue ratios involving doubly deuterated water (D2O) are a sensitive tracer to answer this question. We present strong evidence of inheritance through an enhancement of D2O in the outbursting V883 Ori disk. The high D2O/H2O ratio of $(3.2\pm1.2)\times1e5$ is consistent with values seen in protostellar envelopes and a comet and is two orders of magnitude higher than expected if water is reprocessed. The high deuteration of the heaviest isotopologues D2O/HDO = $(2.3\pm1.0)\timesHDO/H2O$ further establishes the inheritance of water. We conclude that water ice in disks originates from the earliest phases of star formation, providing the missing link between cold dark clouds and (exo-)comets.

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Anatomy of the Class I protostar L1489 IRS with NOEMA - II. A disk replenished by a massive streamer

M. Tanious, R. Le Gal, A. Faure, S. Maret, A. López-Sepulcre, P. Hily-Blant

(abridged) Streamers are newly identified channels that transport mass from large, molecular-cloud scales down to small, protoplanetary-disk scales. To better understand their impact on planet formation, it is essential to study their physical and chemical properties. In this framework, we aim to characterize the longest streamer identified in carbon chain emission within the Class I system L1489 IRS, connecting the nearby prestellar core L1489 to the young stellar object (YSO). We observed multiple transitions of C2H, ortho-c-C3H2, and HC3N in L1489 IRS with NOEMA and IRAM-30m at 3mm and 2mm. Using a variety of radiative transfer methods, including a hyperfine structure (HFS) fitting, rotational diagrams, and proposing a new self-consistent Markov chain Monte Carlo (MCMC) approach combined with the non-LTE RADEX code, we derived the column densities and abundances of those molecules, as well as the H2 number density along the streamer. This enabled us to estimate its mass, infall rate, and its impact on the {star+disk} system's mass. We found lower limits on the streamer mass of \geq (4.67-18.3)e-3 M dot (i.e., \geq 0.65-2.57 times the current disk mass) and an infall rate of \geq (1.94-7.57)e-7 \$M dot\$ yr-1, where the ranges correspond to the different molecular tracers. These values are consistent with those derived in similar Class I objects. This suggests that the disk could be fully replenished by streamer material. Given its mass, the streamer is likely at the origin of the external warped disk seen in this system, as predicted by numerical simulations. Moreover, the first investigations based on the C2H/c-C3H2 and HC3N/c-C3H2 abundance ratios suggest that the streamer chemistry may be inherited from the core. These results suggest, for the first time, that the chemical composition of a Class I object is [...]

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Full-text URL: https://arxiv.org/abs/2510.14022

Oxygen isotopes reveal low-mass star dominance in the Small Magellanic Cloud

Yan Gong, Zhi-yu Zhang, Christian Henkel, C.-H. Rosie Chen, Wenjin Yang, Xindi Tang, Leslie K. Hunt, Axel Weiss, Gang Wu, Yaoting Yan, Konstantin Grishunin, Karl M. Menten

Oxygen isotope abundances and their ratios are fingerprints of stellar evolution and therefore provide a powerful tool in tracing the enrichment history of galaxies. However, their behavior in low-metallicity dwarf galaxies remains largely unexplored. The Small Magellanic Cloud (SMC), a nearby analog of young high-redshift galaxies, offers an ideal laboratory to investigate this regime. Using the Atacama Compact Array, we observed the J=2-1 transitions of 12CO, 13CO, C18O, and C17O from the massive star-forming region LIRS 36 (aka N12A), achieving the first detection of C17O in the SMC. This detection enables the first direct measurement of the 18O/17O abundance ratio of 0.87±0.26 in this galaxy, substantially lower than all values in the literature, including molecular clouds in the Milky Way and other galaxies. Such a low ratio of 18O/17O, together with a high 13CO/C18O ratio, indicates chemical enrichment dominated by low-mass stars, consistent

with the observed paucity of high-mass stars in the SMC. We suggest that the SMC is governed by a top-light integrated galaxy-wide initial mass function, predicted by the SMC's persistently low star-formation activities.

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ATOMIUM: Continuum emission and evidence of dust enhancement from binary motion

T. Danilovich, N. Samaratunge, Y. L. Mori, A. M. S. Richards, A. Baudry, S. Etoka, M. Montargès, P. Kervella, I. McDonald, C. A. Gottlieb, A. Wallace, D. J. Price, L. Decin, J. Bolte, T. Ceulemans, F. De Ceuster, A. de Koter, D. Dionese, I. El Mellah, M. Esseldeurs, M. Gray, F. Herpin, T. Khouri, E. Lagadec, C. Landri, L. Marinho, K. M. Menten, T. J. Millar, H. S. P. Müller, B. Pimpanuwat, J. M. C. Plane, R. Sahai, L. Siess, M. Van de Sande, O. Vermeulen, K. T. Wong, J. Yates, A. Zijlstra

Low- and intermediate-mass stars on the asymptotic giant branch (AGB) account for a significant portion of the dust and chemical enrichment in their host galaxy. Here we present ALMA observations of the continuum emission at 1.24 mm around a sample of 17 stars from the ATOMIUM survey. From our analysis of the stellar contributions to the continuum flux, we find that the semi-regular variables all have smaller physical radii and fainter monochromatic luminosities than the Mira variables. Comparing these properties with pulsation periods, we find a positive trend between stellar radius and period only for the Mira variables with periods above 300 days and a positive trend between the period and the monochromatic luminosity only for the red supergiants and the most extreme AGB stars with periods above 500 days. We find that the continuum emission at 1.2 mm can be classified into four groups. "Featureless" continuum emission is confined to the (unresolved) regions close to the star for five stars in our sample, relatively uniform extended flux is seen for four stars, tentative elongated features are seen for three stars, and the remaining five stars have unique or unusual morphological features in their continuum maps. These features can be explained by binary companions to 10 out of the 14 AGB stars in our sample. Based on our results we conclude that there are two modes of dust formation: well established pulsationenhanced dust formation and our newly proposed companion-enhanced dust formation. If the companion is located close to the AGB star, in the wind acceleration region, then additional dust formed in the wake of the companion can increase the mass lost through the dust driven wind. This explains the different dust morphologies seen around our stars and partly accounts for a large scatter in literature mass-loss rates, especially among semiregular stars with small pulsation periods.

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Glycolaldehyde and ethanol toward the L1157 outflow: resolved images and constraints on glycolaldehyde formation

Juliette Robuschi, Ana López-Sepulcre, Cecilia Ceccarelli, Layal Chahine, Claudio Codella and Linda Podio

Two main formation routes have been proposed for interstellar complex organic molecules (iCOMs): on dust grain surfaces and in the gas phase. Observing such molecules in protostellar outflow shock regions - provided that their ages are wellconstrained - can help distinguish between these pathways by probing chemical evolution over time. This study focuses on the potential daughter-mother relationship of glycolaldehyde (CH2OHCHO) and ethanol (C2H5OH), previously proposed in the literature. We test whether gas-phase reactions converting ethanol into glycolaldehyde derived in these works can explain the observed abundance of the latter in star-forming regions. We target the southern outflow of L1157, which hosts three shock regions, B0, B1 and B2, of increasing ages: about 900, 1500 and 2300 yr. We obtained high-resolution IRAM NOEMA maps of three lines of glycolaldehyde and one line of ethanol. We derived their abundances in the three shocks and used a pseudo time-dependent astrochemical model to simulate gas-phase and grain-surface formation scenarios for glycolaldehyde. Ethanol is assumed to form on grains and be released in the gas by shocks, where it is gradually converted into glycolaldehyde via the ethanol-tree reaction network. We present the first spatially resolved maps of glycolaldehyde and ethanol in the L1157 southern outflow, and more generally toward solar-like star forming regions. The abundance ratio [CH2OHCHO]/[C2H5OH] increases from B1 to B2, consistent with model predictions. However, the model cannot reproduce all three shocked regions simultaneously, suggesting that one of the assumptions of our model, such as the same excitation temperature and grain composition in B0, B1 and B2, or gas temperature evolution, is wrong. Nonetheless, our modeling rules out the possibility that all the observed gaseous glycolaldehyde is a grain-surface product.

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H3+ in irradiated protoplanetary disks: Linking far-ultraviolet radiation and water vapor

J. R. Goicoechea, O. Roncero, E. Roueff, John H. Black, I. Schroetter, and O. Berné

The likely JWST detection of vibrationally excited H3+ emission in Orion's irradiated disk system d203-506 raises the important question of whether cosmic-ray ionization is enhanced in disks within clustered star-forming regions, or whether alternative mechanisms contribute to H3+ formation and excitation. We present a detailed model of the photodissociation region (PDR) component of a protoplanetary disk -comprising the outer disk surface and the photoevaporative wind - exposed to strong external far-ultraviolet (FUV) radiation. We investigate key gas-phase reactions involving excited H2 that lead to the formation of H3+ in the PDR, including detailed state-to-state dynamical calculations of reactions H2(v>=0) + HOC+ -> H3+ + CO and H2(v>=0) + H+ -> H2+ + H. We also consider the effects of photoionization of vibrationally excited

H2(v>=4), a process not previously included in PDR or disk models. We find that these FUV-driven reactions dominate the formation of H3+ in the PDR of strongly irradiated disks, largely independently of cosmic-ray ionization. The predicted H3+ abundance in the disk PDR peaks at $x(H3+)\sim1E-8$, coinciding with regions of enhanced HOC+ and water vapor abundances, and is linked to the strength of the external FUV field (G0). The predicted H3+ column density ($\sim1E13$ cm-2) agrees with the presence of H3+ in the PDR of d203-506. We also find that formation pumping, resulting from exoergic reactions between excited H2 and HOC+, drives the vibrational excitation of H3+ in these regions. We expect this photochemistry to be highly active in disks where $G_0 > 1E3$. The H3+ formation pathways studied here may also be relevant in the inner disk region (near the host star), in exoplanetary ionospheres, and in the early Universe.

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MOLLId: software for automatic identification of spectral molecular lines in the sub-millimeter and millimeter bands and its application to the spectra of protostars from the region RCW 120

A. A. Farafontova, M. S. Kirsanova, S. V. Salii

In this work, we present the program MOLLId (MOLecular Line Identification) for automated molecular lines approximation with gaussian profile. Molecular identification was performed using multi-level comparison of the lines' center frequencies and rest frequencies from the spectroscopic database. The program was tested using identification of the molecular lines in observational spectra of young stellar objects RCW 120 YSO S1 and RCW 120 YSO S2, located near the border of the RCW 120 PDR. In the spectra of the RCW 120 YSO S1 source, 100 lines of 41 molecules were identified over the level of 4-6 sigma. In the spectra of the RCW 120 YSO S2 source, 407 lines of 79 molecules were identified over the level 3-5 sigma. Using Intel Core i7-12700K CPU, identification time is equal to 6 and 8 minutes per spectral range for the YSOs S1 and S2, respectively. From the analysis of CH3OH, CH3CN, CH3CCH molecules identified in RCW 120 YSO S2 we found a two-component structure and estimated the physical parameters in the LTE approximation for each of the components.

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Hydrogen cyanide and hydrocarbons mix on Titan

Fernando Izquierdo-Ruiz, Morgan. L. Cable, Robert Hodyss, Tuan H. Vu, Hilda Sandström, Alvaro Lobato, Martin Rahm

This work reveals a striking exception to the well- established rule in chemistry that polar and nonpolar compounds do not spontaneously mix: insertion of methane, ethane, and other small hydrocarbons into the crystal lattice of hydrogen cyanide (HCN), a highly polar molecule. By mixing these components at cryogenic temperatures, we can observe distinct shifts in vibrational modes using Raman spectroscopy. Our computational pre- dictions confirm that cocrystal structures of HCN and ethane, which match our exper- imental vibrational shifts closely, are thermodynamically and kinetically stable. Given that methane, ethane, and HCN are major components of the atmosphere and surface of Saturn's moon Titan—where they play key roles in shaping chemistry, weather, and landscape—our findings may prove instrumental for explaining Titan's chemical and geological evolution.

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Condensation sequence of circumstellar cluster seeds (CSCCS)

David Gobrecht

Introduction: Traditionally, the condensation sequence of circumstellar dust is predicted based on the thermodynamic stabilities of specific condensates in the macroscopic bulk phase. However, at the (sub-) nanometer scale clusters with noncrystalline structures and significantly different properties are energetically favoured. Methods: For this reason, we study the thermodynamic stabilities of metal oxide clusters with generic stoichiometries of M2O3 and M3O4, where M represents a metal atom. With an upper size limit of 50 atoms, we consider clusters with sizes n = 1-10 for (M2O3)n, and n = 1-7 for (M3O4)n. The M2O3 clusters comprise alumina (Al2O3), Mg-rich pyroxene (MgSiO3) and a size-limited sample of titanates (CaTiO3), whereas the M3O4 clusters include spinel (MgAl2O4), Mg-rich olivine (Mg2SiO4) and calcium aluminates (CaAl2O4). Results: We find that, apart from the alumina monomer, the aluminum-bearing clusters (Al2O3)n, n = 1-10, and (MgAl2O4)n, n = 1-7, are favoured over their silicate counterparts (MgSiO3)n, n = 1-10 and (Mg2SiO4)n, n = 1-7. Also, we find that calcium aluminate clusters, CaAl2O4, are energetically more favourable than magnesium aluminate clusters, MgAl2O4. Furthermore, for a limited data set of (CaTiO3)n, n = 1-2, clusters we find significantly larger stabilities than for the other considered (M2O3)n clusters, namely Al2O3 and MgSiO3. Discussion: Future investigations, in particular on titanates and on Ca-rich silicates, are required to draw a more thorough and complete picture of the condensation sequence at the (sub-)nanoscale.

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Methanol emission tracing ice chemistry and dust evolution in the TW Hya protoplanetary disk

John D. Ilee, Catherine Walsh & Jenny Calahan

Methanol (CH3OH) ice is abundant in space and is a key feedstock for seeding chemical complexity in interstellar and circumstellar environments. Despite its ubiquity, gas-phase methanol has only been detected in one disk around a Solar-type star to date, TW Hya. Here we present new high sensitivity (~1 mJy/beam) observations of TW Hya with ALMA that detect four individual transitions of gas-phase methanol spanning upper level energies from 17 to 38 K. We confirm the presence of gas-phase methanol in the luke-warm molecular layer of the disk (~35.9 K) and with a disk-integrated column density of ~1.8×10^12 cm^-2. A radially-resolved analysis suggests that the gas-phase methanol is centrally compact, peaking within the spatial extent of the mm-sized dust grains (≤80 au). Static gas-grain chemical disk models confirm photodesorption as an important mechanism releasing methanol into the gas phase, with the column density further boosted by the inclusion of grain-surface chemistry, reactive desorption, and an increase in dust-grain surface area assuming fractal grains. However, no model can fully reproduce the observed column density nor the radial distribution, and we suggest that the inclusion of dynamic processes such as vertical mixing and radial drift would be required to do so. Our results demonstrate that the abundance and distribution of the precursors for complex chemistry in the planet-forming regions around Solar-type stars is ultimately controlled by the interplay of grain surface chemistry coupled with the evolution of dust in their disks.

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Announcements

Save the date! - "Cosmic rays 4: the salt of the star formation recipe" (5th-9th October 2026, Pisa, Italy)

This is the fourth edition of the conference that we organised in Florence in 2018, 2022, and 2024. This year we are moving to Pisa! The rationale of the conference can be found below. We are finalising the webpage and the list of invited speakers, and we will soon open registration. We are looking forward to meeting again to talk about all the achievements made over the last two years and share new ideas and challenges for the coming future! Save the date! Please share this information with anyone you think might be interested, and apologise if you receive the mail through several channels. Marco Padovani and Víctor M. Rivilla on behalf of the SOC and the LOC.

Rationale: Cosmic rays are a key ingredient in many fields of astrophysics and in particular in star formation and astrochemsitry. However, despite their great relevance our understanding is still relatively incomplete. Thanks to the data provided by the current infrared, radio and (sub)millimeter telescopes (e.g., JWST, VLA, LOFAR, MeerKAT, ALMA, NOEMA, IRAM 30m, Yebes, APEX, Effelsberg), we have now the opportunity of attaining a comprehensive knowledge about the role of cosmic rays in the physics and chemistry of the interstellar medium, hence about the processes leading to star and planet formation. To properly interpret this vast amount of information, the development of theoretical models, simulations and laboratory experiments, are mandatory. Therefore, this conference aims to allow the interplay between observations, theory, models, simulations, and laboratory, by bringing together experts in all these disciplines. We will share ideas, and we will discuss in dedicated sessions about present results, and about the challenges of the field in the future, thanks to the advent of new powerful facilities such as SKA, ALMA WSU, next generation VLA and ELT.

Scientific organising committee

Marco Padovani (co-chair) - INAF-Osservatorio Astrofisico di Arcetri, Italy Víctor M. Rivilla (co-chair) - Centro de Astrobiología (CAB, CSIC-INTA), Spain Lucia Armillotta - Università degli Studi di Firenze, Italy Daniele Galli - INAF-Osservatorio Astrofisico di Arcetri, Italy Barbara Michela Giuliano - Max Planck Institute for Extraterrestrial Physics (MPE), Germany Evangelia Ntormousi - Scuola Normale Superiore di Pisa, Italy