AstroChemical Newsletter #108

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Abstracts

Full interferometric map of the L1157 southern outflow: Formamide (NH2CHO) can form in the gas, after all

A. López-Sepulcre, C. Codella, C. Ceccarelli, L. Podio, J. Robuschi

The formation mechanism of interstellar formamide (NH2CHO), a key prebiotic precursor, is currently a matter of hot debate within the astrochemistry community, with both gas-phase and grain-surface chemical pathways having been proposed as its dominant formation route. The aim of the present study is to place firm observational constraints on the formation pathways leading to formamide thanks to new interferometric observations of the molecular outflow driven by the protostellar binary L1157. We employed the IRAM NOEMA interferometer to map the entire southern outflow of L1157, which contains three main shocked regions with increasing post-shock age: B0, B1, and B2. This allowed us to measure how the abundance of formamide, that of acetaldehyde (CH3CHO), and the ratio of the two, vary with time in this region. In order to gain a greater understanding of the most likely formation routes of formamide, we ran a grid of astrochemical models and compared these to our observations. A comparison between observations and astrochemical modelling indicates that there are two possible scenarios: one in which the amount of formamide observed can be explained by gas-phase-only chemistry, and more specifically via the reaction H2CO + NH2 –> NH2CHO + H2, and another in which part of the observed formamide originates from surface chemistry and part from gas-phase chemistry. Surface chemistry alone cannot account for the abundance of formamide that we measure. While grain-surface chemistry cannot be ruled out, the present study brings definitive proof that gas-phase chemistry does work in L1157-B and acts efficiently in the production of this molecular species.

A&A (2024) 690, L13
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Full-text URL: https://arxiv.org/abs/2411.00495

Discovery of two cyano derivatives of acenaphthylene (C12H8) in TMC-1 with the QUIJOTE line survey

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We report the discovery in TMC-1 of two cyano derivatives of the PAH acenaphthylene (C12H8). We have found two series of lines with the QUIJOTE line survey that we assign to 1-C12H7CN and 5-C12H7CN. For the 1-isomer, we have detected and assigned 173 rotational transitions with J up to 46 and Ka up to 9, corresponding to 107 independent frequencies. For the 5-isomer, the identification is based on 56 individual lines, corresponding to 117 rotational transitions with J up to 40 and Ka up to 8. Identification of the carriers was achieved through a careful analysis of the derived rotational constants, which permit us to focus on molecules larger than naphthalene but smaller than anthracene and phenanthrene. Moreover, the derived rotational constants indicate that the species are planar; this allows us to discard derivatives of fluorene and acenaphthene, which are non-planar species. Quantum chemical calculations and subsequent chemical synthesis of these molecules, as well as the observation of their rotational transitions in the laboratory, unequivocally support our identifications. We also confirm, via a robust line-by-line detection, the previous claimed detection of 1- and 2-cyanonaphthalene, which were obtained through statistical stacking techniques. The column densities of 1- and 5-cyanoacenaphthylene are (9.5±0.9)e11 cm−2, while those of 1- and 2-cyanonapthalene are (5.5±0.5)e11 cm−2. Hence, it seems that acenaphthylene could be a factor of 1.7 more abundant than naphthalene. These results support a scenario in which PAHs grow in cold dark clouds based on fused five- and six-membered carbon rings.

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Full-text URL: https://arxiv.org/abs/2409.19311

H3+ absorption and emission in local (U)LIRGs with JWST/NIRSpec: Evidence for high H2 ionization rates

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We study the 3.4-4.4μm fundamental rovibrational band of H3+, a key tracer of the ionization of the molecular interstellar medium (ISM), in a sample of 12 local (d< 400 Mpc) ultra/luminous infrared galaxies (U/LIRGs) observed with JWST/NIRSpec. The P, Q, and R branches of the band are detected in 13 out of 20 analyzed regions within these U/LIRGs,

which increases the number of extragalactic H3+ detections by a factor of 6. For the first time in the ISM, the H3+ band is observed in emission in 3 of these regions. In the remaining 10 regions, the band is seen in absorption. The absorptions are produced toward the 3.4-4.4μm hot dust continuum rather than toward the stellar continuum, indicating that they likely originate in clouds associated with the dust continuum source. The H3+ band is undetected in Seyfert-like U/LIRGs where the mildly obscured X-ray radiation from the AGN might limit the abundance of this molecule. For the detections, the H3+ abundances, N(H3+)/N_H = (0.5-5.5)x1e-7, imply relatively high ionization rates between 3e-16 and >4e-15 s-1, which are likely associated with high-energy cosmic rays. In half of the targets the absorptions are blue-shifted by 50-180 km/s, which are lower than the molecular outflow velocities measured using other tracers such as OH 119μm or rotational CO lines. This suggests that H3+ traces gas close to the outflow launching sites before it has been fully accelerated. We used nonlocal thermodynamic equilibrium models to investigate the physical conditions of these clouds. In 7 out of 10 objects, the H3+ excitation is consistent with inelastic collisions with H2 in warm translucent molecular clouds (T_kin~250-500 K and n(H2)~1e2 – 1e3 cm-3). In three objects, dominant infrared pumping excitation is required to explain the absorptions from the (3,0) and (2,1) levels of H3+ detected for the first time in the ISM.

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The salty emission of the intermediate-mass AGB star OH 30.1−0.7

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We analyse continuum and molecular emission, observed with ALMA, from the dust-enshrouded intermediate-mass AGB star OH 30.1 -0.7. We find a secondary peak in the continuum maps, "feature B", separated by 4.6" from the AGB star, which corresponds to a projected separation of 1.8×10^4 au, placing a lower limit on the physical separation. This feature is most likely composed of cold dust and is likely to be ejecta associated with the AGB star, though we cannot rule out that it is a background object. The molecular emission we detect includes lines of CO, SiS, CS, SO2, NS, NaCl, and KCl. We find that the NS emission is off centre and arranged along an axis perpendicular to the direction of feature B, indicative of a UV-emitting binary companion (e.g. a G-type main sequence star or hotter), perhaps on an eccentric orbit, contributing to its formation. However, the NaCl and KCl emission constrain the nature of that companion to not be hotter than a late B-type main sequence star. We find relatively warm emission arising from the inner wind and detect several vibrationally excited lines of SiS (3 = 1), NaCl (up to 3 = 4) and KCl (up to 3 = 2), and emission from low energy levels in the mid to outer envelope, as traced by SO2. The CO emission is abruptly truncated around 3.5" or 14,000 au from the continuum peak, suggesting that mass loss at a high rate may have commenced as little as 2800 years ago.

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A Yebes W band Line Survey towards an Unshocked Molecular Cloud of Supernova Remnant 3C391: Evidence of Cosmic-Ray-Induced Chemistry

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Cosmic rays (CRs) have strong influences on the chemistry of dense molecular clouds (MCs). To study the detailed chemistry induced by CRs, we conducted a Yebes W band line survey towards an unshocked MC (which we named as 3C391:NML) associated with supernova remnant (SNR) 3C391. We detected emission lines of 18 molecular species in total and estimated their column densities with local thermodynamic equilibrium (LTE) and non-LTE analysis. Using the abundance ratio N(HCO+)/N(CO) and an upper limit of N(DCO+)/N(HCO+), we estimated the CR ionization rate of 3C391:NML is ζ≳2.7e-14 s-1 with an analytic method. However, we caution on adopting this value because chemical equilibrium, which is a prerequisite of using the equations, is not necessarily reached in 3C391:NML. We observed lower N(HCO+)/N(HOC+), higher N(HCS+)/N(CS), and higher X(l-C3H+) by an order of magnitude in 3C391:NML than the typical values in quiescent dense MCs. We found that an enhanced CR ionization rate (of order ∼1e-15 or ∼1e-14 s-1) is needed to reproduce the observation with chemical model. This is higher than the values found in typical MCs by 2-3 orders of magnitude.

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Experimental sticking coefficients of CO and N2 on sub-micrometric cosmic grain analogs

Caroline Stadler, Carine Laffon, Philippe Parent

Measuring the sticking coefficient of molecules pertinent to astrochemistry on substrates that mimic interstellar dust grains is crucial for the comprehensive understanding of gas-grain chemical processes. Although astrochemical models assume a sticking coefficient of 1, recent laboratory experiments on H2O and CO2 have revealed significantly lower values when measured on small grain analogs. Our aim is to determine the sticking coefficients of CO and N2 on sub-micrometric silicate and carbon grains. By quantifying realistic sticking coefficients on these dust grain analogs, we can improve the accuracy of astrochemists' predictions of molecular abundances as affected by gas-grain interactions. The molecules of interest were added to various substrates at 10 K in an ultra-high vacuum. The amount of adsorbate that stuck to the substrate was quantified using X-ray photoelectron spectroscopy. These quantities were compared to a reference with a sticking coefficient of 1, allowing the deduction of the sticking coefficient for each substrate. The average sticking coefficients of CO and N2 on grain analogs are 0.17 for CO and 0.14 for N2 on olivine powder, and 0.05 for CO and 0.07 on N2 on soot, instead of the presumed 1. This is in line with the low values previously reported for H2O and CO2. It is thus necessary to reconsider the interactions between gaseous species and dust particles as a low-efficiency process. This reduction in accretion and reaction rates has important implications for how we understand astrochemistry.

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Evidence for Abiotic Dimethyl Sulfide in Cometary Matter

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Technological progress related to astronomical observatories such as the recently launched James Webb Space Telescope (JWST) allows searching for signs of life beyond our solar system, namely, in the form of unambiguous biosignature gases in exoplanetary atmospheres. The tentative assignment of a 1σ–2.4σ spectral feature observed with JWST in the atmosphere of exoplanet K2-18b to the biosignature gas dimethyl sulfide (DMS; sum formula C2H6S) raised hopes that, although controversial, a second genesis had been found. Terrestrial atmospheric DMS is exclusively stemming from marine biological activity, and no natural abiotic source has been identified—neither on Earth nor in space. Therefore, DMS is considered a robust biosignature. Since comets possess a pristine inventory of complex organic molecules of abiotic origin, we have searched high-resolution mass spectra collected at comet 67P/Churyumov–Gerasimenko, target of the European Space Agency's Rosetta mission, for the signatures of DMS. Previous work reported the presence of a C2H6S signal when the comet was near its equinox, but distinction of DMS from its structural isomer ethanethiol remained elusive. Here we reassess these and evaluate additional data. Based on differences in the electron ionization-induced fragmentation pattern of the two isomers, we show that DMS is significantly better compatible with the observations. Deviations between expected and observed signal intensities for DMS are <1σ, while for ethanethiol they are 2σ–4σ. The local abundance of DMS relative to methanol deduced from these data is (0.13 ± 0.04)%. Our results provide the first evidence for the existence of an abiotic synthetic pathway to DMS in pristine cometary matter and hence motivate more detailed studies of the sulfur chemistry in such matter and its analogs. Future studies need to investigate whether or not the present inference of cometary DMS could provide an abiotic source of DMS in a planetary atmosphere.

2024 ApJ 976 74
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Experimental and Computational Study of Ethanolamine Ices under Astrochemical Conditions

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Ethanolamine (NH2CH2CH2OH) has recently been identified in the molecular cloud G+0.693-0.027, situated in the SgrB2 complex in the Galactic center. However, its presence in other regions, and in particular in star-forming sites, is still elusive. Given its likely role as a precursor to simple amino acids, understanding its presence in the star-forming region is required. Here, we present the experimentally obtained temperature-dependent spectral features and morphological behavior of pure ethanolamine ices under astrochemical conditions in the 2 - 12 micrometer (MIR) and 120 - 230 nm (VUV) regions for the first time. These features would help in understanding its photochemical behavior. In addition, we present the first chemical models specifically dedicated to ethanolamine. These models include all the discussed chemical routes from the literature, along with the estimated binding energies and activation energies from quantum chemical calculations reported in this work. We have found that surface reactions: CH2OH + NH2CH2 --> NH2CH2CH2OH and NH2 + C2H4OH --> NH2CH2CH2OH in warmer regions (60 - 90 K) could play a significant role in the formation of ethanolamine. Our modeled abundance of ethanolamine complements the upper limit of ethanolamine column density estimated in earlier observations in hot core/corino regions. Furthermore, we provide a theoretical estimation of the rotational and distortional constants for various species (such as HNCCO, NH2CHCO, and NH2CH2CO) related to ethanolamine that have not been studied in existing literature. This study could be valuable for identifying these species in the future.

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Full-text URL: https://arxiv.org/abs/2409.01307

Fate and detectability of rare gas hydride ions in nova ejecta: A case study with nova templates

M. Sil, A. Das, R. Das, R. Pandey, A. Faure, H. Wiesemeyer, P. Hily-Blant, F. Lique, and P. Caselli

HeH+ was the first heteronuclear molecule to form in the metal-free Universe after the Big Bang. The molecule gained significant attention following its first circumstellar detection in the young and dense planetary nebula NGC 7027. We target some hydride ions associated with the noble gases (HeH+, ArH+, and NeH+) to investigate their formation in harsh environments like the nova outburst region. We use a photoionization modeling (based on previously published best-fit physical parameters) of the moderately fast ONe type nova, QU Vulpeculae 1984, and the CO type novae, RS Ophiuchi and V1716 Scorpii. Our steady-state modeling reveals a convincing amount of HeH+, especially in the dense clump of RS Ophiuchi and V1716 Scorpii. The calculated upper limit on the surface brightness of HeH+ transitions suggests that the James Webb Space Telescope (JWST) could detect some of them, particularly in sources like RS Ophiuchi and V1716 Scorpii, which have similar physical and chemical conditions and evolution. It must be clearly noted that the sources studied are used as templates, and not as targets for observations. The detection of these lines could be useful for determining the physical conditions in similar types of systems and for validating our predictions based on new electron-impact ro-vibrational collisional data at temperatures of up to 20,000 K.

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Anatomy of the Class I protostar L1489 IRS with NOEMA. I. Disk, streamers, outflow(s) and bubbles at 3 mm

Tanious, M., Le Gal, R., Neri, R., Faure, A., Gupta, A., Law, C. J., Huang, J., Cuello, N., Williams, J. P., Ménard, F.

Context. Over the past few years, chemical studies have revealed multiple structures in the vicinity of young stellar objects (YSOs). It has become evident that specific physical conditions are associated with the emission of particular molecular lines, allowing us to use molecular probes of the YSO physics. Consequently, chemical surveys are now necessary to fully constrain the origin of the observed structures. Several surveys have been conducted to explore the chemistry of YSOs, focusing on Class 0 and Class II objects. However, our knowledge of intermediate objects, that are Class I objects, remains limited. Aims: To bridge the gap and establish the relationship between observed structures and molecular line emission at the Class I evolutionary stage, we investigate the spatial distribution of key molecular gas species in the low-mass Class I protostar L1489 IRS (IRAS 04016+2610), a source part of the ChemYSO survey. Methods: We performed a 3 mm line survey at high spatial and high spectral resolution using the NOEMA interferometer and the IRAM-30 m telescope. For the data analysis, we applied and compared two methods: a streamline model and the new python package TIPSY. Results: We present here the ten brightest lines of our survey, in which we identified a new ~3000 au long streamer in HC3N, C2H, and c-C3H2 emission, likely associated with more localized accretion shocks probed in SO. In addition, two ~10 000 au bubbles are seen with the dense molecular tracers HCO+, CS, and HCN around the YSO. We retrieve previously identified structures, like an outflow in HCO+ and another streamer in C2H. Additionally, potential indicators of a second outflow appear in CS and HCN emission, but its nature remains to be confirmed. Conclusions: The late infall identified at large scales may originate from the nearby prestellar core L1489 and is likely responsible for the formation of an external warped disk in this system. The detection of a potential second outflow could be the direct evidence of a binary system. Finally, we hypothesize that the bubbles may result from the magnetic pressure as observed in numerical simulations.

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DOI: 10.1051/0004-6361/202348785
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Reactivity of chondritic meteorites under H2-rich atmospheres: Formation of H2S.

V. Cabedo, G. Pareras, J. Allitt, A. Rimola, J. Llorca, H. H. P. Yiu, M. R. S. McCoustra

Current models of chemical evolution during star and planetary formation rely on the presence of dust grains to act as a third body. However, they generally ignore the reactivity of the dust grains themselves. Dust grains present in the protoplanetary phase will evolve as the solar system forms and, after protoplanets have appeared, they will be constantly delivered to their surfaces in the form of large aggregates or meteorites. Chondritic meteorites are mostly unaltered samples of the dust present in the first stages of the Solar System formation, that still arrive nowadays to the surface of Earth and allow us to study the properties of the materials forming the early Solar System. These materials contain, amongst others, transition metals that can potentially act as catalysts, as well as other phases that can potentially react in different astrophysical conditions, such as FeS. In this work, we present the reactivity of chondritic meteorites under H2-rich atmospheres, particularly towards the reduction of FeS for the formation of H2S and metallic Fe during the early phases of the planetary formation. We present the obtained results on the reaction rates and the percentage of FeS available to react in the materials. Additionally, we include a computational study of the reaction mechanism and the energetics. Finally, we discuss the implications of an early formation of H2S in planetary surfaces.

MNRAS, Volume 535, Issue 3, December 2024, Pages 2714–2723,
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Full-text URL: https://arxiv.org/abs/2410.23012

Detection of carbon dioxide and hydrogen peroxide on the stratified surface of Charon with JWST

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Charon, Pluto's largest moon, has been extensively studied, with research focusing on its primitive composition and changes due to radiation and photolysis. However, spectral data have so far been limited to wavelengths below 2.5 microns, leaving

key aspects unresolved. Here we present the detection of carbon dioxide (CO2) and hydrogen peroxide (H2O2) on the surface of Charon's northern hemisphere, using JWST data. These detections add to the known chemical inventory that includes crystalline water ice, ammonia-bearing species, and tholin-like darkening constituents previously revealed by ground- and space-based observations. The H2O2 presence indicates active radiolytic/photolytic processing of the water ice-rich surface by solar ultraviolet and interplanetary medium Lyman-alpha photons, solar wind, and galactic cosmic rays. Through spectral modeling of the surface, we show that the CO2 is present in pure crystalline form and, possibly, in intimately mixed states on the surface. Endogenically sourced subsurface CO2 exposed on the surface is likely the primary source of this component, with possible contributions from irradiation of hydrocarbons mixed with water ice, interfacial radiolysis between carbon deposits and water ice, and the implantation of energetic carbon ions from the solar wind and solar energetic particles.

2024, Nature Communications, 15, 8247.
DOI: 10.1038/s41467-024-51826-4
Full-text URL: https://www.nature.com/articles/s41467-024-51826-4

Announcements

Funded PhD position in Formation of planetary systems or Simulations of exoplanet climates

The Astrophysics Group in the School of Physics and Astronomy at the University of Leeds are pleased to advertise one fully-funded PhD position in the general areas of exoplanet formation/protoplanetary disks/exoplanet atmospheres/exoplanet climate. The Astrophysics group has researchers working at the forefront of astrophysical observations and simulations of planet formation, and simulations of exoplanet atmospheres and climate. You will work with either Dr John Ilee to model the signatures of forming planets with the Square Kilometre Array (SKA), or with Dr Catherine Walsh to simulate the climate of exo-Earths. This project will be of interest to post-graduate researchers wishing to work at the cutting edge of exoplanetary formation and evolution.

More details can be found on the formal project advertisement page including how to apply:
https://phd.leeds.ac.uk/project/2073-formation-of-planetary-systems-OR-simulations-of-exoplanet-climates
Please contact us if you are interested to find out more about the projects!
Dr John Ilee: j.d.ilee@leeds.ac.uk
Dr Catherine Walsh: c.walsh1@leeds.ac.uk

Global Astrochemistry Lecture Series (GALS) - Astrochemistry: From the Big Bang to Life

Our universe is full of molecules, from the simplest – molecular hydrogen – all the way up to the complex molecular structures essential to the chemistry of life on Earth. A large and diverse array of chemical species has been detected not only on planets but in interstellar clouds, in regions of star formation, in protoplanetary disks, and in comets and meteorites within the solar system. But how and when was all this material formed, and how does it evolve over time? How much molecular content is inherited from one stage of star and planet formation to the next? What role does the chemistry of the universe through cosmic time play in the origins of life? A major unanswered question remains whether the molecules essential to life were produced on the early Earth (endogenous origin), or whether they were produced in the parent interstellar medium or planet-forming disk and delivered to Earth via asteroids, comets and their meteoritic remains (exogenous origin).

This lecture course will be devoted to astrochemistry and the exploration of topics related to the chemical origins of life. In 18 lectures from the world-leading experts, we will discuss the history of the early molecular universe starting from the Big Bang; environmental conditions and key physico-chemical processes in space; astronomical observations (from ground to space) of objects of astrochemical interest; chemical models describing astrophysical environments and their reaction networks; key laboratory techniques and approaches for studying astrochemical processes; chemistry in specific environments, such as the interstellar medium, protoplanetary disks, and atmospheres of (exo)planets; exogenous synthesis and delivery of biomolecule precursors; and, finally, evolution of these precursors on the early Earth. .

GALS is aimed at providing a broad overview of scientific issues, problems, achievements, and open questions in astrochemistry; and at helping senior undergraduate and postgraduate students as well as early career scientists to expand their interests and develop a firm understanding of this area, sufficient to choose an appropriate direction for their future career. The course is open to students and scientists from all over the world..

GALS is an annual event organized by Robin Garrod (University of Virginia, USA), Wolf Geppert (Stockholm University, Sweden), Martin McCoustra (Heriot-Watt University, Scotland), and Alexey Potapov (Friedrich Schiller University Jena, Germany). GALS will comprise of two parts: 14 core lectures and 4 special lectures. There will be a new topic for special lectures every year. For the coming semester, we have chosen JWST..

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Registration: December 01 2024 - January 31 2025.
Webpage: https://www.astrochemistry.de/online-course/