AstroChemical Newsletter #126

July & August 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

Isotopic evidence for a cold and distant origin of 3I/ATLAS,

M. A. Cordiner, N. X. Roth, M. Micheli, G. Villanueva, D. Farnocchia, S. Charnley, N. Biver, D. Bockelée-Morvan, D. Bodewits, C. O. Chandler, J. Crovisier, M. N. Drozdovskaya, K. Furuya, M. S. P. Kelley, S. N. Milam, J. W. Noonan, C. Opitom, M. E. Schwamb, C. A. Thomas

Interstellar objects provide the only directly observable samples of icy planetesimals formed around other stars, and can therefore provide insight into the diversity of physical and chemical conditions occurring during exoplanet formation. Here we report isotopic measurements of the interstellar comet 3I/ATLAS, which reveal an elemental composition unlike any Solar System body. The water in 3I/ATLAS is enriched in deuterium, at a level of D/H = (0.98 ± 0.06)%, which is more than an order of magnitude higher than in known comets, while its range of 12C/13C ratios (141–191 for CO2 and 123–172 for CO) exceeds typical values found in the Solar System, as well as nearby interstellar clouds and protoplanetary disks. Such extreme isotopic signatures indicate formation at temperatures $\lesssim$ 30 K in a relatively metal-poor environment. When interpreted with respect to models for Galactic chemical evolution, the carbon isotopic composition implies that 3I/ATLAS may have accreted as long ago as 12 billion years, following a period of intense, early star formation. 3I/ATLAS thus represents a preserved fragment of an ancient planetary system.

Nature
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Probing the ubiquity of complex ices in protostars with JWST: the first systematic quantification of weak ice bands between 6.8 and 7.9 micron

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Complex organic molecules (COMs) are the key to understanding the chemical evolution from simple interstellar molecules to potential prebiotic material. Although COMs have been extensively studied in the gas phase toward protostars, their counterparts in ices, where they are thought to form at earlier stages, remain far less constrained. A number of diagnostic features of complex ices lie between 6.8 and 8.8 um, a region known as the "COM ice fingerprint range," but previous infrared facilities lacked the sensitivity and spectral resolution required to quantify the weak bands therein. With the unprecedented sensitivity and resolving power of JWST, these limitations can now be overcome. Here, we present the first large-sample quantitative study of the absorption features at 7.02, 7.24, 7.40, and 7.67 um, using MIRI-MRS spectra of 21 protostars. The CH4 band at 7.67 um is the strongest band and shows remarkably uniform peak positions (7.67-7.68 um) and FWHMs (0.06-0.08 um), suggesting CH4 ice as its dominant carrier. The 7.24 and 7.40 um bands exhibit larger source-to-source variations in peak positions and FWHMs, but their occurrence and intensities are strongly correlated with each other. Comparisons with existing and new laboratory spectra suggest HCOO- as the most likely carrier of these two bands, yet HCOO- cannot fully reproduce their intensity ratios, implying additional contributions from other species such as C2H5OH, CH3CHO, and CH3COCH3. Our results reveal, for the first time, the potential ubiquity of weak features of complex ices in protostars, which have remained largely undetected due to observational limitations.

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An ACA map of a molecular cloud interacting with supernova remnant W28

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Supernova remnants (SNRs) strongly influence the physical and chemical properties of the molecular clouds (MCs) with which they interact. We carried out a high-resolution observation toward W28F, a chemically rich MC interacting with SNR W28, with the Atacama Compact Array (ACA) in Band 7. Significant emission (> 10 sigma) of CO, CH3OH, p-H2CO, SiO and SO is detected. We reveal the clumpy structures of the shocked MC, with different spatial distributions between CH3OH and SiO. We select six molecular clumps to conduct spectral decomposition and non-local-thermodynamic-equilibrium analysis with the CH3OH and p-H2CO lines. The best-fit results show a H2 density of nH2 ~ (1-3)e5 cm-3 and a gas temperature of Tgas ~ 50-170 K in most of the fitted components. The H2 density and gas temperature show a clear anti-

correlation across different regions, with the thermal pressure consistent with that of the adjacent X-ray-emitting hot plasma. This is consistent with the picture that the SNR shocks propagate into multi-phase gas, with a pressure balance existing between different phases. We propose that the high abundance ratio between E-CH3OHand A-CH3OH (> 0.9) suggests extra gas-phase processes to enhance this ratio, such as proton exchange with H3+ and HCO+. The chemical segregation between CH3OH and SiO, in both the spatial and spectral regime, can be explained by the fact that CH3OH traces slow shocks while SiO traces fast shocks.

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A new hot core in the outer Galaxy: Impact of metallicity on the formation of complex organic molecules

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Many complex organic molecules (COMs) in star-forming regions are believed to form on dust grains. We thus expect both the reduced metallicity and dust-to-gas ratio in the outer Galaxy to have an impact on the chemical composition of these regions. We investigate if certain COMs are more sensitive than others to metallicity by measuring the chemical composition of hot cores in the outer Galaxy. We used NOEMA to perform an imaging spectral line survey of G135.27+2.79, located at a galactocentric distance of 13.1 kpc. We derived the rotational temperatures and column densities of the detected molecules while assuming local thermodynamic equilibrium and compared the chemical composition of G135.27+2.79 to other sources and to the predictions of the three-phase astrochemical code MAGICKAL. G135.27+2.79 hosts three continuum cores, labeled MM1, MM2, and MM3. Most species in MM1 trace a hot, compact region, confirming MM1 as a hot core. The chemical composition of MM1 correlates rather well with that of the inner and outer Galaxy hot cores G31.41+0.31 and WB89-789 SMM1, but its molecular abundances relative to methanol lie in between, which may reflect the influence of metallicity on COM formation. The model results agree reasonably well, though with a few notable exceptions, with the COM abundances of MM1 relative to methanol and with the abundance ratios between MM1 and G31.41+0.31. Sensitivity to the reduced metallicity and dust-to-gas ratio varies between molecules, with carbon chains and nitriles most negatively affected. The lower dust-to-gas ratio leads to slower adsorption under low-metallicity conditions so that more carbon is locked up into CO in the gas. Slow adsorption means that CO is hydrogenated more efficiently on grains, enhancing CO-related COM abundances above expectations. These results demonstrate that metallicity has a significant impact on the formation of COMs.

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Metal Oxide Clusters in Gas Giant Exoplanet Atmospheres

Deepak Bisht, Christiane Helling, David Gobrecht, Ludmila Carone, Helena Lecoq-Molinos, Peter Woitke, Markus Aichhorn, Jan Philip Sindel, and Amit Reza

This study investigates the thermal stability and absorption of metal oxide clusters in exoplanetary atmospheres. Utilizing our thermochemical data, we analyze eight distinct cluster families: magnesium oxide (MgO), silicon monoxide (SiO), titanium monoxide (TiO), vanadium monoxide (VO), titanium dioxide (TiO2), vanadium dioxide (VO2), aluminum oxide (Al2O3), and vanadium pentoxide (V2O5). Equilibrium cluster populations as a function of gas temperature and pressure reveal distinct stability regimes. Under solar elemental abundances, (TiO2)N and (Al2O3)N are favored at higher temperatures, while (MgO)N and (SiO)N dominate at lower temperatures. Computed absorption spectra exhibit strong size- and composition-dependent absorption features in the mid-infrared (8-50 um), many of which fall within the wavelength range accessible to JWST/MIRI. We further coupled cluster thermodynamics with 3D general circulation model (GCM) outputs to investigate the cluster stability across the ultra-hot Jupiters (UHJs) WASP-121 b and WASP-18 b, the hot Jupiter (HJ) WASP-39 b, and the warm Jupiter (WJ) WASP-69 b. In WASP-121 b and WASP-18 b, extreme dayside temperatures suppress large-cluster stability, yielding atmospheres dominated by metal ions at low pressures and neutral metals at depth, with limited cluster survival on the nightside and morning terminator. In WASP-39 b, larger clusters are not thermochemically favoured despite the enhanced metallicity; instead, equilibrium chemistry stabilises smaller species, with only TiO showing a tendency toward stable larger cluster forms, likely due to its open d-orbitals. In contrast, WASP-69 b favors the formation of larger metal oxide clusters across an extended pressure range, highlighting WJs as a favorable environment for metal oxide cluster stability.

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Detection of CO2 ice in the planetary nebula NGC 6302

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Using JWST/MIRI observations, we report the detection of CO2 ice in the dusty torus of the planetary nebula NGC 6302, an environment generally considered hostile to fragile molecular species and ices due to intense UV irradiation. This detection

accompanies cold (20–50 K) gas-phase CO2 along the same sightlines. The ice absorption profile exhibits a double-peak profile, which is characteristic of pure crystalline CO2 ice. The CO2 gas-to-ice ratio is higher by more than an order of magnitude than in young stellar objects, which indicates distinct ice formation or processing mechanisms in evolved stellar environments. This discovery demonstrates that the dusty torus provides sufficient shielding to harbor ice chemistry, and that ice-mediated surface reactions must be incorporated into chemical models of planetary nebulae.

Astronomy & Astrophysics, Volume 708, id.L13, 7 pp.
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Mapping Interstellar Ice Inventory toward Class 0 Protostars in Star-forming Region Orion A with JWST Data

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We present a detailed study of the spatial distribution and chemical composition of interstellar ices toward six Class 0 protostars (HOPS-56, HOPS-60, HOPS-73, HOPS-91, HOPS-96, and HOPS-108) in the Orion A molecular cloud. Using high-resolution spectroscopic data from the JWST NIRspec and MIRI MRS instruments (4.3 - 8.1 μm), we have constructed the first pixel by pixel absorption maps with a resolution of ∼100AU for key ice species, including 13CO2, OCN−, CO, H2O, NH+4, and H2CO. CH4 and OCS were analyzed toward the continuum peaks. The column densities were derived by fitting the observed spectra with laboratory ice analogs. We employed radiative transfer modeling, which confirmed the reliability of our column density estimates within the protostellar envelopes. Our analysis reveals significant variations in ice abundances and distributions, reflecting the physical structure and energetic processes within the envelopes. Specifically, we observe the influence of protostellar heating and outflows on the ice mantles, most notably in HOPS-60. The total ice composition is consistent with astrochemical models and covers ∼90% of observed ice inventory suggesting that ice is primarily formed during the prestellar stage and subsequently inherited by the protostellar envelope. Based on the abundance relative to water, the sources can be categorized into two distinct groups, possibly indicating evolutionary differences or variations in envelope density and temperature profiles.

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The reaction of P+ with H2O (D2O): a pathway for the formation of PO and PO+ in the ISM and circumstellar envelopes

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Interstellar phosphorus shows uncertain depletion patterns and an unidentified main reservoir, with only a few P-bearing molecules detected despite their key astrochemical and astrobiological relevance. In particular, recent observations of PO+ with a high abundance with respect to PO suggest that ion–molecule chemistry may play a crucial role, motivating a reassessment of its formation pathways in the ISM and circumstellar envelopes. The role of the reaction between P+ and water (D2O) for the synthesis of PO+ and POH+ is explored in a joint experimental and theoretical study. Furthermore, new possible routes leading to the conversion of i) POH+ into PO (via a non-dissociative proton-transfer reaction with ammonia) and of ii) PO into PN (via the adiabatic barrierless reaction of N(4S) with PO are proposed. The reaction P+ plus D2O is studied experimentally by measuring absolute cross sections (CSs) and branching ratios (BR), as a function of collision energy. Experiments are supported by a theoretical investigation combining high-level electronic structure calculations of the multidimensional triplet and singlet potential energy surfaces with a kinetic investigation to derive BRs and channel-specific rate constants as a function of temperature in the 10-5000 K range. The P+ + D2O reaction leads mostly to POD+ plus D (BR=90%) with PO+ plus D2 being a minor channel (BR=10%). From the total reaction CS as a function of collision energy, estimates for the rate constant as a function of temperature have been obtained, with values ranging from 1.2e−9 cm3s−1 (at 10 K) to 7.5e−10 cm3s−1 (at 5000 K). The proton transfer reaction between POH+ and NH3 is found to be efficient with rate constants in the range (1.1 − 2.7)e−9 cm3s−1. As a final consideration, the reaction of P+ with water should be considered in astrochemical models where phosphorus can be released in the gas phase as a cation, from the energetic processing of icy interstellar grains due to shocks. The reaction leads to POH+ as the main reaction product and relevant interstellar isomer, an important precursor for PO formation not only via dissociative recombination with electrons, but also by proton transfer to NH3. The direct formation of PO+ as a secondary channel can explain the high PO+/PO ratio detected in the ISM.

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Calcium-bearing cyanopolyynes in IRC+10216

T. J. Millar

In recent years, a number of metal-containing, carbon-chain species have been detected in the external circumstellar

envelope of the carbon-rich AGB star IRC+10216. The most common metal detected in such species is Mg, for which molecules as large as MgC5N, MgC5N+, MgC6H, and MgC6H+ have been observed. In this paper, we calculate the likely abundances of the Ca-bearing cyanopolyynes, CaC(2n+1)N for n = 1-4, drawing the conclusion that the observed abundance of CaNC must be made from much larger Ca-terminated cyanopolyyne ions, which requires considerable rearrangement in their dissociative recombination. We pay particular attention to the detectability of CaC3N whose rotational spectrum has recently been measured.

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Detection of C_{60} Combination Bands in the Near-IR Spectrum of Tc 1

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We report the detection of a set of new near-infrared emission features between 3.5 and 5.2 μm in JWST/NIRSpec observations of Tc 1, the planetary nebula known for displaying the cleanest and most prominent mid-infrared cosmic fullerene spectrum. These broad features share the same spatial distribution as the well-known C_{60} and C_{70} mid-infrared emission bands, peaking in an asymmetric ring approximately 5–6" from the central star. Through comparison with new anharmonic quantum chemical calculations, we demonstrate that these features arise from C_{60} combination bands, marking their first detection in an astrophysical environment. The total energy radiated in the combination bands amounts to ~17% of the total energy emitted from all C_{60} modes, with direct implications for fullerene cooling models. These near-infrared combination bands offer a promising new window for identifying and studying the molecular astrophysics of C_{60} in sources where mid-infrared spectra are more complex.

Morgan M. Giese et al. 2026, ApJL, 1004, L32
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Detecting Nitrogen Carriers in the Inner Regions of Protoplanetary Disks

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Nitrogen is a key element for building habitable worlds, yet only a small fraction of the available N-budget of planet-forming disks has been detected. In particular, the lack of any IR NH3 detection is striking, as this molecule is predicted to be rather abundant in the warm, inner regions of protoplanetary disks, and therefore potentially readily incorporated into (giant) planets' atmospheres. We present a combined modeling and observational study of N-bearing molecules in planet-forming disks, using detailed thermo-chemical disk models that investigate the sensitivity of N-containing molecules to the bulk elemental composition of the disk. Our models predict a strong increase in HCN flux with high C/H, and conversely a strong increase in flux from NO when O/H is high. The flux from NH3 is not very sensitive to O/H, but does decrease at high C/H due to competition with HCN. However, the absolute NH3 flux predicted by our model is not large enough to be detected with JWST-MIRI, even when N/H is enhanced by an order of magnitude. The flux from NO, on the other hand, is potentially detectable, and could therefore provide further insights into the N-budget of the inner disk. Using a cross-correlation technique, we search for NH3 and NO detections in three disks, GW Lup, Sz 98, and V1094 Sco. We do not find any NH3 detections, and only one tentative NO detection in V1094 Sco, though this needs further study to be confirmed. Additionally, we demonstrate that future facilities in the FIR may provide a better opportunity to detect NH3 and thereby draw a comparison to the NH3 budget known to be present in interstellar ices.

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Single-dish observations and non-LTE analysis of CH3OH, HCN, and CO line emission in the Oort cloud comet C/2017 K2 (PANSTARRS)

M. S. Kirsanova, Ya. N. Pavlyuchenkov, A. O. H. Olofsson, M. S. Lerner

We present pre-perihelion observations of methanol, carbon monoxide, and hydrogen cyanide in the Oort cloud comet C/2017 K2 (PANSTARRS), performed with the APEX 12-m and Onsala 20-m telescopes from April to July 2022. As the comets heliocentric distance decreased from 3.4 to 2.7 AU, CH3OH line intensities increased substantially (by factors of 1.1-4.0), with the most pronounced enhancement in lines with the upper-level energies Eu > 40K. In contrast, the brightness of the CO and HCN lines remained constant. We estimate the best-fit gas kinetic temperatures Tgas > 100 K and water production rate of Q(H2O)=(3-10)e28 1/s. The derived methanol-to-water abundance ratio approx. 0.01-0.04, depending on the observed period. Our results demonstrate that non-LTE effects are dominant in the coma and must be accounted for to accurately derive molecular production rates. We also report weak non-thermal excitation, including potential maser activity in the CH3OH 8(0)-7(1) line.

accepter by MNRAS

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Direct Absorption Spectroscopy at 1.1 THz: New Measurements of CrH (X6Σ+)

Rajat Ravi, Deacon J Nemchick, Brian J Drouin, Lucy M Ziurys

The pure rotational spectrum of the 52CrH radical in its X6Σ+ state at 1.1 THz has been recorded with direct absorption methods using a cascaded chain multiplier source. The N = 3 ←2 transition has been measured in multiple spin components for ΔJ = 0, ± 1, and the proton hyperfine structure resolved. The transition was also recorded for the 53Cr isotopologue in natural abundance and both the proton and 53Cr hyperfine splittings measured—the first observation of this species by rotational spectroscopy. The data, including previously measured N = 1 ← 0 and 2 ← 1 frequencies for the main isotopologue, were analyzed with a Hund's case (b) Hamiltonian that included third-order spin-rotation and fourth-order spin–spin terms. Rotational, fine structure, and proton hyperfine constants were determined for CrH, as well as 53Cr hyperfine parameters for 53CrH. In particular, the higher-order parameters γs and θ were established to a high degree of accuracy. The hyperfine constants for both nuclei are consistent with the unpaired electrons being principally located on the chromium nucleus. The Fermi contact term bF for the 53Cr nucleus suggests that the unpaired σ electron occupies an orbital mostly 3d in character.

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Temperature-programmed desorption of SO2 from water ice surfaces: Adsorption energy distributions

F. Benoit, A. B. Hacquard, J.-H. Fillion, M. Bertin

Context. Sulphur-bearing species play a key role in the chemical evolution of the interstellar medium and icy Solar System bodies such as the Jovian moons, yet the sulphur budget remains poorly constrained. Sulphur dioxide is considered one of the main sulphur reservoirs in icy environments, making its interaction with water ice surfaces highly relevant for astrochemical models. Aims. This work aims to extract adsorption energy distributions of SO2 on water ice substrates as a relevant model for astrophysical environments to better constrain its thermal behaviour and solid-gas exchange for astrochemical simulations. Methods. We performed a systematic experimental study of temperature-programmed desorption of SO2 deposited on three types of surfaces – polycrystalline gold, compact amorphous solid water (c-ASW), and crystalline water under ultra-high vacuum conditions – to then extract, using a Polanyi-Wigner model, the adsorption energy distributions of SO2 on each surface. Results. We performed the extraction of the adsorption energy distribution of SO2 deposited on water ice substrates. These exhibit a bimodal structure: a first physisorbed layer and a second, more strongly bound population. Only minor differences are observed between c-ASW and crystalline water ice in the behaviour of the distributions. We also provide mean values, most probable values, and width of the distribution. On average, the binding energy of SO2 on water ice surface is 439 +/- 41 meV.

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Announcements

Nautilus and KIDA training school

September 22 and 23, 2026 (Bordeaux, France)

Nautilus is a gas–grain astrochemical model. It is a three-phase model, which means that in addition to the gas phase, it treats ices as two separate phases: a surface and a bulk. It can be used in a variety of interstellar environments. Associated with Nautilus, the KIDA astrochemical database provides kinetic data for Nautilus based on laboratory and theoretical studies. Both Nautilus and KIDA are open to the public. Considering the number of new users each year, we propose a two-day training course on these tools. The program will include one day of lectures presenting the tools, followed by a hands-on session and time to work on users' specific problems on the second day.

The two-day school will be held in Bordeaux on September 22 and 23, 2026. The number of participants is limited to 20 and registrations will be accepted on a first come, first served basis. You can register through the link below before September 13.
A small amount of money will be available to partially fund the student travel.

https://nautilus.sciencesconf.org [via Valentine Wakelam]