

AstroChemical Newsletter #120

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Abstracts

Isotopomer-Specific Carbon Isotope Ratio of Complex Organic Molecules in Star-Forming Cores

Ryota Ichimura, Hideko Nomura, Kenji Furuya, Tetsuya Hama, T. J. Millar

The recent observation of complex organic molecules (COMs) in interstellar ices by the James Webb Space Telescope (JWST), along with previous gas-phase detections, underscores the importance of grain surface and ice mantle chemistry in the synthesis of COMs. In this study, we investigate the formation and carbon isotope fractionation of COMs by constructing a new astrochemical reaction network that distinguishes the position of ^{13}C within species (e.g., $\text{H}^{13}\text{COOCH}_3$ and $\text{HCOO}^{13}\text{CH}_3$ are distinguished). We take into account the position of ^{13}C in each species in gas and solid phase chemistry. This new model allows us to resolve isotopomer-specific $^{12}\text{C}/^{13}\text{C}$ ratios of COMs formed in the star-forming cores. We consider thermal diffusion-driven radical-radical reactions on the ice surface and non-thermal radiolysis chemistry in the bulk (surface + mantle) ice. We find that carbon isotope fractionation of the functional groups in COMs appears through both non-thermal radiolysis in cold environments and thermal diffusion in warm environments, depending on the COMs. In particular, COMs containing methyl groups show isotopomer differences in $^{12}\text{C}/^{13}\text{C}$ ratios that reflect their formation pathways and environments. These isotopomer-resolved fractionation patterns provide a diagnostic tool to probe the origins of COMs in star-forming cores. Our results suggest that future comparisons between high-sensitivity isotopic observations and isotopomer-specific models will be helpful for constraining the relative contributions of thermal and non-thermal formation processes of COMs.

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High-energy astrochemistry in the molecular interstellar medium

Brandt A. L. Gaches, Serena Viti

In the past decade, there has been a significant shift in astrochemistry with a renewed focus on the role of non-thermal processes on the molecular interstellar medium, in particular energetic particles (such as cosmic ray particles and fast electrons) and X-ray radiation. This has been brought about in large part due to new observations of interstellar complex organic molecules (iCOMs) in environments that would inhibit their formation, such as cold, dense gas in prestellar cores or in the highly energetic environments in galactic centers. In parallel, there has been a plethora of new laboratory investigations on the role of high-energy radiation and electrons on the chemistry of astrophysical ices, demonstrating the ability of this radiation to induce complex chemistry. In recent years, theoretical models have also begun to include newer cosmic-ray-driven processes in both the gas and ice phases. In this review, we unify aspects of the chemistry driven by X-ray radiation and energetic particles into a "high-energy astrochemistry", defining this term and reviewing the underlying chemical processes. We conclude by examining various laboratories where high-energy astrochemistry is at play and identify future issues to be tackled.

Accepted by ACS Earth and Space Chemistry (Eric Herbst Festschrift)

Full-text URL: <https://arxiv.org/abs/2512.10060>

X-ray and UV photochemical rates of CO ices

C. Laffon, Ph. Parent

X-rays are usually a minor component of the interstellar radiation field, but they can dominate locally near galactic or stellar sources and thus influence the chemistry of icy dust grains. In this work, laboratory experiments quantify how CO ice responds to both UV photons and X-rays through two key processes: photodesorption, which releases CO back into the gas phase, and photodissociation, which breaks CO into reactive fragments. At 10 K, UV-driven photodesorption rates agree with previous studies, whereas X-rays induce photodesorption that is about an order of magnitude more efficient. X-ray-induced photodissociation is even more effective, with rates two orders of magnitude higher than under UV irradiation, and both processes scale with the X-ray absorption cross section of CO. Importantly, CO destruction by X-rays is rapidly balanced by reformation reactions within the ice, leading to a steady state in which only a limited fraction (~25%) of the initial CO is lost. As a result, once this equilibrium is established, the evolution of CO ice is governed mainly by UV and X-ray photodesorption rather than by net chemical destruction.

A&A, 700, A43 (2025)

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Zooming into the water snow line: High-resolution water observations of the HL Tau disk

M. Leemker, S. Facchini, P. Curone, L. Rampinelli, M. Benisty, A. Garufi, and E. Humphreys

Water is one of the central molecules for the formation and habitability of planets. In particular, the region where water freezes-out, the water snowline, could be a favorable location to form planets in protoplanetary disks. We use high resolution ALMA observations to spatially resolve H₂O, H₁₃CO⁺ and SO emission in the HL Tau disk. A rotational diagram analysis is used to characterize the water reservoir seen with ALMA and compare this to the reservoir visible at mid- and far-IR wavelengths. We find that the H₂O 183 GHz line has a compact central component and a diffuse component that is seen out to ~75 au. A radially resolved rotational diagram shows that the excitation temperature of the water is ~350 K independent of radius. The steep drop in the water brightness temperature outside the central beam of the observations where the emission is optically thick is consistent with the water snowline being located inside the central beam (< ~6 au) at the height probed by the observations. Comparing the ALMA lines to those seen at shorter wavelengths shows that only 0.02%-2% of the water reservoir is visible at mid- and far-IR wavelengths, respectively, due to optically thick dust hiding the emission whereas 35-70% is visible with ALMA. An anti-correlation between the H₂O and H₁₃CO⁺ emission is found but this is likely caused by optically thick dust hiding the H₁₃CO⁺ emission in the disk center. Finally, we see SO emission tracing the disk and for the first time in SO a molecular outflow and the infalling streamer out to ~2". The velocity structure hints at a possible connection between the SO and the H₂O emission. Spatially resolved observations of H₂O lines at (sub-)mm wavelengths provide valuable constraints on the location of the water snowline, while probing the bulk of the gas-phase reservoirs.

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Effect of lowering gas-grain sticking coefficients on cold-core molecular abundances

C. Stadler, C. Laffon, P. Parent, A. Taillard, V. Wakelam

In cold and dense regions of the interstellar medium, gas-phase molecules collide with dust grains and may stick to their surfaces, initiating the growth of icy mantles. Astrochemical models usually assume a sticking coefficient of unity, meaning that every collision leads to adsorption. However, recent laboratory experiments indicate that sticking is often much less efficient. In this study, gas-grain chemical simulations are used to explore how reduced sticking coefficients affect the chemical evolution of cold cores. By varying the sticking coefficient between 0.1, 0.3, and 1, and comparing the resulting abundances of key species such as CO and CH₃OH with observations of several well-studied cold cores, we show that lower sticking coefficients delay ice growth and shift the timing of abundance peaks. For CO, reduced sticking strongly lowers the ice-to-gas ratio. Importantly, using more realistic sticking probabilities can reproduce observed gas-phase abundances as well as, or even better than, the standard assumption of perfect sticking, although it modifies the inferred chemical age of the cores.

A&A 700, A83 (2025)

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Deuterium fractionation and CO depletion in Barnard 5

I. Petrashkevich, A. Punanova, P. Caselli, J. E. Pineda, O. Sipilä, A. I. Vasyunin

Deuterium fractionation provides a key diagnostic of the physical and chemical evolution of prestellar and protostellar cores, where it is strongly linked to CO depletion in cold, dense gas. We present the first spatially resolved maps of deuterium fraction and CO depletion in the Barnard 5 (B5) region of the Perseus molecular cloud, covering both a starless core and the protostellar core hosting the Class 0/I source IRAS 03445+3242. Using IRAM 30m observations of N₂H⁺(1-0), N₂D⁺(1-0), H₁₃CO⁺(1-0), and DCO⁺(2-1), complemented by C₁₈O(2-1) data, we derive column density, deuterium fraction, and CO depletion maps. We find that the deuterium fraction in both mentioned nitrogen- and carbon-bearing species increases from the protostellar to the starless core, reaching RD(N₂H⁺)=0.43±0.10 and RD(HCO⁺)=0.09±0.02 in the starless core, compared with 0.15±0.03 and 0.05±0.01, respectively, in the protostellar core. The CO depletion factor also rises from 4.1±0.1 to 5.0±0.1 across the same transition. While the embedded YSO reduces deuteration in the dense inner gas, the less dense envelope traced by HCO⁺ is only slightly affected at our resolution. Our analysis confirms that CO freeze-out and the presence of a protostar jointly regulate deuterium chemistry in star-forming regions.

Accepted for publication in The Astrophysical Journal

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ALMA Band 7 Observations of Water Lines in the Protoplanetary Disk of V883 Ori

Hiroto Nakasone, Shota Notsu, Tomohiro C. Yoshida, Hideko Nomura, Takashi Tsukagoshi, Tomoya Hirota, Mitsuhiro Honda, Eiji Akiyama, Alice S. Booth, Jeong-Eun Lee, Seokho Lee

The FU Orionis star V883 Ori provides a unique opportunity to probe the water snowline in a protoplanetary disk. During an accretion burst, the enhanced stellar luminosity heats the disk, sublimating ices and bringing volatile species into the gas-

phase. The water snowline, located at 80 au in the midplane, represents a key boundary for dust growth and volatile delivery to forming planets. We present Atacama Large Millimeter/submillimeter Array Band 7 observations of V883 Ori that detect two targeted water isotopologue transitions: para-H₂(18O) at 322 GHz and HDO at 335 GHz. After correcting for Keplerian rotation, we detect HDO and H₂(18O) at 23.6 σ and 9.3 σ , respectively. Rotational-diagram analysis using a Markov Chain Monte Carlo approach yields $T_{\text{rot}}=116.89\pm12.81$ K and $N=(4.90\pm1.69)\times10^{15}$ cm⁻² for H₂(18O), and $T_{\text{rot}}=87.46\pm4.95$ K and $N=(4.47\pm0.62)\times10^{15}$ cm⁻² for HDO. These results imply water vapor abundances of $N_{\text{H}_2\text{O}}/N_{\text{H}_2}\sim3\text{e-}7\text{--}5\text{e-}6$ and an HDO/H₂(18O) ratio of $(0.4\text{--}2.0)\text{e-}3$ just inside the water snowline, broadly consistent with inheritance from protostellar envelopes. The HDO line in Band 7 is significantly weaker than predicted from Band 6 extrapolation, showing only $\sim 26\%$ of the expected strength. This attenuation can be explained by a more compact, hotter emitting region with an effective radius of ~ 53 au and/or frequency-dependent dust absorption that enlarges the apparent inner cavity at higher frequency. Our results highlight both the diagnostic power of water isotopologue lines and the need for higher angular resolution observations to resolve the water snowline and test these scenarios.

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Announcements

6th KROME School on Astrochemistry

We are pleased to announce the 6th KROME School on astrochemistry, a training school aimed at PhD students and early-career researchers interested in computational astrochemistry and star and planet formation.

The school will provide an introduction to the physical and chemical processes shaping molecular clouds, protoplanetary disks, and planetary atmospheres, with a strong focus on numerical and modeling approaches. Lectures from experts in the field will be complemented by tutorials and hands-on sessions designed to help participants build practical skills and confidence in using modern computational tools.

Dates: 13-17 July 2026

Location: Villa del Grumello, Lake Como, Como, Italy

Website: <https://krome.lakecomoschool.org/application/>

Topics include

- Astrochemical networks
- Dust evolution and surface chemistry
- Radiation-thermochemical modeling
- Cosmic rays
- Numerical methods in star and planet formation
- Synthetic observations

Invited speakers

- Til Birnstiel (LMU Munich, Germany)
- Paola Caselli (MPE, Germany)
- Cornelis Dullemond (ZAH, Heidelberg, Germany)
- Barbara Ercolano (LMU Munich, Germany)
- Troels Haugbølle (Niels Bohr Institute, University of Copenhagen, Denmark)
- Dwayne Heard (University of Leeds, UK)
- Pierre Hily-Blant (Université Grenoble Alpes, France)
- Inga Kamp (Leiden University, Netherlands)
- Yamila Miguel (Leiden Observatory, Netherlands)
- Marco Padovani (INAF-Arcetri, Italy)
- Christian Rab (LMU Munich, Germany)
- Daniel R. Reynolds (UMBC, USA)
- Dmitry Semenov (ITA, Heidelberg University, Germany)
- Serena Viti (Leiden Observatory, Netherlands)

Registration and applications

- Application deadline: 31.03.2026
- Notification of acceptance: 15.04.2026
- Registration deadline: 31.05.2026

The KROME School is particularly suited for students who wish to strengthen their background in computational modeling and gain insight into current research directions in astrochemistry and planet formation.

For full details, please visit: <https://krome.lakecomoschool.org>
[via Stefano Bovino]

KIDA survey

The Kinetic Database for Astrochemistry (KIDA <https://kida.astrochem-tools.org>) is a database of gas phase reaction rates and grain surface processes quantities compiled from the astrochemical literature. You can help us guide the future developments of the project by responding to this short survey: <https://framaforms.org/kida-survey-1706605349>

There are 10 questions and it should only take a few minutes to answer.

Thank you for your feedback
[via Pierre Gratier]