

AstroChemical Newsletter #122

March 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

Irradiation of methanol ice on a sulfur-rich dust analogue at 25 K: A mid-infrared spectroscopic study

D.V. Mifsud, Z. Kaňuchová, O. Auriacombe, P. Herczku, R. Rácz, S.T.S. Kovács, D. Qasim, B. Sulik, Z. Juhász, I. Vajda, I. Rajta, U. Raut, S. Biri, S. Ioppolo, and N.J. Mason

Despite possibly representing a comparatively large reservoir of sulfur in extraterrestrial environments, the role of sulfur allotropes in the radiation-driven chemistry occurring in low-temperature ices in astrophysical media (e.g., pre-stellar nebulae or the outer Solar System) is an underexplored topic. Previous work has shown that the irradiation of astrophysical ice analogues composed of simple molecules on top of layers of allotropic sulfur results in the formation of simple, inorganic sulfur-bearing molecules in the ice phase. Our present work seeks to qualitatively determine whether the analogous irradiation of methanol on top of allotropic sulfur may lead to the formation of organosulfur molecules, as well as H₂S. Using in situ mid-infrared absorption spectroscopy, we have found compelling evidence for the formation of SO₂, CS₂, H₂SO₄, and a number of sulfur oxyanions, as well as tentative evidence for H₂S formation. Evidence for the formation of thiol molecules was inconclusive. Our experimental results are discussed in the context of their applicability to sulfur astrochemistry.

Phys. Chem. Chem. Phys., 2026, Advance Article

DOI: [10.1039/D5CP03973H](https://doi.org/10.1039/D5CP03973H)

Full-text URL: <https://pubs.rsc.org/en/content/articlelanding/2026/cp/d5cp03973h>

Identification of solid N₂O in interstellar ices using open JWST data

V. Karteyeva, R. Nakibov, I. Petrashkevich, M. Medvedev, A. Vasyunin

Context. Only six molecules containing an N-O bond are detected in the gaseous phase of the interstellar medium. One of them is nitrous oxide (N₂O), which was unsuccessfully searched for in solid form since the launch of the Infrared Space Observatory (ISO) mission. The observational capabilities of the James Webb Space Telescope (JWST) present the possibility of identifying solid interstellar N₂O. Aims. We aim to identify nitrous oxide in open JWST spectra of interstellar ices toward a sample of Class 0, 0/I, and flat protostars using the relevant laboratory mixtures of N₂O-bearing interstellar ice analogs. Methods. A set of laboratory infrared transmission spectra was obtained for the following mixtures: N₂O:CO₂ = 1:20, N₂O:CO = 1:20, N₂O:N₂ = 1:20, N₂O:CO₂:CO = 1:15:5, and N₂O:CO₂:N₂ = 1:15:13 at 10–23 K. A search for N₂O in JWST NIRSpec spectra toward 50 protostars was performed by fitting the 4.44–4.47 μm (2250–2235 cm⁻¹) NN-stretch absorption band with new laboratory mixtures of N₂O-bearing ices. Results. We claim the first secure identification of N₂O in 16 protostars. The fitting results show that N₂O is formed predominantly within the apolar layer of the ice mantles, which are rich in CO, CO₂, and N₂. The abundance of solid N₂O is estimated at 0.2–2.1% relative to solid CO. We present the band strengths for N₂O in the mixtures corresponding to the apolar layer. We also report the identification of the C-N stretch band at 4.42 μm (2260 cm⁻¹), which we tentatively assign to HNCO, the simplest C-N bond carrier.

A&A, 706 (2026) L4

DOI: [10.1051/0004-6361/202557939](https://doi.org/10.1051/0004-6361/202557939)

Full-text URL: <https://arxiv.org/abs/2601.03705>

MINDS. Anatomy of a Water-rich, Inclined, Brown Dwarf Disk: Lack of Abundant Hydrocarbons

G. Perotti, N. T. Kurtovic, Th. Henning, G. Olofsson, A. M. Arabhavi, K. Schwarz, J. Kanwar, R. van Boeke, I. Kamp, I. Pascucci, E. F. van Dishoeck, M. Güdel, P-O. Lagage, D. Barrado, A. Caratti o Garatti, A. M. Glauser, F. Lahuis, V. Christiaens, R. Franceschi, D. Gasman, S. L. Grant, H. Jang, T. Kaeufer, M. Morales-Calderón, M. Temmink, and M. Vlasblom

2MASS J04381486+2611399 (or J0438) is one of the few young brown dwarfs (BDs) with a highly inclined ($i \sim 70^\circ$) disk. Here we report results from JWST Mid-Infrared Instrument (MIRI) Medium Resolution Spectroscopy, Hubble Space Telescope (HST) Advanced Camera for Surveys, and Atacama Large Millimeter/ submillimeter Array (ALMA) Band 7 observations. Despite its late spectral type (M7.25), the spectrum of J0438 resembles those of inner disks around earlier-type stars (K1–M5, T Tauri stars), with a volatile reservoir lacking hydrocarbons (except for acetylene, C₂H₂) and dominated by water. Other identified species are H₂, CO₂, HCN, [Ar⁺], and [Ne⁺]. The dominance of water over hydrocarbons is driven by multiple factors such as disk dynamics, young disk age, low accretion rate, and possible inner disk clearing. J0438 appears highly dynamic, showing a seesaw-like variability and extended emission in H₂ S(1), S(3), S(5), [Ne⁺], and CO (J = 3–2). Interestingly, the CO emission reaches up to 400 au from the BD, suggesting ongoing infalling/outflowing activity

impacting the disk chemistry. These observations underscore the combined power of MIRI, HST, and ALMA in characterizing the chemical diversity and dynamics of BD disks.

2026, ApJ, 997:281

DOI: [10.3847/1538-4357/ae2793](https://doi.org/10.3847/1538-4357/ae2793)

Full-text URL: <https://arxiv.org/abs/2504.11424>

exoALMA. XIX. Confirmation of Non-thermal Line Broadening in the DM Tau Protoplanetary Disk

Caitlyn Hardiman, Christophe Pinte, Daniel J. Price, Thomas Hilder, Iain Hammond, Taïssa Danilovich, Sean M. Andrews, Richard Teague, Giovanni Rosotti, Mario Flock, Gianni Cataldi, Jaehan Bae, Marcelo Barraza-Alfaro, Myriam Benisty, Nicolás Cuello, Pietro Curone, Ian Czekala, Stefano Facchini, Daniele Fasano, Misato Fukagawa, Maria Galloway-Sprietsma, Himanshi Garg, Cassandra Hall, Jane Huang, John D. Ilee, Andres F. Izquierdo, Kazuhiro Kanagawa, Geoffroy Lesur, Giuseppe Lodato, Cristiano Longarini, Ryan Loomis, Francois Menard, Ryuta Orihara, Jochen Stadler, Hsi-Wei Yen, Gaylor Wafflard-Fernandez, David J. Wilner, Andrew J. Winter, Lisa Wölfer, Tomohiro C. Yoshida, Brianna Zawadzki

Turbulence is expected to transport angular momentum and drive mass accretion in protoplanetary disks. One way to directly measure turbulent motion in disks is through molecular line broadening. DM Tau is one of only a few disks with claimed detection of nonthermal line broadening of 0.25cs–0.33cs, where cs is the sound speed. Using the radiative transfer code *mcFost* within a Bayesian inference framework that evaluates over five million disk models to efficiently sample the parameter space, we fit high-resolution (0.15", 28 m s⁻¹) 12CO J = 3–2 observations of DM Tau from the exoALMA Large Program. This approach enables us to simultaneously constrain the disk structure and kinematics, revealing a significant nonthermal contribution to the line width of ~0.4cs, inconsistent with purely thermal motions. Using the CO-based disk structure as a starting point, we reproduce the CS J = 7–6 emission well, demonstrating that the CS (which is more sensitive to nonthermal motions than CO) agrees with the turbulence inferred from the CO fit. Establishing a well-constrained background disk model further allows us to identify residual structures in the moment maps that deviate from the expected emission, revealing localized perturbations that may trace forming planets. This framework provides a powerful general approach for extracting disk structure and nonthermal broadening directly from molecular line data and can be applied to other disks with high-quality observations.

Hardiman et al 2026 ApJL 997 L47

DOI: [10.3847/2041-8213/ae313a](https://doi.org/10.3847/2041-8213/ae313a)

Full-text URL: <https://arxiv.org/abs/2602.01620>

The HITRAN2024 molecular spectroscopic database

I.E. Gordon, L.S. Rothman, R.J. Hargreaves, F.M. Gomez, T. Bertin, C. Hill, R.V. Kochanov, Y. Tan, P. Wcisło, V.Yu. Makhnev, P.F. Bernath, M. Birk, V. Boudon, A. Campargue, A. Coustenis, B.J. Drouin, R.R. Gamache, J.T. Hodges, D. Jacquemart, E.J. Mlawer, A.V. Nikitin, V.I. Perevalov, M. Rotger, S. Robert, J. Tennyson, G.C. Toon, H. Tran, V.G. Tyuterev, E.M. Adkins, A. Barbe, D.M. Bailey, K. Bielska, L. Bizzocchi, T.A. Blake, C.A. Bowesman, P. Cacciani, P. Čermák, A.G. Császár, L. Denis, S.C. Egbert, O. Egorov, A.Yu. Ermilov, A.J. Fleisher, H. Fleurbaey, A. Foltynowicz, T. Furtenbacher, M. Germann, E.R. Guest, J.J. Harrison, J.-M. Hartmann, A. Hjältén, S.-M. Hu, X. Huang, T.J. Johnson, H. Jóźwiak, S. Kassı, M.V. Khan, F. Kwabia-Tchana, F. Lee, D. Lisak, A.-W. Liu, O.M. Lyulin, N.A. Malarich, L. Manceron, A.A. Marinina, S.T. Massie, J. Mascio, E.S. Medvedev, V.V. Meshkov, G.Ch. Mellau, M. Melosso, S.N. Mikhailenko, D. Mondelain, H.S.P. Müller, M. O'Donnell, A. Owens, A. Perrin, O.L. Polyansky, P.L. Raston, Z.D. Reed, Z.D. Rey, C. Richard, G.B. Rieker, C. Röske, S.W. Sharpe, E. Starikova, N. Stolarczyk, A.V. Stolyarov, K. Sung, F. Tamassia, J. Terragni, V.G. Ushakov, S. Vasilchenko, B. Vispoel, K.L. Vodopyanov, K.L. Wagner, S. Wójciewicz, S.N. Yurchenko, N.F. Zobov

The HITRAN database is a curated compilation of validated molecular spectroscopic parameters, established in the early 1970s. It is used by various computer codes to predict and simulate the transmission and emission of light in gaseous media (with an emphasis on terrestrial and planetary atmospheres). The HITRAN compilation is composed of six major components. These components include the line-by-line spectroscopic parameters required for high-resolution radiative-transfer codes, experimentally derived absorption cross-sections (for molecules where it is not yet feasible for representation in a line-by-line form), collision-induced absorption data, aerosol indices of refraction, and general tables (including partition sums) that apply globally to the data. Responding to community requests, HITRAN2024 also incorporates — for the first time — a water-vapor continuum model. This paper describes the details of the choices of data and their compilation for the 2024 quadrennial edition of HITRAN. The HITRAN2024 edition takes advantage of recent experimental and theoretical data that were meticulously validated, in particular, against laboratory and atmospheric spectra. The new edition replaces the previous HITRAN edition of 2020 (including various updates during the intervening years). The extent of the updates of the line-by-line section in the HITRAN2024 edition ranges from updating a few lines of specific molecules/isotopologues to complete replacements of the lists, and also the introduction of additional isotopologues and six new (to HITRAN) molecules: H₃⁺, CH₃, S₂, COFCl, HONO, ClNO. Many new vibrational bands were added, extending the spectral coverage and completeness of the line lists. In addition, the accuracy of the parameters for major atmospheric absorbers has been increased substantially, often bringing the uncertainties down to unprecedented levels below 0.1%. The HITRAN2024 edition is available through www.hitran.org as well as the HITRAN Application Programming Interface (HAPI). The functionality of the tools to work with the HITRAN data has been extended for the new edition.

Journal of Quantitative Spectroscopy and Radiative Transfer 353, 109807 (2026)

PDRs4All: XVIII. The evolution of the PAH ionisation and PAH size distribution across the Orion Bar

Alexandros Maragkoudakis, Christiaan Boersma, Els Peeters, Louis J. Allamandola, Pasquale Temi, Vincent J. Esposito, Jesse D. Bregman, Alessandra Ricca, Felipe Alarcón, Olivier Berné, Mridusmita Buragohain, Jan Cami, Amélie Canin, Ryan Chown, Emmanuel Dartois, Asunción Fuente, Javier R. Goicoechea, Emilie Habart, Olga Kannavou, Baria Khan, Thomas S.-Y. Lai, Takashi Onaka, Dries Van De Putte, Ilane Schroetter, Ameet Sidhu, Alexander G. G. M. Tielens, Boris Trahin, Yong Zhang

We investigate the evolution of the PAH population's charge state and size across key physical zones in the Orion Bar, which include the HII region, the atomic PDR (APDR), and three HI/H2 dissociation fronts (DF1, DF2, and DF3). Utilising the NASA Ames PAH Infrared Spectroscopic Database (PAHdb) and the pyPAHdb spectral modelling tool, we analysed the MIRI-MRS observations of the Orion Bar from the "PDRs4All" ERS Program. pyPAHdb modelling reveals the fractional contribution of the different PAH charge states and sizes to the total PAH emission across the Orion Bar. Cationic PAH emission peaks in the APDR region, where neutral PAHs have minimal contribution. Emission from neutral PAHs peaks in the HII region that consists of emission from a face-on PDR associated to the background OMC-1 molecular cloud, and in the molecular cloud regions past DF2. PAH anions are observed deep within the DF2 and DF3 zones. The average PAH size ranges between $\sim 60\text{--}74$ Nc. The modelling reveals regions of top-down PAH formation at the ionisation front, and bottom-up PAH formation within the molecular cloud region. The PAH ionisation parameter γ ranges between $\sim 2\text{--}9 \times 10^4$. Intensity ratios tracing PAH ionisation scale well with γ in regions encompassing edge-on or face-on PDR emission, but their correlation weakens within the molecular cloud zone. Modelling of the $5\text{--}15\ \mu\text{m}$ PAH spectrum with pyPAHdb achieves comprehensive characterization of the net contribution of neutral and cationic PAHs across different environments, whereas empirical PAH proxy intensity ratio tracers can be highly variable and unreliable outside regions dominated by PDR emission. The derived average PAH size in the different physical zones is consistent with a view of PAHs being more extensively subjected to ultraviolet processing closer to the ionisation front, and less affected within the molecular cloud.

Accepted for publication in A&A

Full-text URL: <https://arxiv.org/abs/2601.23282>

MAJORS II: HCO⁺ & HCN Abundances in W40

René Plume, David J. Eden, Malcolm J. Currie, Lawrence K. Morgan, Xue-Jian Jiang, James DiFrancesco, Masatoshi Imanishi, Kee-Tae Kim, Tie Liu, Raffaele Rani, Alessio Traficante, Jane Cohen, Neal J. Evans II, Luis C. Ho, Eun Jung Chung, Sihan Jiao, Chang Won Lee, Dana Alina, Toby Moore, Jonathan M. C. Rawlings, Florian Kirchschrager, Sudeshna Patra, Andrew J. Rigby, Hsien Shang, Jihye Hwang, Patricio Sanhueza, Mark G. Rawlings, Kianoosh Tahani, Junfeng Wang, Kate Pattle, James S. Urquhart, Quang Nguyen-Luong, Sarah E. Ragan, Yang Su, Xindi Tang, Agata Karska, Michael G. Burton

We present observations of HCN and HCO⁺ J = 3–2 in the central 424"×424" region of the W40 massive star forming region. The observations were taken as part of a pilot project for the MAJORS large program at the JCMT telescope. By incorporating prior knowledge of N(H₂) and TK, assuming a constant density, and using the RADEX radiative transfer code we found that the HCN and HCO⁺ abundances range from $X(\text{HCN}) = [0.4\text{--}7.0]e\text{-}8$ and $X(\text{HCO}^+) = [0.4\text{--}7.3]e\text{-}9$. Additional modelling using the NAUTILUS chemical evolution code, that takes H₂ density variations into account, however, suggests the HCN and HCO⁺ abundances may be fairly constant. Careful modelling of three different positions finds $X(\text{HCN}) = [1.3\text{--}1.7]e\text{-}8$, $X(\text{HCO}^+) = [1.3\text{--}3.1]e\text{-}9$. Cross-comparison of the two models also provides a crude estimate of the gas density producing the HCN and HCO⁺ emission, with H₂ densities in the range $5e4\text{--}5e5\ \text{cm}^{-3}$, suggesting that the HCN and HCO⁺ emission does indeed arise from dense gas. High UV intensity (e.g. $G_0 > \text{a few thousand}$) has no effect on the abundances in regions where the visual extinction is large enough to effectively shield the gas from the UV field. In regions where $A_V < 6$, however, the abundance of both species is lowered due to destructive reactions with species that are directly affected by the radiation field.

2026, MNRAS, accepted Jan 23

DOI: [10.1093/mnras/stag186](https://doi.org/10.1093/mnras/stag186)

Full-text URL: <https://arxiv.org/abs/2601.19971>

Millimeter and Submillimeter Spectroscopy of Methylallene, CH₃CHCCH₂

Holger S. P. Müller, Frank Lewen, Jean-Claude Guillemin, Stephan Schlemmer

Small polycyclic aromatic hydrocarbons and somewhat larger cyano derivatives were detected in the cold dark cloud TMC-1 recently. Their formation from smaller hydrocarbons is not well understood, in part because abundances of many species are not known. Methylallene, CH₃CHCCH₂, may be one of the building blocks, but its rotational spectrum was characterized only to a very limited extent. We recorded rotational transitions in the 36 - 501 GHz region to extend the existing line list of methylallene and thus enable searches for the molecule in space. Quantum-chemical calculations were carried out to evaluate initial spectroscopic parameters. We obtained transition frequencies with $J \leq 61$ and $K_a \leq 21$ and resolved the internal rotation splitting of the CH₃ group at least partially. As a result, a full set of distortion parameters up to sixth order along with two octic ones were determined, as well as parameters describing the internal rotation of the methyl group. The spectroscopic parameters are accurate enough to identify methylallene up to 720 GHz, sufficient for searches even in the

warm interstellar medium.

Mol. Phys. (2026), in press.

DOI: [10.1080/00268976.2026.2625421](https://doi.org/10.1080/00268976.2026.2625421)

Full-text URL: <https://arxiv.org/abs/2601.22872>

Rotational Spectroscopy as a Tool to Study Vibration-Rotation Interaction: Investigations of (13)CH₃CN and CH₃(13)CN up to v₈ = 2 and a Search for v₈ = 2 Transitions toward Sagittarius B2(N)

Holger S. P. Müller, Arnaud Belloche, Frank Lewen, Stephan Schlemmer

Methyl cyanide, CH₃CN, is present in diverse regions in space, in particular in the warm parts of star-forming regions where it is a common molecule. Rotational transitions of (13)CH₃CN and CH₃(13)CN in their v₈ = 1 lowest excited vibrational states are quite prominent in Sagittarius B2(N). In order to be able to search for transitions of the next higher vibrational state v₈ = 2, we recorded spectra of samples enriched in (13)CH₃CN and CH₃(13)CN up to v₈ = 2 in the 35 to 1091 GHz region and reinvestigated existing spectra of CH₃CN in its natural isotopic composition between 1085 and 1200 GHz. Perturbations caused by near-degeneracies in K = 4 of v₈ = 2,0 and K = 2 of v₈ = 2,-2 yielded accurate information on the energy spacing of 22.93 and 21.79 cm⁻¹ between the l-components of (13)CH₃CN and CH₃(13)CN, respectively. Fermi-type interaction between K = 13 and 14 of v₈ = 1,-1 and v₈ = 2,+2 probe the energy differences between the two states of both isotopomers. In addition, a DK -2, D_l+1 interaction between the ground vibrational state of (13)CH₃CN and v₈ = 1,+1 provides information on their energy spacing. Furthermore, we obtained improved or extended ground state rotational transition frequencies of (13)CH₃(13)CN and extensive data for (13)CH₃C(15)N and CH₃(13)C(15)N. Finally, we report the results of our search for transitions of (13)CH₃CN and CH₃(13)CN in their v₈ = 2 states toward Sagittarius B2(N).

ACS Earth Space Chem. (2026) 10, 578–591

DOI: [10.1021/acsearthspacechem.5c00353](https://doi.org/10.1021/acsearthspacechem.5c00353)

Full-text URL: <https://arxiv.org/abs/2601.22824>

Infrared spectra of methane-containing ice mixtures for JWST data analyses

Varvara Karteyeva, Ruslan Nakibov, Igor Petrashkevich, Mikhail Medvedev, Anton Vasyunin

Context. Solid methane (CH₄) is an important molecule in interstellar and planetary environments, serving as a precursor to complex organic compounds and a potential biosignature in exoplanetary studies. Despite its significance, laboratory data on low-temperature phase of methane below 10 K remain limited. Aims. We aim to obtain spectra of methane in binary mixtures at 10 K and compare it to the spectra obtained at 6.7 K. These temperatures correspond to phases II and II* of pure methane and are representative of dark molecular clouds and protostars at early stages. We also aim to test the obtained data applicability to JWST data interpretation. Methods. Laboratory reference spectra were obtained on the ISEAge setup via FTIR spectroscopy in transmission mode. A weighted χ^2 minimization is used for the fitting. Results. We present infrared spectra with corresponding band strengths of pure methane and binary mixtures with methane: CH₄:H₂O, CH₄:CO₂, CH₄:CH₃OH, CH₄:NH₃ at 6.7 K and 10 K showing a 20% increase in mixtures compared to commonly used 10 K band strength value of pure methane. We also test the usability of the spectra on open JWST data by probing the spatial distribution of methane in B335. We also present additional experiments concerning the phase transition of methane between phase II* and phase II. Conclusions. Our results reveal distinct spectral features for methane in non-H₂O environments, enabling more accurate interpretation of JWST observations. The dataset of spectra, publicly available on Zenodo, can be used for fitting JWST data.

9 pages, 4 figures, 2 tables, accepted to Astronomy&Astrophysics

Full-text URL: <https://arxiv.org/abs/2602.14604>

PRODIGE - envelope to disk with NOEMA: VII. (Complex) organic molecules in the NGC1333 IRAS4B1 outflow: A new laboratory for shock chemistry

Laura A. Busch, J. E. Pineda, P. Caselli, D. M. Segura-Cox, S. Narayanan, C. Gieser, M. J. Maureira, T.-H. Hsieh, Y. Lin, M. T. Valdivia-Mena, L. Bouscasse, Th. Henning, D. Semenov, A. Fuente, Y.-R. Chou, L. Mason, P. C. Cortés, L. W. Looney, I. W. Stephens, M. Tafalla, A. Dutrey, W. Kwon, P. Saha

Shock chemistry is an excellent tool to shed light on the formation and destruction mechanisms of complex organic molecules (COMs). The L1157-mm outflow is the only low-mass protostellar outflow that has extensively been studied in this regard. Using the data taken as part of the PRODIGE (PROTostars & Disks: Global Evolution) large program, we aim to map COM emission and derive the molecular composition of the protostellar outflow driven by the Class 0 protostar NGC1333 IRAS4B1 to introduce it as a new laboratory to study the impact of shocks on COM chemistry. In addition to typical outflow tracers such as SiO and CO, outflow emission is seen from H₂CO, H₂NCO, and HC₃N, as well as from the COMs CH₃OH, CH₃CN, and CH₃CHO, and even from deuterated species such as DCN, D₂CO, and CH₂DOH. Maps of integrated intensity ratios between CH₃OH and DCN, D₂CO, and CH₃CHO reveal gradients with distance from the protostar. Intensity ratio maps of HC₃N and CH₃CN with respect to CH₃OH peak in the southern lobe where temperatures are highest. Rotational temperatures derived towards two positions, one in each lobe, are found in the range ~50-100 K. Abundances with respect to CH₃OH are higher by factors of a few than for the L1157-B1. In conclusion, for the first time, we securely detected the COMs CH₃CN, CH₃CHO, and CH₂DOH in the IRAS 4B1 outflow, serendipitously with limited sensitivity and bandwidth.

Targeted observations will enable the discovery of new COMs and a more detailed analysis of their emission. Morphological differences between molecules in the IRAS 4B1 outflow lobes and their relative abundances provide first proof that this outflow is a promising new laboratory for shock chemistry, which will offer crucial information on COM formation and destruction as well as outflow structure and kinematics.

Accepted for publication in A&A

Full-text URL: <https://arxiv.org/abs/2602.17177>

H2 Ortho-Para Spin Conversion on Inhomogeneous Grain Surfaces. II. impact of the rotational energy difference between adsorbed ortho-H2 and para-H2 and implication to deuterium fractionation chemistry

K. Furuya, T. Sugimoto, K. Iwasaki, M. Tsuge, N. Watanabe

We investigate how the H₂ ortho-to-para ratio (OPR) and deuterium fractionation in star-forming regions are affected by nuclear spin conversion (NSC) on dust grains. Particular focus is placed on the rotational energy difference between ortho-H₂ (o-H₂) and para-H₂ (p-H₂) on grain surfaces. While the ground state of o-H₂ has a higher rotational energy than that of p-H₂ by 170.5 K in the gas phase, this energy difference is expected to become smaller on solid surfaces, where interactions between the surface and adsorbed H₂ molecules affect their rotational motion. A previous study by Furuya et al. (2019) developed a rigorous formulation of the rate for the temporal variation of the H₂ OPR via the NSC on grains, assuming that adsorbed o-H₂ has higher rotational energy than adsorbed p-H₂ by 170.5 K, as in the gas phase. In this work, we relax the assumption and re-evaluate the rate, varying the rotational energy difference between their ground states. The re-evaluated rate is incorporated into a gas-ice astrochemical model to study the evolution of the H₂ OPR and the deuterium fractionation in prestellar cores and the outer, cold regions of protostellar envelopes. The inclusion of the NSC on grains reduces the timescale of the H₂ OPR evolution and thus the deuterium fractionation, at densities of $>1\text{e}4\text{ cm}^{-3}$ and temperatures of $<14\text{-}16\text{ K}$ (depending on the rotational energy difference), when the ionization rate of H₂ is $1\text{e-}17\text{ s}^{-1}$.

Accepted in ApJ

Full-text URL: <https://arxiv.org/abs/2602.13122>

Simulation of proton radiolysis of H₂O and O₂ ices with the Nautilus code

Tian-Yu Tu, Valentine Wakelam, Jean-Christophe Loison, Marin Chabot, Emmanuel Dartois, Yang Chen

The radiolysis effect of cosmic rays (CRs) plays an important role in the chemistry in molecular clouds. CRs can dissociate the molecules on dust grains, producing reactive suprathermal species and radicals which facilitate the formation of large molecules. We add the radiolysis process and some relevant reactions into the Nautilus astrochemical code. By adjusting some parameters, we investigate the sensitivity of the simulation results of the H₂O ice on the removal of reaction-diffusion competition, the removal of non-diffusive chemistry, and the desorption energies of the suprathermal species. We find the model, with a few adjustments of the chemistry, can reproduce the steady-state $[\text{H}_2\text{O}_2]/[\text{H}_2\text{O}]$ and $[\text{O}_3]/[\text{O}_2]_0$ abundance ratios in the H₂O and O₂ radiolysis experiments at any CR flux in the experiments. These adjustments in the model do not fully reproduce the fluence required to reach the steady state. It tends also to overestimate the destruction of H₂O as measured in H₂O radiolysis experiments. We show that reducing the G-values of H₂O radiolysis, which implies an increase in the efficiency of immediate reformation of water locally after ion impact, leads to simulated H₂O destruction rates closer to the experiments. The effect of reaction-diffusion competition on the simulation results of H₂O ice is significant at $\zeta \leq 1\text{e-}14\text{ s}^{-1}$. The non-diffusive chemistry affects the simulation results at 16 K but not 77K, while the results are sensitive to the desorption energies of suprathermal H, O, O₃ and OH at 77 K. Our results show that the steady-state $[\text{H}_2\text{O}_2]/[\text{H}_2\text{O}]$ and $[\text{O}_3]/[\text{O}_2]_0$ in experiments can be reproduced by fine-tuning the chemical model, but still call for more constraints on the intermediate pathways in the radiolysis processes, especially the ion chemistry in the ice bulk, as well as activation barriers and branching ratios of the reactions in the network.

Accepted for publication in A&A

Full-text URL: <https://arxiv.org/abs/2602.19996>

Announcements

Expressions of interest for two PhD positions (4-year each) at the Molecular Astrophysics Department of IFF-CSIC (Madrid, Spain)

Two fully funded PhD positions are available at the Molecular Astrophysics Department of the Instituto de Física Fundamental in Madrid in the context of the ERC Starting Grant project "ISOCOSMOS". Isomeric imbalances are precious proxies to diagnose a variety of astronomical environments, where the very low temperatures essentially impose a strict kinetic control on molecular inventories. In this project, we aim to understand and leverage the isomeric ratios observed in interstellar environments, proposing new isomers for interstellar detection, rationalizing their chemical routes of formation and destruction, and ultimately using them as probes of the physical conditions of their host environments.

The two PhD candidates will focus on the theoretical modelling of isomer-selective processes in interstellar environments, working on two complementary aspects:

(i) isomer-specific gas-phase reactions (e.g., ion-neutral, neutral-neutral reactions) and tunneling-mediated isomerization in

vacuum,

(ii) isomerization and isomer-selective reactions on icy dust grain surfaces, for example through tunneling-mediated hydrogen addition and abstraction reactions.

The candidates will employ state-of-the-art quantum chemistry and molecular dynamics methods to sample the potential energy surfaces of relevant reactions, connecting the resulting surfaces with the derivation of reaction rate constants and inclusion of the data in our astrochemical kinetic models. Finally, the results will be compared with astronomical observation campaigns carried out in our institute.

The candidates will work under the supervision of Dr. Germán Molpeceres in both projects, with co-supervision of Dr. Octavio Roncero for the gas-phase reaction project.

Candidate profile and requirements

The candidate must hold a Master's degree in Physics, Chemistry, or a closely related field. In accordance with CSIC regulations, a Master's title is required to formalize the contract. Consequently, applications from candidates who do not hold a Master's degree, or who do not plan to obtain it before the end of the 2025–2026 academic year (July 2026), cannot be considered.

The ideal candidate will have a strong background in quantum chemistry, together with solid programming (Python, Fortran) and data visualization skills. A good understanding of chemical kinetics and reaction dynamics is also highly desirable, as is familiarity with machine learning techniques applied to molecular sciences. A genuine interest in astrophysics is essential, although prior experience in the field is not strictly required.

What we offer

We offer two fully funded 4-year PhD positions, with a competitive salary according to the Spanish National Research Council (CSIC) standards. The candidates will have access to dedicated computational facilities at the IFF-CSIC as well as centralized CSIC supercomputing resources. The candidates will also have the opportunity to attend international conferences and workshops, as well as to visit collaborating institutions abroad. Estimated start date: July 2026 - February 2027

Application process

Applicants should send a CV, a motivation letter, the contact details of at least one referee, and the position of preference (gas-phase or surface chemistry) to Dr. Germán Molpeceres. The starting date is flexible within 2026 and the beginning of 2027. If the MSc degree has not yet been obtained, applicants should indicate the expected completion date. Applications will be reviewed on a rolling basis until the position is filled.

First announcement: Final COST NanoSpace Joint Scientific Meeting

When: 15-17 September 2026

Where: IACTEC, Tenerife, Canary Islands, Spain

Registration Deadline: 30 June 2026

Contact email: nanospacefjsm2026@iac.es

Website: <https://meetings.iac.es/nanospacefjsm2026/>

The Final Joint Scientific Meeting of the COST Action NanoSpace (CA21126; <https://research.iac.es/proyecto/nanospace/>) will take place 15-17 September 2026, at IACTEC, La Laguna, Tenerife, Canary Islands, Spain. You can find all detailed information about the venue, registration (participation is free), abstract submission, etc., in the meeting website: <https://meetings.iac.es/nanospacefjsm2026/>. The event will bring together leading scientists, researchers, and innovators to explore the pivotal role of carbon-based molecular nanostructures in space science and technology.

The Final COST NanoSpace Joint Scientific Meeting will focus on the fundamental and applied research of diverse carbon-based molecular nanostructures — including fullerenes, graphene, carbon nanotubes, and their derivatives — within the broader context of space science and exploration. The meeting will address key questions related to the formation, evolution, properties, and potential applications of these nanocarbon materials under space-relevant conditions. Discussions will be structured around the major Working Group (WG) topics, and including thematic areas such as: (i) formation and characterization; (ii) space radiation and stability; (iii) astrobiology and planetary science; (iv) applications in space technology; (v) laboratory studies; and (vi) catalysis in space, among others. By bringing together experimental, theoretical, and observational perspectives, the meeting aims to foster interdisciplinary dialogue and consolidate the scientific advances achieved within the COST Action NanoSpace.

This is the Final Joint Action Meeting (in person), focused on the main Action scientific results achieved by the interaction and collaboration among the diversity of disciplines (laboratory astrophysics, theoretical chemistry and physics, astronomy, astrobiology, material science, among others) and researchers (especially from Inclusiveness Target Countries and Young Researchers) of the Action. The program will be composed by scientific sessions separated by WG topic, and short special sessions on the NanoSpace Knowledge Hub, NanoSpace games, and NanoSpace links with industry are also planned.

The deadline for registration and abstract submission is 30th June 2026.

THERE IS NO REGISTRATION FEE and the NanoSpace COST Action will provide financial support (i.e., reimbursement

after the event) for a significant number of participants (at least ~60-80), with high priority to PhD students and Young Researchers presenting a contribution (contributed talk or poster) and researchers with a primary affiliation in an institution located in an Inclusiveness Target Country (ITC) / Near Neighbour Country (NNC) participating in the Action. Please check the meeting website (<https://meetings.iac.es/nanospacefjism2026/>) for news and updates about the final list of invited speakers, hotel registration links, etc. More detailed information will be given in the second announcement. Looking forward to have a wonderful final meeting! Kind regards, Anibal Garcia-Hernández (Chair of the COST Action NanoSpace)

Postdoc in Molecular Astrophysics with JWST (3 yr) at DCBP, Universität Bern

PROJECT DESCRIPTION

What sets the chemical composition of planet-forming materials? By studying the composition of the earliest sites of star and planet formation with JWST, we can begin to unravel how natal environments predetermine planetary composition.

The goal is to observationally study prestellar cores and protostellar environments with JWST, in order to obtain a chemical inventory of the interstellar ices therein. To start, NIRCAM and NIRSpec data are already available for reduction and analysis. Of particular interest to the project are complex organic species and their precursors. Over the course of the project, emphasis will be placed on securing statistically significant samples. As a postdoctoral researcher, you will be given significant autonomy and will help develop future research areas. You will immediately become part of international consortia with ample opportunity to collaborate and expand your network. This is a fixed-term, 3-year position funded by the European Research Council (ERC) 2025 Consolidator Grant (CoG).

You will join a brand-new ambitious Molecular Astrophysics Group at the Department of Chemistry, Biochemistry and Pharmaceutical Sciences (DCBP) at Universität Bern (UniBe), founded on May 1st, 2026. With us, you will have a major impact on shaping the group's culture and approach to science for the coming years. As a more experienced member of a new and growing research group, you will be expected to take on roles with more responsibilities, while benefiting from more facetime with your supervisor and short internal decision making. Powerful computers to facilitate work on JWST data will be made available. The Molecular Astrophysics Group will be an international team with scientific excellence, mutual empowerment, and collective resilience as its core values.

WHAT YOU WILL DO

- Reduce and analyze JWST NIRCAM and NIRSpec data
- Develop and apply data reduction pipelines
- Lead publications in high-impact journals
- Contribute to and lead future observing proposals
- Present results at international conferences and consortia meetings
- Co-supervise MSc/PhD students (optional)

REQUIREMENTS

- PhD degree in a relevant field (astronomy, astrophysics, chemistry, physics)
- Research experience backed by a publication record
- Programming skills (e.g., Python)
- Interest to develop leadership skills and work autonomously
- [preferred] Research experience with JWST data and molecular astrophysics
- [preferred] Experience developing pipelines for observational data reduction

START DATE

June 1st, 2026 or later by agreement

APPLICATION INSTRUCTIONS

Applications will be considered on a rolling basis until filled. Apply by March 31st, 2026 for full consideration. Send the following documents in a single PDF to maria.drozdovskaya@unibe.ch

1. Motivation Letter (1 pg. max)
2. CV
3. Publication List
4. Contact information of 3 references (that may be contacted for a reference letter at a later stage)

PhD in Molecular Astrophysics and Star Formation (4 yr) at DCBP, Universität Bern

PROJECT DESCRIPTION

How chemically complex do molecules in star-forming regions get and how do they form? Unbiased spectral surveys executed with the most powerful interferometers such as the Atacama Large Millimeter/submillimeter Array (ALMA) allow us to robustly identify 100s of molecules and constrain their abundances in regions containing infant stars. Meanwhile, state-of-the-art physicochemical models permit us to disentangle the individual chemical pathways towards chemical complexity and identify the most conducive physical environments. The first goal is to observationally study star-forming regions with ALMA, in order to identify chemically complex molecules, their isotopologs, and their abundances. The second goal is to model the physical processes of star and protoplanetary disk formation alongside chemical process that produce and destroy complex organic molecules. ALMA data and initial modelling framework are already available. By the end of the project, you are expected to defend your PhD thesis and emerge with dual expertise in, both, radio observations and physicochemical modelling. You will immediately become part of international consortia with ample opportunity to collaborate and build your network. This is a fixed-term, 4-year position funded by the European Research Council (ERC) 2025 Consolidator Grant (CoG).

You will join a brand-new ambitious Molecular Astrophysics Group at the Department of Chemistry, Biochemistry and

Pharmaceutical Sciences (DCBP) at Universität Bern (UniBe), founded on May 1st, 2026. With us, you will have a major impact on shaping the group's culture and approach to science for the coming years. As a member of a new and growing research group, you will benefit from close supervision by your supervisor and more senior group members, and short internal decision making. Powerful computers to facilitate work on ALMA data will be made available. The Molecular Astrophysics Group will be an international team with scientific excellence, mutual empowerment, and collective resilience as its core values.

WHAT YOU WILL DO

- Analyze ALMA data and learn data reduction pipelines
- Develop physical models of star formation and networks for interstellar chemistry
- Lead publications in high-impact journals
- Contribute to and lead future observing proposals
- Present results at international conferences and consortia meetings

REQUIREMENTS

- MSc degree in a natural science or engineering (astronomy, astrophysics, chemistry, physics, or another relevant field)
- Programming experience (e.g., Python)
- Interest in chemical composition and physicochemical processes transpiring in star-forming regions
- Competence in spoken and written English (C1 or higher)
- Exposure to basic astronomy is preferred

START DATE

June 1st, 2026 or later by agreement

APPLICATION INSTRUCTIONS

Applications will be considered on a rolling basis until filled. Apply by March 31st, 2026 for full consideration. Send the following documents in a single PDF to maria.drozdovskaya@unibe.ch

1. Motivation Letter (2 pg. max), including reasons for pursuing a PhD in general and for choosing the research field of molecular astrophysics
2. CV
3. Complete list and transcripts of all Bachelor- and Master-level courses, with a translation if not in English, German, French, Russian, or Dutch (notarized translation is not needed)
4. Contact information of 2 references (that may be contacted for a reference letter at a later stage)

Postdoc in Molecular Astrophysics with JWST (1 yr) at DCBP, Universität Bern

PROJECT DESCRIPTION

What is the chemical composition of interstellar ices in molecular clouds, protostellar regions, and protoplanetary disks? With JWST, this can now be determined at an unprecedented accuracy.

The idea is to assemble an inventory of interstellar ice species and their abundances across the full evolutionary range of star- and planet-forming regions. Upon agreement, a specific evolutionary stage and corresponding JWST data set will be selected for a focused project achievable within the 1-yr timeframe. This is a short-term (1-yr with a potential extension depending on funding) postdoc opportunity, which could be ideal for a more experienced postdoc in need of bridge funding or an ambitious early postdoc, while applying for own independent funding, for example. Ample support will be provided for such pursuits of independent funding. As a more senior member of the group, you will be given significant autonomy and will help develop future research areas. You will have the opportunity to become part of international consortia with many opportunities to collaborate and expand your network. The initial fixed-term, 1-year position is funded by the European Research Council (ERC) 2025 Consolidator Grant (CoG).

You will join a brand-new ambitious Molecular Astrophysics Group at the Department of Chemistry, Biochemistry and Pharmaceutical Sciences (DCBP) at Universität Bern (UniBe), founded on May 1st, 2026. With us, you will have a major impact on shaping the group's culture and approach to science for the coming years. As a more experienced member of a new and growing research group, you will be expected to take on roles with more responsibilities, while benefiting from more facetime with your supervisor and short internal decision making. Powerful computers to facilitate work on JWST data will be made available. The Molecular Astrophysics Group will be an international team with scientific excellence, mutual empowerment, and collective resilience as its core values.

WHAT YOU WILL DO

- Reduce and analyze JWST data
- Lead publications in high-impact journals
- Present results at international conferences and consortia meetings
- Co-supervise MSc/PhD students (optional)

REQUIREMENTS

- PhD degree in a relevant field (astronomy, astrophysics, chemistry, physics)
- Research experience backed by a publication record
- Programming skills (e.g., Python)
- Interest to pursue independent funding
- Research experience with JWST data and/or molecular astrophysics

START DATE

June 1st, 2026 or later by agreement

APPLICATION INSTRUCTIONS

Applications will be considered on a rolling basis until filled. Apply by March 31st, 2026 for full consideration. Send the following documents in a single PDF to maria.drozdovskaya@unibe.ch

1. Motivation Letter (1 pg. max)
2. CV
3. Publication List
4. Contact information of 3 references (that may be contacted for a reference letter at a later stage)

Laboratory Astrophysics Newsletter First Issue

We are excited to present the Laboratory Astrophysics Newsletter, whose goal is to enhance communication and interactions between experimentalists, theoreticians, modelers, and observers in the fields of Astrophysics and Planetary Science around the world. The Laboratory Astrophysics Newsletter is intended to be released quarterly. Each issue will focus on a particular theme in the Laboratory Astrophysics field and include sections such as a cover image, a scientist interview, a description of facilities, recent publications in the field, and/or announcements for upcoming meetings. The theme of the first issue was Cold Solar System Objects. You can find it at: <https://www.nasa.gov/ames/science/laboratory-astrophysics-newsletter/>

In future issues, we look forward to featuring various Laboratory Astrophysics themes and include interviews of scientists and presentations of facilities around the world.

We welcome contributions. You can share publications and announcements through our contributions form, and join our mailing list or contact us at: labastronewsletter@mail.nasa.gov.

Keep an eye out for our next issue, in March 2026, and please let us know what you would like future themes to be or if you would like to contribute!