AstroChemical Newsletter #128

October 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

Deuteration of Organic Molecules as a Probe of Starless Core and Filament Evolution in Barnard 10

H. Andras-Letanovszky, Y. L. Shirley, L. J. Steffes, B. Svoboda, H. Gruber, S. Scibelli, E. Vertachnik

The deuterium fractionation of molecules in starless cores is sensitive to their dynamical histories, which recent magnetohydrodynamical simulations have shown to be extremely varied. The deuterated isotopologues of formaldehyde (H2CO) and methanol (CH3OH) probe deuterium fractionation in simple organic molecules. This complete survey targets 11 low-mass starless cores in the small, quiescent Barnard 10 (B10) region of the Taurus Molecular Cloud. The cores were observed using the 12m Arizona Radio Observatory telescope with a 100% detection rate in transitions of o/pH2CO, HDCO, pD2CO, A/E-CH3OH, and CH2DOH and the dense gas tracer N2H+. The HDCO and pD2CO column densities and deuterium fractions are not correlated with those of the grain-surface deuteration tracer CH2DOH, indicating significant gas-phase formation of deuterated formaldehyde. The observed deuterium fractions do not correlate with evolutionary indicators (e.g. core central density) or physical conditions (e.g. core mass). We also find that cores within the northwestern filament have lower deuterium fractions than cores of similar densities in the other two filaments. These could indicate differential core evolution both between and within entire filaments. Comparing the deuterium fractions of the B10 sample to published sources across different evolutionary stages suggests the inheritance of D2CO from starless cores, although more surveys of organic deuteration are needed to conclusively determine inheritance.

Accepted for publication in Publications of the Astronomical Society of the Pacific (PASP).
DOI: 10.1088/1538-3873/ae9a00
Full-text URL: https://arxiv.org/abs/2609.00308

Resolving dense photodissociation regions: the structure of photochemical fronts in three-dimensional gas distributions

Brandt A. L. Gaches, Thomas G. Bisbas, Lothar Brendel, Zhengping Zhu

For decades, the Orion Bar has been the prototypical photodissociation region. Viewed nearly edge-on, it offers a unique window into the stratified chemical structure of the atomic-to-molecular transition of the interstellar medium. Understanding its photochemistry is essential to interpreting key observations originating from dense photo-dissociation regions. ALMA and JWST observations reveal that H2 photodissociation front overlaps with the C+ recombination front and exhibits a complex spatial morphology. Despite considerable theoretical effort, existing modeling approaches based on simplified geometrical assumptions have difficulties reproducing the spatial emission structure. Our aim is to investigate the response of photochemistry in realistic three-dimensional density distributions, using the Orion Bar as a representative application. We present the first fully three-dimensional high-resolution model of an Orion Bar analogue that resolves the relevant photochemical fronts using the upgraded steady-state 3D-PDR photo-dissociation region code, which allows for the treatment of plane-irradiatation and for the solution of the non-LTE H2 rovibrational levels. We find that the H2 dissociation front is characterized by a complex surface that overlaps with the C+ recombination front. Our 3D model can reproduce the complex morphology of H2 emission seen in observations, in particular the arc- and filament-like features, and provides a physical explanation of its chemistry. The overlapping H2 dissociation and C+ recombination fronts and the spatial emission morphology can be explained due to the three-dimensional gas distribution, resulting in shadowing and shielding by dense substructures. Our results mark a turning point for astrochemistry, where three-dimensional steady-state models can deliver fundamentally new insights into the chemistry of the interstellar medium. (Abridged)

Accepted to A&A.
DOI: 10.1051/0004-6361/202660769
Full-text URL: https://arxiv.org/abs/2608.04116

Inventories of Rich Carbon-Chain Chemistry in Prestellar and Starless Cores in the Perseus Molecular Cloud

A. Pokorny-Yadav, S. Scibelli, J. Ferrer Asensio, Y. Shirley, A. Megías, I. Jiménez-Serra

Carbon-chain molecules serve as an important reservoir of reactive organic matter that will eventually be incorporated into protoplanetary disks, planets, and cometary material. Prestellar and starless cores are composed of cold (~ 10 K) and dense (~ 10e5 cm−3) clumps of gas and dust within molecular clouds, and are nurseries for low-mass stars and planetary systems. Surveys of starless cores have focused on the study of complex organic molecules, COMs, whereas observations of carbon-chains in starless cores are limited. We analyze the carbon-chain inventories of 15 prestellar and starless cores in

the Perseus Molecular Cloud. Using Yebes 40m single-dish observations, we detect CS, CCS, CCCS, HC3N, DC3N, and HC5N in at least 10/15 cores and HC7N in 4/15 cores. Our study also finds related isotopologues, where 13CS, C34S, C13CS, CC34S, H13CCCN, HC13CCN, HCC13CN, HC13CCCCN, HCC13CCCN, HCCC13CCN, HCCCCC15N, and DCCCCCN are detected. We report detection statistics, compare column density ratios with Taurus, Serpens, and protostar sources, examine DC3N/HC3N deuterium fractionation, and investigate the relative abundances and correlations between cyanopolyyne (HCnN) and sulfur-bearing (CnS) carbon-chains. The diverse suite of species detected reveals the richness of carbon-chain chemistry in Perseus and illustrates how local environmental conditions, such as density, temperature, and proximity to protostellar activity, shape each core's molecular inventory and relative evolutionary phase. Our findings provide a glimpse into the carbon-chain reservoir of starless and prestellar cores in Perseus, which may ultimately be inherited by emerging protoplanetary disks and later integrated into planetary systems and biologically relevant material.

Accepted for publication in MNRAS (2026)
DOI: 10.1093/mnras/stag1509
Full-text URL: https://arxiv.org/abs/2608.05264

Rotational spectroscopy of cyclopentadiene oxide

Bettina Heyne, Mariyam Fatima, Holger S. P. Müller, Prachi Misra, Stephan Schlemmer, Jean-Claude Guillemin

The first rotational study of cyclopentadiene oxide (C5H6O, CPO) is presented. Three spectrometers were employed for measurements between 11.5 and 500 GHz. In these measurements, 1986 lines could be assigned, whose quantum numbers ranged to a maximum value of J = 75 and Ka = 56. Quantum chemical calculations were performed and provided starting values for deriving spectroscopic parameters. Rotational parameters, as well as quartic and sextic distortion parameters, are presented which shall enable an astronomical search of this heterobicycle.

Phys. Chem. Chem. Phys., in press.
DOI: 10.1039/d6cp02156e
Full-text URL: https://doi.org/10.1039/d6cp02156e

Sulphur within the extreme environment of the central molecular zone of NGC 253: a chemical modelling approach

Bouvier, M. ; Dutkowska, K. M. Dutkowska; Viti, S. ; Mangum, J. G. ; Behrens, E. ; Eibensteiner, C.

Sulphur(S)-bearing species are ubiquitous in Galactic star-forming regions, from dense cold cores to outflows and shocks linked to protostellar activity. A recent observational study investigated the origin of S-bearing species towards the central molecular zone (CMZ) of NGC 253 and showed that Sulphur emission is linked to the presence of forming stars. However, more extensive modelling of these observations are required to determine the exact origin of the Sulphur emission (e.g. shock or thermal evaporation). Using chemical modelling, we examine how S-bearing species behave in the more extreme environment of the starburst galaxy NGC 253, and more generally, how they can help us improve our understanding of the emission linked with the dense star-forming gas in external galaxies. We use the gas-grain time-dependent chemical model UCLCHEM to model static warm clouds and C-type shocks under the physical conditions found in the CMZ of NGC 253. We compare observed abundances and abundance ratios to the modelled output abundances. We found that depending on the model type (shock, post-shock or static cloud), the highest abundance reached by the S-bearing species varies significantly. Hence, we can use their observed abundances of S-bearing species to distinguish between shocked, post-shocked or a quiescent (non-shocked) gas. We also confirm observationally-based conclusions on their emission origins, including in the case of unresolved emission. Comparing GMC-scale observations with chemical modelling is a powerful method to investigate and constrain the origin of molecular emission towards extragalactic star-forming regions. Sulphur-bearing species are useful to distinguish between different types of ISM components (shocked/post-shocked/quiescent gas).

Accepted in A&A
Full-text URL: https://arxiv.org/abs/2609.01162

Formation scenarios of dense starless cores from their ice composition

J. Kalvāns

Context. Dense, dark, starless cores of molecular clouds form in large-scale processes. The evolution of physical conditions in forming dense cores is often regulated by external phenomena and cannot be easily reproduced with models considering only the core and its immediate environment. Aims. The aim is to determine likely formation paths for dense cores that, when applied in an astrochemical model, produce column-density ratios of interstellar ice species in agreement with observations. Thus, we chemically determined how a typical core’s central density evolves during its formation period. Methods. Compliance with observations of calculated ice composition was investigated for five central density growth paths: exponential, linear, sigmoid (S-type), asymptotic growth, and gravitational infall. Timescales of 1, 2, and 3 Myr were considered. An increase of the central density was accompanied by a contraction of the 1D spherical molecular cloud with a constant mass. Chemistry was simulated with a multi-grain multi-layer model with dynamical desorption energy for surface species. Results. Exponential, infall, linear, and sigmoid density-growth models were apparently able to replicate observed ice composition, each with its own timescale. The results indicate that core formation likely occurs on a 2 Myr timescale that includes a 1 Myr stage of active contraction. Gravitational infall produces an agreement with observations when it is delayed by a factor of about 0.3. The possibility of ice photoprocessing in steady-state cores after their formation, as well as other local conditions, induces uncertainty in the actual formation path of individual objects. Conclusions. The study presents and

tests a simple, optimisable way of creating dense cores for astrochemical modelling purposes.

2026, Astronomy & Astrophysics, Volume 713, A124
DOI: 10.1051/0004-6361/202553962
Full-text URL: https://www.aanda.org/articles/aa/full_html/2026/09/aa53962-25/aa53962-25.html

When two worlds collide: How collisions between silicate and carbonaceous nanograins can drive complex chemistry

Alexandros Kyriazis, Albert Rimola and Stefan T. Bromley

Context. Observations have revealed the presence of silicate and carbonaceous material in interstellar grains, however, these components are generally assumed to belong to distinct dust populations. While some dust models do incorporate mixed silicate-carbonaceous grains, there is little evidence to support grain mixing mechanisms. In this work, we use atomistic simulations to investigate collisions between silicate and carbonaceous nanograins at velocities representative of a range of astrophysical environments. Aims. Our overall objective is to determine how collision velocity governs the interactions between silicate and carbonaceous nanograins. We aim to: (i) identify collisional regimes capable of producing mixed silicate-carbonaceous grains and/or chemically complex molecular species; and (ii) quantify fragmentation threshold velocities related to dust destruction. Methods. We performed molecular dynamics simulations employing a machine-learning force field to model head-on collisions between silicate and carbonaceous nanograins of comparable masses. Collision velocities span 1 to 11 km/s. For all collisions, we tracked the extent of grain-grain mixing and the formation of molecular fragments. Results. We identified four velocity regimes: (1) <=1.5 km/s, where grains bounce off one another; (2) ~1.5-3.5 km/s, where sticking between the grains starts to occur; (3) ~3.5-7.5 km/s, where grains tend to aggregate and form inter-grain chemical bonds, yielding stable mixed grains; and (4) >=7.5 km/s, where fragmentation dominates. The latter regime produces CO as the main product, along with hydrocarbons, complex organic molecules, molecular silicates, and mixed carbonaceous-silicate clusters. The fragmentation threshold velocity for these collisions is found to be approximately 7.5 km/s. Conclusions. We show that collision velocities govern both the physical and chemical outcomes of silicate-carbonaceous nanograin interactions. In the fragmentation regime, collisions provide a viable pathway for generating mixed grains and a wide range of molecular species, many of which have been observationally detected. Here, we provide a simple credible mechanism linking the physics of grain processing with observed complex interstellar chemistry.

A&A, 713, A125 (2026)
DOI: 10.1051/0004-6361/202661452
Full-text URL: https://arxiv.org/abs/2607.22213

Vacuum-ultraviolet photoionization of a grandPAH molecule: The interplay of alkyl groups and large polycyclic aromatic hydrocarbons upon photoionization

Helgi Rafn Hrodmarsson, Ugo Jacovella, Serge Pluta, Xuelin Yao, Akimitsu Narita, Klaus Müllen, Martin Schwell, Harold Linnartz, Laurent Nahon, and Alexandre Giuliani

So-called grandPAH molecules are proposed to be omnipresent in various interstellar regions as they are large enough to be photostable against strong interstellar radiation fields. They are also notoriously difficult to synthesize and sublimate. Measuring their gas phase spectra and molecular properties is thus very difficult. We report on the experimental photoionization of a defined grandPAH cation (C60H18(C12H25)4 m/z 1415 amu). The molecule consists of a large PAH containing 60 sp2 carbon atoms and four long alkyl groups (-C12H25) attached to peripheral positions. The alkyl chains wrap around the aromatic core and stabilize the dication leading to a lowering of the ionization energy. The ion yield spectrum of the grandPAH was recorded from 8.1 to 25 eV using an ion trap coupled to vacuum-ultraviolet (VUV) synchrotron radiation. To accurately extrapolate the experimental results toward the unsubstituted grandPAH itself, we perform a series of calculations to quantify this lowering of the ionization energy. The adiabatic ionization energy of the grandPAH cation was determined as 8.50 ± 0.35 eV. This dual experimental and theoretical methodology can be used to perform other spectroscopic measurements of large, alkylated PAHs to extract properties of the unsubstituted PAH. The implications of these results are discussed in the context of the behavior of large PAHs in interstellar and/or interplanetary dust particles as well as PAH units embedded in insoluble organic material which are found in meteorites.

A&A, 2026, aa60570-26
DOI: 10.1051/0004-6361/202660570
Full-text URL: https://www.aanda.org/articles/aa/abs/2026/09/aa60570-26

Non-equilibrium formation of the elusive dibridged diboranyl (B2H5) radical and boranes in low-temperature diborane ices

Jia Wang, Joshua H. Marks, Chaojiang Zhang, Andrew M. Turner, Mason McAnally, Miori Nogamida,Ralf I. Kaiser

Boranes are prototypical electron-deficient species central to boron chemistry and chemical vapor deposition. Despite extensive studies of diborane (B2H6), key reactive intermediates—particularly the monobridged and dibridged diboranyl (B2H5) radicals—have remained incompletely characterized because of their high reactivity. Here, we report the experimental identification of the hitherto elusive dibridged diboranyl radical together with its monobridged isomer in low-temperature diborane ices exposed to energetic electron irradiation. The radicals were identified in irradiated diborane and fully deuterated diborane-d6 ices at 40 K via Fourier transform infrared spectroscopy, revealing the formation of the

monobridged radical through B–H bond cleavage, followed by isomerization to the dibridged isomer. Additionally, utilizing vacuum ultraviolet photoionization reflectron time-of-flight mass spectrometry combined with isotopic labeling experiments, complex boranes ranging from B6H10 to B12H26 were detected in the gas phase during temperature-programmed desorption. The formation of these increasingly complex boranes is proposed to proceed through sequential boron-insertion reactions involving BH and BH3 addition coupled with hydrogenation pathways. These findings highlight the critical role of non-equilibrium chemistry in the synthesis of reactive diboranyl radicals and complex boranes in low-temperature ices, providing fundamental insight into boron chemistry under extreme conditions.

Chem. Sci. (2026) 17 (32): 15528–15537
DOI: 10.1039/d6sc04215e
Full-text URL: https://doi.org/10.1039/d6sc04215e

Thioacetaldehyde (CH3CHS) on interstellar ices: a key molecule to unravel two chemical dichotomies in the ISM

M. Mallo, M. Sanz-Novo, M. Agúndez, J. Cernicharo, G. Esplugues, V.M. Rivilla, I. Jiménez-Serra, C. Cabezas, G. Molpeceres

Thioacetaldehyde (CH3CHS), recently detected in TMC-1, has an abundance approximately 36 times lower than its oxygen analog, acetaldehyde (CH3CHO). This makes the CH3CHS/CH3CHO pair the one with the largest column density difference among the detected oxygen/sulfur analogue pairs in this cloud. We investigate the hydrogenation pathways of CH3CHS to address two chemical dichotomies in the ISM: (i) the differenciation between CH3CHS and CH3CHO, and (ii) the apparent absence of both CH3CHS in the G+0.693-0.027 molecular cloud and ethyl mercaptan (CH3CH2SH), in TMC-1. Our results reveal a complex scheme that involves multiple competing reactions, highlighting an efficient sequence of consecutive hydrogenations that can lead to CH3CH2SH. This finding suggests that the high S/O ratio observed for thioacetaldehyde in TMC-1 (∼36), and even more pronounced in G+0.693-0.027 (≥112), may result from its conversion via hydrogenation on the ice surface, contrary to the case of CH3CHO, which is more resistant to that chemical process. The straightforward hydrogenation of CH3CHS on ices, which can also take place even in the gas-phase at 150 K, provides a reliable explanation for its non-detection in G+0.693-0.027, where grain-surface chemistry is expected to play an important role, favoring the conversion of CH3CHS into CH3CH2SH, which is indeed detected in G+0.693-0.027. In contrast, TMC-1 represents a more pristine gas-phase environment, where grain-surface chemistry has a lower impact. Under these conditions, CH3CHS can persist, while CH3CH2SH remains undetected. Overall, our results show the entirely different reactivity that contributes to the chemical complexity of two of the largest interstellar sulfur factories.

Accepted for publication in MNRAS
DOI: 10.1093/mnras/stag1773
Full-text URL: https://arxiv.org/abs/2609.20506

Collisional excitation of cyclopentadiene by helium. A complete set of rate coefficients and astrophysical applications

S. Demes, F. Lique, M. Agúndez, J. Cernicharo

Complex organic molecules, including large cyclic species, are prevalent in interstellar space and play a key role in various astrochemical processes. Cyclopentadiene (c-C5H6) is a five-membered cyclic hydrocarbon recently detected in TMC-1 and some other interstellar molecular clouds. While accurate spectroscopic data were available, collisional rate coefficients for its rotational transitions were missing so far, introducing a potential limitation in the interpretation of the observations. This study aims to provide a comprehensive set of state-to-state thermal rate coefficients for the rotational excitation of c-C5H6 due to collisions with helium, crucial for non-local thermodynamic equilibrium (non-LTE) radiative transfer modelling in astrophysical environments, and to examine how far the molecule is from thermalisation under the physical conditions of cold molecular clouds. The research employed accurate quantum scattering calculations using the close-coupling (CC) and coupled states (CS) methods, based on a highly-correlated three-dimensional potential energy surface for the [c-C5H6 + He] collisional complex. Calculations were performed for a wide range of rotational states (from j = 0 to j <= 25) and kinetic temperatures (from 10 to 50 K). We calculated a complete set of thermal rate coefficients for both ortho- and para-C5H6. Radiative transfer simulations demonstrated that most rotational levels of cyclopentadiene are fully thermalized under typical cold cloud conditions and exhibit minor non-LTE effects. Nevertheless, this study is the first to utilise accurate state-to-state rate coefficients for radiative transfer simulation of a large, five-membered cyclic species detected in space. This allows to draw some general conclusions and paves the way for future studies of complex astromolecules that will enable a more precise interpretation of upcoming detections.

Accepted in A&A
DOI: 10.1051/0004-6361/202662015
Full-text URL: https://arxiv.org/abs/2609.01314

Effect of Ice Charging on the Astrochemistry of Interstellar Sulfur Bearing Species on Amorphous Solid Water

T. Vorsselmans, I. Grubova, K. Verhagen, T. Guldentops, R. Buimer, C. King, E. C. Neyts

We aim to derive statistically robust and physically interpretable BE distributions for atomic S and the sulfur-bearing

molecules H2S, SO2, and OCS on neutral and negatively charged ASW, and assess how excess negative charge alters their retention and potential role in the sulfur reservoir of cold dense molecular clouds. Basis set superposition error (BSSE) and zero-point energy (ZPE) corrected BEs of S, SO2, OCS and H2S, are calculated by density functional theory (DFT), using the ORCA software. Molecule-specific DFT levels of theory were first selected from benchmark calculations on neutral and charged small water complexes, against coupled-cluster reference energies. The selected protocols were then applied to study adsorption on neutral and charged ASW clusters. A range of adsorption sites were sampled on five independent amorphous ice clusters, yielding BE distributions that account for the site heterogeneity of ASW. Neutral ASW yields broad, site-dependent BE distributions consistent with previous water-ice estimates. On charged ASW, three general cases are identified: the BE will either always increase due to electron transfer (S-atom, SO2), the BE increases slightly without any electron transfer (H2S) or the BE remains the same unless an electron transfer occurs under specific conditions (OCS). These findings are inherently linked to the molecular properties of these molecules.

Accepten in A&A
DOI: 10.1051/0004-6361/202661939
Full-text URL: https://arxiv.org/abs/2607.09364

Physical conditions in PDRs revealed by IGRINS ro-vibrational H2 observations

A. Piluso, V. Maillard, R. Meshaka, E. Bron, F. Le Petit, K. Kaplan, P. Palud, E. Habart, E. Roueff, J. Le Bourlot

We compare H2 high ro-vibrational observations of 5 PDRs (S140, IC63, Horsehead Nebula, NGC 2023 and Orion Bar) obtained with the IGRINS spectrograph to PDR models produced with the Meudon PDR code, in order to estimate the physical conditions and to constrain the physical and chemical processes that govern PDRs. We use newly flux-calibrated and extinction-corrected IGRINS H2 observations covering the 1.45-2.45 um range at a resolution of 45000, and adjust Meudon PDR models using both a simple chi2 minimization approach and a robust method using Bayesian inversion followed by posterior exploration via an advanced MCMC technique. The PDR models use specific incident FUV spectra for each PDRs based on theoretical stellar spectra from the Pollux database. The Meudon PDR code is able to reproduce more than 85% of the observed H2 ro-vibrational line intensities within a factor of two. We find that (1) a realistic modeling of the incident FUV field (both in term of geometry and of spectral shape) and (2) the inclusion of recent data on collisional de-excitation rates for high vibrational levels of H2 are key to this success. H2 ro-vibrational emission lines are found to provide good constraints on both the thermal pressure and the incident FUV field strength, G0, although with a non-negligible remaining degeneracy in most PDRs. Additional constraints, such as the spatial scales of the PDR derived from ALMA or JWST observations, are found to be able to lift this degeneracy. For low excitation PDRs, the observations provide evidence that nascent H2 molecules formed on grains have relatively low rotational energy and high vibrational energy, as predicted by theoretical and experimental studies of the surface formation of H2.

Accepted in Astronomy & Astrophysics
DOI: 10.48550/arXiv.2609.24630
Full-text URL: https://arxiv.org/abs/2609.24630

High Water D/H Ratio of the Interstellar Object 3I/ATLAS is Consistent with a Low-metallicity Origin

K. Furuya, M. Cordiner, D. Bockelée-Morvan, D. Bodewits, C. O. Chandler, M. N. Drozdovskaya, N. X. Roth, G. Villanueva

Recent JWST observations have revealed unusually high 12C/13C ratios in carbon-bearing molecules of the interstellar object 3I/ATLAS, consistent with formation in a lower-metallicity environment than the present-day local ISM. 3I/ATLAS also exhibits an exceptionally high water D/H ratio, exceeding those in solar system comets and nearby low-mass star-forming regions. Here we investigate whether this high water D/H ratio can be reproduced in a low-metallicity formation scenario, using gas–ice astrochemical models. Assuming that the water observed in 3I/ATLAS was inherited from the parent molecular cloud and core, we perform a grid of astrochemical models covering the cloud-to-core stages, varying the gas density, UV radiation field, cosmic-ray ionization rate, and metallicity, while solving thermal balance for the gas temperature. We find that lower metallicity enhances H3+ deuteration and, more importantly, its transfer to water ice. In contrast, the water D/H ratio depends nonmonotonically on the strength of UV and the CR ionization rate, because of competing chemical and thermal effects. In our models, the observed water D/H ratio is most readily reproduced at subsolar metallicities and relatively high cloud densities of ~1e4 cm-3 without strong constraints on either the UV radiation field or the ionization rate, as long as the ionization rate is lower than 1e-15 s−1. The D/H ratio of methane normalized by that of water is not sensitive to the metallicity, being consistent with the similar values observed in 67P/Churyumov–Gerasimenko and 3I/ATLAS. These results suggest that water deuteration may provide a complementary probe of the metallicity and physical condition of the parent molecular cloud and dense core of interstellar objects.

2026 ApJL, 1009, L25
DOI: 10.3847/2041-8213/aea221
Full-text URL: https://arxiv.org/abs/2609.12370

A Cyanopolyyne-rich but COM-poor Massive Protostar: The First Hot Carbon Chain Chemistry Source G28.28-0.36

Kotomi Taniguchi, Masao Saito, Prasanta Gorai, Olli Sipila, Kazuhito Dobashi, Paola Caselli, Tirupati Kumara

Sridharan, Tomomi Shimoikura, Jonathan C. Tan

We present molecular emission line data from the massive young stellar object (MYSO) G28.28-0.36 (G28.28) obtained with the Atacama Large Millimeter/submillimeter Array Band 3. Cyanopolyynes (HC3N and HC5N) and three complex organic molecules (COMs; CH3OH, CH3CN, and CH3CHO) are detected from the MYSO G28.28. In addition, strong emission regions of cyanopolyynes are identified between G28.28 and a nearby ultracompact H II region. The HC5N emission is coincident with the dust continuum peak, where an excitation temperature of 100 K is derived from CH3CN. These results suggest that the Hot Carbon Chain Chemistry (HCCC) mechanism produces cyanopolyynes in the hot region around G28.28. We find that G28.28 exhibits a unique chemical feature: cyanopolyynes are abundant, but COMs are deficient, unlike the other MYSOs studied previously. These results imply that G28.28 is a counterpart of the Warm Carbon Chain Chemistry (WCCC) low-mass source L1527. G28.28 is the first HCCC source identified so far.

Accepted by The Astrophysical Journal
Full-text URL: http://arxiv.org/abs/2609.30654

Announcements

Cosmic rays in the molecular interstellar medium

March 15 to 19, 2027 – Duisburg, Germany
https://indico.cenide.de/e/crismchem2027

Energetic particles, dubbed cosmic rays, with a wide range of compositions, are important in driving chemical and thermodynamic processes in the molecular interstellar medium. Cosmic ray protons and electrons are important regulators of gas-phase chemistry through non-thermal ionizations and excitations. Heavy fast ions play a vital role in the radiation chemistry in interstellar ices and the build of chemical complexity in ices to prebiotic molecules. In the dense, shielded regions, the cosmic ray-driven ionization sets the electron fraction, controlling the strength of non-ideal magneto-hydrodynamic processes.

The physics and chemistry of cosmic ray irradiation is naturally an inter- and multidisciplinary problem. Their acceleration and transport exist in the realm of high-energy astrophysics and plasma physics. Understanding their role in interstellar molecular chemistry requires investigations into fundamental microphysics, such as electron-molecular interactions, and laboratory and computational chemistry. Finally, placing the role of these small-scale processes in the larger astrophysical picture requires macroscopic chemical models and observations across a wide range of photon energies.

The conference aims to bring together an interdisciplinary group of experts, from astronomy, chemistry, and physics, to improve our understanding of radiation chemistry from the microscopic (nanometer) to macroscopic (parsec) scales. The conference will include a range of talks across different specializations, and discussion sections to bring these diverse communities together under a common goal and set of curiosities.

Note: To avoid conference fees, the conference is limited to about 50 participants. Therefore, we urge all participants that if they cannot make it to the conference to inform the SOC with sufficient notice.

Themes:
Astronomical observations in a range of cosmic ray environments
Cosmic-ray astrochemical modeling
Cosmic-ray acceleration and transport through the interstellar medium
Theoretical chemistry investigations into radiation chemistry
Laboratory investigations into the radiation chemistry of ices
Material and surface physics investigations of ion irradiation

Timetable:
Start: 13:00 Monday, March 15, 2027
End: 13:00 Friday, March 19, 2027

Registration and abstract submission open
Abstract deadline: Nov 30, 2026
Abstract decision: Mid Jan, 2027
Registration deadline: Feb 1, 2027

SOC:
Brandt Gaches (Universität Duisburg-Essen, DE, chair)
Thomas Bisbas (Zhejiang Laboratory, CN)
Emmanuel Dartois (Univ. Paris-Saclay, FR)
Elena Redaelli (European Southern Observatory, DE)
Marika Schleberger (Universität Duisburg-Essen, DE)
Julia Tjus (Ruhr-Universität Bochum, DE)
[via Brandt Gaches]

Postdoctoral researcher in theoretical astrochemistry

The Emmy Noether Junior Group led by Dr. Brandt Gaches at the University of Duisburg-Essen is looking to hire a postdoctoral researcher to investigate the microphysics and chemistry of cosmic-ray interactions with icy dust grains. The group focuses on high-energy astrochemical processes, in particular the interaction of cosmic rays with dense molecular gas. The group uses a range of methods, in particular chemical modelling and theory. The group also leads the Astrochemistry Low-energy electron Cross-Section database.

The position is funded through the DFG-funded Emmy Noether group "Towards the next generation in cosmic-ray astrochemistry", hosted at the University of Duisburg-Essen.

Official link: https://www.uni-due.de/karriere/stelle.php?kennziffer=461-26

Your main tasks

As the postdoctoral researcher on this project, you will help build an atomic-scale understanding of the interaction of energetic particle irradiation with icy dust grains. Your work will include:
+ calculating the energy deposition and electron distribution in icy mantles following particle irradiation
+ using ab initio molecular dynamics simulations to quantitatively investigate chemistry immediately after particle irradiation
+ characterising the chemical structure of the simulated irradiated ices and the composition of the desorbed gas-phase molecules
+perform a broad parameter study for different radiation particle types, ice mantle compositions, and ice thicknesses
The results of this research will lead to a significant increase in our understanding of the buildup of complex organic molecules via cosmic-ray irradiation.

Your profile
+ Must hold a PhD in astrophysics, physics, chemistry, or a relevant field by the start of the position
+ Proficient knowledge of astrochemistry
+ Excellent command of written and spoken English
+ Proficient in C/C++ and/or Fortran
+ Preferred: Experience in quantum chemistry methods, in particular ab initio molecular dynamics
+ Preferred: Experience with the Geant4 physics package, or similar
+ Preferred: A high degree of independence, self-initiative and creativity

We offer you
+ a position in the public sector with reliable working conditions in a varied, multifaceted field of work and in a research-intensive environment
+ an interesting, meaningful role with significant scope for creativity
+ an appealing work environment characterized by respectful and appreciative collaboration
+ a diverse range of continuing education and professional development opportunities
+ various canteens and cafés run by the Studierendenwerk on our campuses
+ attractive discounts through Corporate Benefits
+ a family-friendly university culture (e.g., childcare options, counselling for family caregiving responsibilities, etc.)
+ a prime location and infrastructure with excellent public transportation access and free parking
+ flexible working hours and the option to work from home
+ 30 days of vacation with a 5-day workweek, plus additional days off on Christmas Eve and New Year’s Eve
+ fair pay in accordance with the collective bargaining agreement (TV-L), including an annual bonus and a company-sponsored supplemental pension plan
+ numerous sports and wellness programs (including university sports)

Application deadline: 2026-11-15

Application
We look forward to receiving your digital application including the usual documents:
+ Motivation letter, CV, including publication list. The publication list does not need to include citation count, or other statistics such as h-index, as these will not be used for consideration.
+ Brief (max 3 pages) statement of research experience and interests.
+ Names and contact information for three referees willing to send letters of recommendation.
+ Academic certificates. If you have not yet defended your Ph.D., but will by the start date, please attach a signed (digital is acceptable) letter from your advisor stating the expected defense date.
Please specify the reference number and submit your application to Dr. Brandt Gaches, Universität Duisburg-Essen, Fakultät für Physik, 47057 Duisburg, E-mail: brandt.gaches@uni-due.de.
[via Brandt Gaches]

Postdoctoral Opening, Velocity Map Imaging from Icy Surfaces

A post-doctoral position is open in the CIRS-group at Sorbonne Université (MONARIS, PARIS, France) to work with our SPICES-VMI set-up (see details below) to study the photodesorption dynamics in the vacuum-UV. Photodesorption (photon induced desorption) from ices has been suggested as a major (non-thermal) desorption process explaining the observations

of molecules in the cold interstellar medium. The determination of photodesorption yields from interstellar ice analogues has been the subject of many studies in the last decade, however, the mechanisms explaining the desorption are still poorly understood. We propose a novel experimental approach to shed insights onto the photodesorption dynamics from ices.

The SPICES-VMI instrument allows 3D-velocity map imaging (VMI) of neutral particles ejected from a cold surface (10-100 K). Typically thin films of physisorbed small molecules (CO, N2, H2O ..) or larger (aminoacids) organics of astrophysical interest will be irradiated with monochromatic photons in the range between 5-20 eV (VUV-laser or synchrotron radiation). It will lead to the desorption of parent molecules or fragments, velocity and angular distributions of which will be measured.

The candidate will be involved in a scientific program including:
• 3D-velocity map imaging (VMI) following photodesorption from ices in order to investigate the role of the polarization state of light.
• Commissioning of an upgraded tunable UV/VUV system (four-wave frequency mixing) and application to photodesorption studies above 10 eV

Depending on the agenda he/she will have the opportunity to participate to complementary photodesorption campaigns, aiming at identifying the effects of light polarization on the desorption from chiral molecules, using the SOLEIL synchrotron facility (DESIRS beamline).
The appointment period is initially for one year. The fellowship includes a gross monthly salary ranging between €2900-€3500 depending on the experience of the candidate. Candidates should have a Ph.D. in Chemical Physics or Physics or Chemistry. Experience in molecular/quantum dynamics and/or laser spectroscopy is expected, and an ability to perform collaborative work within an international team. Experience in velocity imaging techniques is not mandatory but will be positively considered.

Knowledge of French is not mandatory, but a fluent level of spoken and written English is required.

Applicants should submit a letter of interest, at least two reference names, a CV, and a publication list to Prof. J.-H. Fillion (jean-hugues.fillion@sorbonne-universite.fr), Department of Physics, Sorbonne Université at Paris, France. Review of applications will begin on November 1st, 2026, and will continue until the position is filled

[via Jean-Hugues Fillion]