AstroChemical Newsletter #113

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Abstracts

H2S ice sublimation dynamics: experimentally constrained binding energies, entrapment efficiencies, and snowlines

Julia C. Santos, Elettra L. Piacentino, Jennifer B. Bergner, Mahesh Rajappan, Karin I. Öberg

Hydrogen sulfide (H2S) is thought to be an important sulfur reservoir in interstellar ices. It serves as a key precursor to complex sulfur-bearing organics, and has been proposed to play a significant role in the origin of life. Although models and observations both suggest H2S to be present in ices in non-negligible amounts, its sublimation dynamics remain poorly constrained. In this work, we present a comprehensive experimental characterization of the sublimation behavior of H2S ice under astrophysically-relevant conditions. The sublimation behavior of H2S was monitored with a quadrupole mass spectrometer (QMS) during temperature-programmed desorption (TPD) experiments. These experiments are used to determine binding energies and entrapment efficiencies of H2S, which are then employed to estimate its snowline positions in a protoplanetary disk midplane. We derive mean binding energies of 3159±46 K for pure H2S ice and 3392±56 K for submonolayer H2S desorbing from a compact amorphous solid water (cASW) surface. These values correspond to sublimation temperatures of around 64 K and 69 K in the disk midplane, placing its sublimation fronts at radii just interior to the CO2 snowline. We also investigate the entrapment of H2S in water ice and find it to be highly efficient, with ~75-85% of H2S remaining trapped past its sublimation temperature for H2O:H2S mixing ratios of ~5-17:1. We discuss potential mechanisms behind this efficient entrapment. Our findings imply that, in protoplanetary disks, H2S will mostly be retained in the ice phase until water crystallizes, at radii near the water snowline, if it forms mixed into water ice. This has significant implications for the possibility of H2S being incorporated into icy planetesimals and its potential delivery to terrestrial planets, which we discuss in detail.

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Complex Organic Molecules towards the central molecular zone of NGC 253

M. Bouvier, S. Viti, J. G. Mangum, C. Eibensteiner, E. Behrens, V. M. Rivilla, Á. López-Gallifa, S. Martín, N. Harada, S. Muller, L. Colzi, K. Sakamoto

Interstellar complex organic molecules (iCOMs) may have a link to prebiotic species, key building blocks for life. In Galactic star-forming (SF) regions, spatial variations of iCOMs emission could reflect the source physical structure or different chemical formation pathways. Investigating iCOMs in extragalactic SF regions may thus provide crucial information about these regions. As an active extragalactic SF region, the central molecular zone (CMZ) of the nearby galaxy NGC 253 provides an ideal template for studying iCOMs under more extreme conditions. We aim to investigate the emission of a few selected iCOMs and understand if a difference between the iCOMs could reflect on the source's chemical or physical structure. Using the high angular resolution (∼27 pc) observations from the ALCHEMI ALMA large program, we imaged the emission of selected iCOMs and precursors; CH3CHO, C2H5OH, NH2CHO, CH2NH, and CH3NH2. We estimated the iCOMs gas temperatures and column densities using a rotational diagram analysis, and by performing a non-LTE analysis for CH2NH.The iCOM emission concentrates mostly towards the inner part of the CMZ of NGC 253 and can be reproduced with two gas components. Different emission processes can explain iCOM emission towards the CMZ of NGC 253: at Giant Molecular Cloud (GMC) scales (∼27 pc), the iCOMs could trace large-scale shocks whilst at smaller scales (few pc), both shock and heating processes linked with ongoing star formation may be involved. Using column density correlation trends and known formation pathways, we find that more than one formation path could be involved to explain the iCOM emission. Finally, we found chemical differences between the GMCs, such as a decrease of abundance for the N-bearing species towards one of the GMCs or different excitation conditions for NH2CHO and CH3CHO towards two of the GMCs.

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Discovery of an intriguing chemically rich outflow in the OMC-2/3 filament

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Studying chemically rich protostellar outflows and their jet provides an important insight into the low-mass star formation process and its related chemistry. Whilst well-known shock tracers such as SiO can be used to study the jet properties and give information about the dynamics of the system, interstellar complex organic molecules (iCOMs) have been useful in constraining the age of shocked gas, for example. Yet, the number of outflows mapped in iCOMs is still limited. In this work, we study the outflow driven by the protostar FIR6c-a (HOPS 409) located in the OMC-2/3 filament. We report the detection

of the red-shifted jet, left undetected in previous studies, as well as the detection of the iCOMs methanol (CH3OH) and methyl cyanide (CH3CN) for the first time towards this outflow. Using SiO, we derived some jet properties (i.e., collimation and dynamical time). We found a clear dichotomy between the blue- and red-shifted jets, likely due to the density of the medium in which the jets propagate. In addition, we identified two bow shocks within the blue-shifted part of the outflow, which we attribute to two different ejection events. Finally, using the CH3OH and CH3CN abundance ratio and chemical modelling, we constrained the outflow age to be ≥1000 yr old and, surprisingly, found that a cosmic-ray ionization rate of 1e-14 s-1 is needed to reproduce the observed ratio towards the source.

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Scattering resonances in the rotational excitation of HDO by Ne and normal-H2: theory and experiment

Ricardo Manuel García-Vázquez, Astrid Bergeat, Otoniel Denis-Alpizar, Alexandre Faure, Thierry Stoecklin and Sébastien B. Morales

The rotational excitation of singly deuterated water molecule (HDO) by a heavy atom (Ne) and a light diatomic molecule (H2) is investigated theoretically and experimentally in the near-threshold regime. Crossed-molecular beam measurements with a variable crossing angle are compared to close-coupling calculations based on high-accuracy potential energy surfaces. The two lowest rotational transitions 000→ 101 and 000→ 111 are probed in detail and a good agreement between theory and experiment is observed for both transitions in the case of HDO + Ne where scattering resonances are however blurred out experimentally. In the case of HDO-H2, the predicted theoretical overlapping resonances are faithfully reproduced by experiment for the 000→ 111 transition while the calculated strong signal for the 000→ 101 transition is not detected. Future works are needed to reconcile this discrepancy.

Faraday Discuss., 2024, 251, 205–224
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Full-text URL: https://cnrs.hal.science/hal-04662082v1

Rotationally Resolved Spectrum of the Degenerate Antisymmetric C–H Stretching Band of c-C3H3+

Divita Gupta, Philipp C Schmid, Thomas Salomon, Oskar Asvany, Stephan Schlemmer

The rotationally resolved spectrum of the degenerate ν4 antisymmetric C–H stretching band of the cyclopropenyl cation, c-C3H3+, the smallest aromatic hydrocarbon cation, has been recorded employing leak-out-spectroscopy (LOS) in a cryogenic 22-pole ion trap instrument operated at T = 42 K. About 370 lines were measured in the region 3110–3150 cm–1 and assigned to rovibrational transitions of the fundamental antisymmetric C–H stretching band. Spectroscopic parameters have been refined compared to the previous experimental work from the group of Harold Linnartz [Zhao et al., Astrophys. J. Lett. 2014, 791, L28] and previous high-level theoretical predictions [Huang et al., J. Phys. Chem. A 2011, 115, 5005–5016]. Details of the spectral signatures allow for a thorough comparison of action spectroscopy in low-temperature ion traps to cavity ring down spectroscopy in a free-jet cooled discharge.

ACS Earth and Space Chemistry 2025
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Conformational isomerism of methyl formate: new detections of the higher-energy trans conformer and theoretical insights

Miguel Sanz-Novo, Germán Molpeceres, Víctor M. Rivilla, Izaskun Jiménez-Serra

In recent astrochemical studies it has become crucial to study all the complete conformational panorama of the molecule, some of which are potentially detectable in the interstellar medium (ISM). In this context, the isomeric ratio can be used as a powerful tool to distinguish between different formation routes of molecules with increasing levels of complexity. While the most stable cis conformer of methyl formate (CH3OCHO, MF) is ubiquitous in the ISM, there is just one tentative detection of the higher-energy trans form toward the envelope of the star-forming region Sgr B2(N). Here, we present the detections of trans-methyl formate toward the Galactic Center molecular cloud G+0.693-0.027 and the protostellar shock L1157-B1, providing definite observational evidence of its presence in the ISM. Numerous unblended or slightly blended a-type Ka = 0, 1 transitions belonging to the A-substate of trans-MF have been identified in both sources. We derive a molecular column density for trans-methyl formate of N = (8.2 ± 0.4) e12 cm−2 and N = (1.6 ± 0.3) e12 cm−2, respectively, yielding a molecular abundance with respect to H2 of ∼6e−11 and ∼8e−10. Therefore, we obtain cis/trans isomeric ratios of ∼72 and ∼34 toward G+0.693 and L1157-B1, which are ∼7 and 3 times larger than that found in the Sgr B2(N) region. These results are compared with new grain-surface theoretical computations, which suggest that a stereospecific formation of trans-MF via the CH3O + HCO route on grain surfaces can qualitatively explain the observed cis/trans abundance ratio. Nevertheless, we show that additional stereospecific gas-phase routes could also play a crucial role in maintaining the intricate balance between formation and destruction of trans-MF, ultimately leading to its detection.

Accepted in Astronomy and Astrophysics
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Full-text URL: https://arxiv.org/abs/2503.23045

A search for the three isomers of cyano-1,3-butadiene in TMC-1: Implications for bottom-up routes involving 1,3-butadiene

M. Agundez, C. Cabezas, N. Marcelino, B. Tercero, R. Fuentetaja, P. de Vicente, J. Cernicharo

The molecule 1,3-butadiene (CH2CHCHCH2) could play a key role in the synthesis of the cyclic molecules cyclopentadiene and benzene in cold dense clouds. Since 1,3-butadiene is non-polar, we searched for its cyano derivative, which exists in the form of three different polar isomers, in the cold dense cloud TMC-1. We used the most recent data obtained with the Yebes 40m telescope in the Q band (31.0-50.3 GHz) in the frame of the QUIJOTE project. We do not detect any of the two isomers of 1-cyano-1,3-butadiene, and derive 3sigma upper limits to their column densities of 1.2e10 cm-2 and 2.0e10 cm-2 for E- and Z-1-cyano-1,3-butadiene, respectively. Our results are not consistent with those from Cooke et al. (2023), who determine a column density of 3.8e10 cm-2 for E-1-cyano-1,3-butadiene in TMC-1 using GBT data and a line stack technique. At the current level of sensitivity of our data, there is tentative evidence for the presence of the third cyano derivative isomer, 2-cyano-1,3-butadiene, although a firm detection must await more sensitive data. We derive an upper limit to its column density of 3.1e10 cm-2. This isomer cannot be formed in the reaction between CN and 1,3-butadiene, according to experimental and theoretical studies, and thus we speculate whether it could arise from neutral-neutral reactions like C2H3 + CH2CHCN and CH2CCN + C2H4. From the upper limit on the abundance of 1-cyano-1,3-butadiene derived here, we estimate that the abundance of 1,3-butadiene in TMC-1 is below 1e-11 - 1e-10 relative to H2. The low abundance inferred for 1,3-butadiene makes it unlikely that it plays an important role in bottom-up routes to cyclopentadiene and benzene.

A&A, accepted
DOI: 10.1051/0004-6361/202554343
Full-text URL: https://arxiv.org/abs/2503.23841

Announcements

First announcement: COST NanoSpace AI in Astrochemistry Training School

When: 5-8 August 2025
Where: Aalto University, Helsinki, Finland
Registration Deadline: 30 May 2025
Contact email: agarcia@iac.es , miguel.caro@aalto.fi
Website: https://ocamm.fi/event/cost-nanospace-ai-in-astrochemistry-training-school-2025/
Dear colleagues,
We are very happy to announce the “COST NanoSpace AI in Astrochemistry Training School”; a COST/Aalto Summer School on artificial intelligence (AI) and machine learning (ML) tools in astrochemistry. The School will be held 5-8 August 2025 in Aalto University, Helsinki, Finland.
All detailed information about the COST NanoSpace AI in Astrochemistry Training School; i.e., programme, organising committees, registration, logistics, etc. can be found on the school’s website at: https://ocamm.fi/event/cost-nanospace-ai-in-astrochemistry-training-school-2025/ (also available via the NanoSpace website).
The list of topics and lecturers/trainers is the following:
• Fundamentals of ML - Miguel Caro, Aalto Univ., Finland
• Basics of Neural Networks - Xabier Pérez Couto, A Coruña Univ., Spain
• Gaussian Processes and Regressors - Mads-Peter V. Christiansen, Aarhus Univ., Denmark
• Intelligent Molecular Structure Search Algorithms – Isabelle Braems, IMN-CNRS, France
• ML for Chemical Intuition - Brett McGuire, MIT, USA
• ML for Radio Interferometry - Ryan Loomis, NRAO, USA
• ML Binding Energies of Astrochemically Molecules and/or Interpretable ML Techniques for Astrochemistry - Johannes Heyl, UCL, UK
• Neural Networks for Astrochem - Lorenzo Branca, Heidelberg Univ., Germany
• ML for Protoplanetary Disk Chemistry and/or ML for Star Formation Chemistry – (to be confirmed)
• ML for Interatomic Potentials - Rina Ibragimova, Aalto Univ., Finland
• ML for Radiation Damage in Space - Andrea Sand, Aalto Univ., Finland
Short description of the COST NanoSpace AI in Astrochemistry Training School:
This AI in Astrochemistry Training School is organized by the COST Action NanoSpace (CA21126) in collaboration with the Aalto University, Department of Chemistry and Materials Science. The main goal of the AI in Astrochemistry Training School is to provide PhD students and young researchers, specialized knowledge and address the urgent need for training on AI tools in astrochemistry. The program will include several sessions on AI and ML tools and its actual or potential applications in astrochemistry (e.g., intelligent structure search algorithms, neural networks for astrochemistry, as well as ML for chemical intuition, radio observations, proto-planetary disk chemistry, interatomic potentials, and radiation damage in space), as well as series of practical exercises.
The School will be in person with attendance limited to 50-55 trainees and with priority given to PhD students and Young Researchers, who are strongly encouraged to participate. There is no registration fee and the NanoSpace COST Action will provide financial support (i.e. reimbursement after the event, covering full or partial travel, accommodation, and subsistence

costs) for a significant number of participants (at least ~20-25), with high priority to those with a primary affiliation in an institution located in an Inclusiveness Target Country (ITC) / Near Neighbour Country (NNC) participating in the Action. The information requested in the registration form below will be used to select the final list of registered participants as well as those eligible for financial support, which will be notified in advance of the Training School (i.e., by mid-June 2025). The attendees are expected to arrange their own travel and accommodation. Looking forward to meet you in Aalto!
Kind regards,
Domingo Anibal García-Hernández, NanoSpace Action Chair on behalf of the Organizing Committee

Astrophysics: The James Webb Space Telescope. From First Light to New World Views.

The James Webb Space Telescope (JWST) is revolutionizing many areas in astronomy, from the earliest distant galaxies to nearby planets around stars other than our Sun. This book, based on a workshop held at the Pontifical Academy of Sciences in early 2024, provides one of the first compilations of those new results. It includes papers on Astrochemistry in Star- and Planet-forming regions by Andrea Banzatti, Olivier Berne, Inga Kamp, Melissa McClure, Colette Salyk, Lukasz Tychoniec, and Yao-Lun Yang; in the Solar System by Stefanie Milam, Henrik Melin and Jonathan Lunine; and in Exoplanet Atmospheres by Jonathan Fortney, Nikku Madhusudhan, Nikole Lewis, Michiel Min, Sasha Hinkley and Rene Doyon.

At the same time, this book also reflects on the impact that this new knowledge has on society at large, from technological and economic benefits to philosophical perspectives, including a sense of awe and wonder that looking at the sky with a powerful telescope brings (in the words of a poet). JWST's beautiful images have inspired billions of people across the world. How did they come about? What lessons do they provide for other outreach and public engagement projects? How do we preserve the pristine night sky? And how can a large international and multidisciplinary project like JWST, that took thirty years to build, succeed?

The book is published as Pontificiae Academiae Scientiarum Scripta Varia 155, edited by Ewine F. van Dishoeck. It can be downloaded at: https://www.pas.va/en/publications/scripta-varia/sv155pas.html

Videos of most presentations and interviews can be found at https://www.pas.va/en/events/2024/astrophysics.html