AstroChemical Newsletter #76

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Abstracts

Successive deuteration in low-mass star-forming regions: the case of D2-methanol (CHD2OH) in IRAS 16293-2422

Maria N. Drozdovskaya, Laurent H. Coudert, Laurent Margulès, Audrey Coutens, Jes K. Jørgensen, Sébastien Manigand

Accurate quantification of the column density of di-deuterated methanol is a key missing puzzle piece in the otherwise thoroughly constrained family of D-bearing methanol in the deeply embedded low-mass protostellar system and astrochemical template source IRAS16293-2422. A spectroscopic dataset for astrophysical purposes is built for CHD2OH and made publicly available to facilitate accurate characterization of this species in astrochemical surveys. The newly computed line list and partition function are used to search for CHD2OH towards IRAS16293-2422 A and B in data from ALMA-PILS. Only non-blended, optically thin lines of CHD2OH are used for the synthetic spectral fitting. The constructed spectroscopic database contains line frequencies and strengths for 7417 transitions in the 0 to 500 GHz frequency range. ALMA-PILS observations in the 329-363 GHz range are used to identify 105 unique, non-blended, optically thin line frequencies of CHD2OH for synthetic spectral fitting. The derived excitation temperatures and column densities yield high D/H ratios of CHD2OH in IRAS 16293-2422 A and B of 7.5±1.1% and 7.7±1.2%, respectively. Deuteration in IRAS 16293-2422 is not higher than in other low-mass star-forming regions. Di-deuterated molecules consistently have higher D/H ratios than their monodeuterated counterparts in all low-mass protostars, which may be a natural consequence of H-D substitution reactions as seen in laboratory experiments. The Solar System's natal cloud, as traced by comet 67P/Churyumov-Gerasimenko, may have had a lower initial abundance of D, been warmer than the cloud of IRAS16293-2422, or been partially reprocessed. In combination with accurate spectroscopy, a careful spectral analysis, and a consideration of the underlying assumptions, successive deuteration is a robust window on the physicochemical provenance of star-forming systems.

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Atomic Shocks in the Outflow of L1551 IRS 5 Identified with SOFIA-upGREAT Observations of [O I]

Y.-L. Yang, N. J. Evans, A. Karska, L. E. Kristensen, R. Aladro, J. P. Ramsey, J. D. Green, J.-E. Lee

We present velocity resolved SOFIA/upGREAT observations of [OI] and [CII] lines toward a Class I protostar, L1551 IRS 5, and its outflows. The SOFIA observations

detect [OI] emission toward only the protostar and [CII] emission toward the protostar and the red-shifted outflow. The [OI] emission has a width of ~100 km s−1 only in the blue-shifted velocity, suggesting an origin in shocked gas. The [CII] lines are narrow, consistent with an origin in a photodissociation region. Differential dust extinction from the envelope due to the inclination of the outflows is the most likely cause of the missing red-shifted [OI] emission. Fitting the [OI] line profile with two Gaussian components, we find one component at the source velocity with a width of ~20 km s−1 and another extremely broad component at -30 km s−1 with a width of 87.5 km s−1, the latter of which has not been seen in L1551 IRS 5. The kinematics of these two components resemble cavity shocks in molecular outflows and spot shocks in jets. Radiative transfer calculations of the [OI], high-J CO, and H2O lines in the cavity shocks indicate that [OI] dominates the oxygen budget, making up more than 70% of the total gaseous oxygen abundance and suggesting [O]/[H] of ~1.5e−4. Attributing the extremely broad [OI] component to atomic winds, we estimate the intrinsic mass loss rate of (1.3±0.8)x1e−6 Msun yr−1. The intrinsic mass loss rates derived from low-J CO, [OI], and HI are similar, supporting the model of momentum-conserving outflows, where the atomic wind carries most momentum and drives the molecular outflows.

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A pathway to peptides in space through the condensation of atomic carbon

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Organic molecules are widely present in the dense interstellar medium, and many have been synthesized in the laboratory on Earth under the conditions typical for an interstellar environment. Until now, however, only relatively small molecules of biological interest have been demonstrated to form experimentally under typical space conditions. Here we prove experimentally that the condensation of carbon atoms on the surface of cold solid particles (cosmic dust) leads to the formation of isomeric polyglycine monomers (aminoketene molecules). Following encounters between aminoketene molecules, they polymerize to produce peptides of different lengths. The chemistry involves three of the most abundant species (CO, C and NH3) present in star-forming molecular clouds, and proceeds via a novel pathway that skips the stage of amino acid formation in protein synthesis. The process is efficient, even at low temperatures, without irradiation or the presence of water. The delivery of biopolymers formed by this chemistry to rocky planets in the habitable zone might be an important element in the origins of life.

Nat Astron (2022).
DOI: 10.1038/s41550-021-01577-9
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Deuterium fractionation as a multi-phase component tracer in the Galactic Centre

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The Central Molecular Zone (CMZ) contains most of the mass of our Galaxy but its star formation rate is one order of magnitude lower than in the Galactic disc. This is likely related to the fact that the bulk of the gas in the CMZ is in a warm (>100 K) and

turbulent phase with little material in the pre-stellar phase. We present in this Letter observations of deuterium fractionation (D/H ratios) of HCN, HNC, HCO+, and N2H+ towards the CMZ molecular cloud G+0.693-0.027. These observations clearly show, for the first time, the presence of a colder, denser, and less turbulent narrow component, with a line width of about 9 km s−1, in addition to the warm, less dense and turbulent broad component with a line width of about 20 km s−1. The very low D/H ratio <6e−5 for HCO+ and N2H+, close to the cosmic value (about 2.5e−5), and the high D/H ratios >4e−4 for HCN and HNC derived for the broad component, confirm the presence of high-temperatures deuteration routes for nitriles. For the narrow component we have derived D/H ratios >1e−4 and excitation temperatures of 7 K for all molecules, suggesting kinetic temperatures <30 K and H2 densities >5e4 cm−3, at least one order of magnitude larger than for the broad component. The method presented in this Letter allows to identify clouds on the verge of star formation, i.e. under pre-stellar conditions, towards the CMZ. This method can also be used for the identification of such clouds in external galaxies.

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Gas-Phase Reactivity of OH Radicals With Ammonia (NH3) and Methylamine (CH3NH2) at Around 22K

Daniel González, Bernabé Ballesteros, André Canosa, José Albaladejo and Elena Jiménez

Interstellar molecules containing N atoms, such as ammonia (NH3) and methylamine (CH3NH2), could be potential precursors of amino acids like the simplest one, glycine (NH2CH2COOH). The gas-phase reactivity of these N-bearing species with OH radicals, ubiquitous in the interstellar medium, is not known at temperatures of cold dark molecular clouds. In this work, we present the first kinetic study of these OH-reactions at around 22 K and different gas densities [(3.4–16.7) × 1e16 cm−3] in helium. The obtained rate coefficients, with ± 2σ uncertainties, can be included in pure gas-phase or gas-grain astrochemical models to interpret the observed abundances of NH3 and CH3NH2. We observed an increase of k1 and k2 with respect to those previously measured by others at the lowest temperatures for which rate coefficients are presently available: 230 and 299 K, respectively. This increase is about 380 times for NH3 and 20 times for CH3NH2. Although the OH + NH3 reaction is included in astrochemical kinetic databases, the recommended temperature dependence for k1 is based on kinetic studies at temperatures above 200 K. However, the OH + CH3NH2 reaction is not included in astrochemical networks. The observed increase in k1 at ca. 22 K does not significantly change the abundance of NH3 in a typical cold dark interstellar cloud. However, the inclusion of k2 at ca. 22 K, not considered in astrochemical networks, indicates that the contribution of this destruction route for CH3NH2 is not negligible, accounting for 1/3 of the assumed main depletion route (reaction with HCO+) in this IS environment. k1(OH + NH3) = (2.7 ± 0.1) × 10−11 cm3 s−1 k2(OH + CH3NH2) = (3.9 ± 0.1) × 10−10 cm3 s−1

Frontiers in Astronomy and Space Sciences, 8, 802297 (2022)
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CH3CN deuteration in the SVS13-A Class I hot-corino. SOLIS XV

E. Bianchi, C. Ceccarelli, C. Codella, A. López-Sepulcre, S. Yamamoto, N. Balucani, P. Caselli, L. Podio, R. Neri, R. Bachiller, C. Favre, F. Fontani, B. Lefloch, N. Sakai, D. Segura-Cox

We studied the line emission from CH3CN and its deuterated isotopologue CH2DCN towards the prototypical Class I object SVS13-A, where the deuteration of a large number of species has already been reported. Our goal is to measure the CH3CN deuteration in a Class I protostar, for the first time, in order to constrain the CH3CN formation pathways and the chemical evolution from the early prestellar core and Class 0 to the evolved Class I stages. We imaged CH2DCN towards SVS13-A using the IRAM NOEMA interferometer at 3mm in the context of the Large Program SOLIS (with a spatial resolution of 1.8"x1.2"). The NOEMA images have been complemented by the CH3CN and CH2DCN spectra collected by the IRAM-30m Large Program ASAI, that provided an unbiased spectral survey at 3mm, 2mm, and 1.3mm. The observed line emission has been analysed using LTE and non-LTE LVG approaches. The NOEMA/SOLIS images of CH2DCN show that this species emits in an unresolved area centered towards the SVS13-A continuum emission peak, suggesting that methyl cyanide and its isotopologues are associated with the hot corino of SVS13-A, previously imaged via other iCOMs. In addition, we detected 41 and 11 ASAI transitions of CH3CN and CH2DCN, respectively, which cover upper level energies (Eup) from 13 to 442 K and from 18 K to 200 K, respectively. The derived [CH2DCN]/[CH3CN] ratio is ~ 9%. This value is consistent with those measured towards prestellar cores and a factor 2-3 higher than those measured in Class 0 protostars. Contrarily to what expected for other molecular species, the CH3CN deuteration does not show a decrease in SVS13-A with respect to measurements in younger prestellar cores and Class 0 protostars. Finally, we discuss why our new results suggest that CH3CN was likely synthesised via gas-phase reactions and frozen onto the dust grain mantles during the cold prestellar phase.

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Non-Energetic Formation of Ethanol via CCH Reaction with Interstellar H2O Ices. A Computational Chemistry Study

Jessica Perrero, Juan Enrique-Romero, Berta Martínez Bachs, Cecilia Ceccarelli, Nadia Balucani, Piero Ugliengo, Albert Rimola

Ethanol (CH3CH2OH) is a relatively common molecule, often found in star forming regions. Recent studies suggest that it could be a parent molecule of several so-called interstellar complex organic molecules (iCOMs). Yet, the formation route of this species remains debated. In the present work, we study the formation of ethanol through the reaction of CCH with one H2O molecule belonging to the ice, as a test case to investigate the viability of chemical reactions based on a "radical + ice component" scheme as an alternative mechanism for the synthesis of iCOMs, beyond the usual radical-radical coupling. This has been done by means of DFT calculations adopting two clusters of 18 and 33 water molecules as ice models. Results indicate that CH3CH2OH can potentially be formed by this proposed reaction mechanism. The reaction of CCH with H2O on the water ice clusters can be barrierless (thanks to the help of boundary icy water molecules acting as proton transfer assistants) leading to the formation of vinyl alcohol precursors (H2CCOH and CHCHOH). Subsequent hydrogenation of vinyl alcohol yielding ethanol is the only step presenting a low activation energy barrier. We finally discuss the astrophysical implications of these findings.

In press, ACS Earth and Space Chemistry
Full-text URL: https://arxiv.org/abs/2202.11406

Absolute measurements of state-to-state rotational energy transfer between CO and H2 at interstellar temperatures

Hamza Labiad, Martin Fournier, Laura A. Mertens, Alexandre Faure, David Carty, Thierry Stoecklin, Piotr Jankowski, Krzysztof Szalewicz, Sébastien D. Le Picard, and Ian R. Sims

Experimental measurements and theoretical calculations of state-to-state rate coefficients for rotational energy transfer of CO in collision with H2 are reported at the very low temperatures prevailing in dense interstellar clouds (5–20 K). Detailed agreement between quantum state-selected experiments performed in cold supersonic flows using time-resolved infrared–vacuum-ultraviolet double-resonance spectroscopy and close-coupling quantum scattering calculations confirms the validity of the calculations for collisions between the two most abundant molecules in the interstellar medium.

Phys. Rev. A 105, L020802 (2022)
DOI: 10.1103/PhysRevA.105.L020802
Full-text URL: https://arxiv.org/abs/2202.00342

Announcements

EAS 2022 Symposium 9 - The astrochemical heritage: from molecular clouds to planetary surfaces

EAS 2022 Symposium 9 (S9), entitled "The astrochemical heritage: from molecular clouds to planetary surfaces", held in person in Valencia (Spain), from 30th June to July 1st, as part of the EAS 2022 general assembly (June 27th - July 1st).

The full conference program can be found here:
https://eas.unige.ch/EAS_meeting/images/EAS2022_Timetable_sessions.pdf

Event description: This S9 Symposium will bring together the multidisciplinary community working on the chemical complexity in the interstellar medium (molecular clouds, pre-stellar cores, star-forming regions, protoplanetary disks) and the Solar System (comets, asteroids and planetary surfaces). The most recent results from ground-based telescopes and space missions, laboratory works, theoretical calculations and chemical models will be presented and discussed. This symposium will provide a complete view of our current knowledge of the chemical heritage of star and planet formation, and will contribute to design the strategy to best exploit the potential of future facilities in the coming decades.

Website:
The website of the symposium with relevant info can be found here:
https://eas.unige.ch/EAS2022/session.jsp?id=S9

Confirmed Invited Speakers:
• Rosario Brunetto
• José Cernicharo
• Maria Drozdovskaya
• Jon Holdship

• John Ilee
• Thanja Lamberts
• Niels Ligterink
• Zita Martins
• Melissa McClure
• Brett McGuire
• Mattia Melosso
• Dana Qasim

The SOC will award up to 18 contributed talks as well as ePosters.

The abstract submission: https://eas.unige.ch/EAS_meeting/abstract_submission.jsp
The registration page can be found here:
https://eas.unige.ch/EAS_meeting/registration.jsp
via Víctor M. Rivilla, on behalf of the SOC:
• Víctor M. Rivilla (Centro de Astrobiología, CSIC-INTA, Madrid, Spain) - Chair
• Arnaud Belloche (Max-Planck Institute for Radio Astronomy, Germany)
• Paola Caselli (Max-Planck Institute for Extraterrestrial Physics, Munich, Germany)
• Cristina Puzzarini (University of Bologna, Italy)
• Serena Viti (Leiden University, The Netherlands / University College London, United Kingdom)
• Catherine Walsh (University of Leeds, United Kingdom)