AstroChemical Newsletter #110

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Abstracts

Unveiling the ice and gas nature of active centaur (2060) Chiron using the James Webb Space Telescope

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Context. (2060) Chiron is a large centaur that has been reported active on multiple occasions at relatively large heliocentric distances, including during aphelion passage. Studies of Chiron’s coma during active periods have resulted in the detection of C≡N and CO outgassing. Additionally, Chiron is surrounded by a disk of debris that varies with time. Significant work remains to be undertaken to comprehend the activation mechanisms on Chiron and the parent molecules of the gas phases detected. Aims. This work reports the study of the ices on Chiron’s surface and coma and seeks spectral indicators of volatiles associated with the activity. Additionally, we discuss how these detections could be related to the activation mechanism for Chiron and, potentially, other centaurs. Methods. In July 2023, the James Webb Space Telescope (JWST) observed Chiron when it was active near its aphelion. We present JWST/NIRSpec spectra from 0.97 to 5.27 μm with a resolving power of ∼1000, and compare them with laboratory data for identification of the spectral bands. Results We report the first detections on Chiron of absorption bands of several volatile ices, including CO2, CO, C2H6, C3H8, and C2H2. We also confirm the presence of water ice in its amorphous state. A key discovery arising from these data is the detection of fluorescence emissions of CH4, revealing the presence of a gas coma rich in this hyper-volatile molecule, which we also identify to be in non-local thermal equilibrium (non-LTE). CO2 gas emission is also detected in the fundamental stretching band at 4.27 μm. We argue that the presence of CH4 emission is the first proof of the desorption of CH4 due to a density phase transition of amorphous water ice at low temperature in agreement with the estimated temperature of Chiron during the JWST observations (61 K). Detection of photolytic and proton irradiation products of CH4 and CO2 on the surface, in the coma ice grains, or in the ring material is also detected via a forest of absorption features from 3.5 to 5.3 μm.

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A JWST/DiSCo-TNOs portrait of the primordial Solar System through its trans-Neptunian objects

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The detection of molecules on the coldest and outermost objects in our Solar System has long been limited by the terrestrial atmosphere and sensitivity of the available instrumentation. However, near-infrared observations by the James Webb Space Telescope have provided an unprecedented view of the molecular diversity on the surfaces of trans-Neptunian objects (TNOs). Using the low spectral resolution PRISM mode on the near-infrared spectrograph as part of the Cycle 1 large programme, ‘Discovering the Surface Composition of trans-Neptunian objects’, we report the detection of several molecular ices throughout the TNO population, including H2O, CO2, 13CO2, CO, CH3OH and complex molecules and refractory materials containing aliphatic C–H, C≡N, O–H and N–H bonds. As a result of the imprint that these molecules leave on the spectra, three main compositional groups consistently emerge from multiple independent cluster analyses. Our results unlock the long-standing question of the interpretation of colour diversity, providing the much-needed compositional information. The marked separation of the three spectral clusters reveals sharp variations in the surface molecular constituents. The C/O and (CH + NH)/(C + O) ratios on the surface of TNOs are the primary indicators of the spectral differences among the three TNO compositional groups observed. We propose that these objects are fossil remnants of icy planetesimals, and that the three compositional groups provide a picture of the ice retention lines in the Solar System that likely occurred in the outer protoplanetary disk, possibly just before a major planetary migration.

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Time evolution of o-H2D+, N2D+, and N2H+ during the high-mass star formation process

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Deuterium fractionation is a well-established evolutionary tracer in low-mass star formation, but its applicability to the high-mass regime remains an open question. In this context, the abundances and ratios of different deuterated species have often been proposed as reliable evolutionary indicators for different stages of the high-mass star formation process. In this study, we investigate the role of N2H+ and key deuterated molecules (o-H2D+ and N2D+) as tracers of the different stages of the high-mass star formation process. We assess whether their abundance ratios can serve as reliable evolutionary indicators. We conducted APEX observations of o-H2D+ (110–111), N2H+ (4-3), and N2D+ (3-2) in a sample of 40 high-mass clumps at different evolutionary stages, selected from the ATLASGAL survey. Molecular column densities and abundances relative to H2, X, were derived through spectral line modelling, both under local thermodynamic equilibrium (LTE) and non-LTE conditions. The o-H2D+ column densities show the smallest deviation from LTE conditions when derived under non-LTE assumptions. In contrast, N2H+ shows the largest discrepancy between the column densities derived from LTE and non-LTE. In all the cases discussed, we found that X(o-H2D+) decreases more significantly with each respective evolutionary stage than in the case of X(N2D+); whereas X(N2H+) increases slightly. Therefore, the validity of the X(o-H2D+)/X(N2D+) ratio as a reliable evolutionary indicator, recently proposed as a promising tracer of the different evolutionary stages, was not observed for this sample. While the deuteration fraction derived from N2D+ and N2H+ clearly decreases with clump evolution, the interpretation of this trend is complex, given the different distribution of the two tracers. Our results suggest that a careful consideration of the observational biases and beam-dilution effects are crucial for an accurate interpretation of the evolution of the deuteration process during the high-mass star formation process.

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Submillimeter-Wave Spectroscopy of the CH3O Radical

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The methoxy radical, CH3O, has long been studied experimentally and theoretically by spectroscopists because it displays a weak Jahn-Teller effect in its electronic ground state, combined with a strong spin-orbit interaction. In this work, we report an extension of the measurement of the pure rotational spectrum of the radical in its vibrational ground state in the submillimeter-wave region (350−860 GHz). CH3O was produced by H-abstraction from methanol using F-atoms, and its spectrum was probed in absorption using an association of source-frequency modulation and Zeeman modulation spectroscopy. All the observed transitions together with available literature data in v=0 were combined and fit using an effective Hamiltonian allowing to reproduce the data at their experimental accuracy. The newly measured transitions involve significantly higher frequencies and rotational quantum numbers than those reported in the literature (f<860 GHz and N≤15 instead of 272 GHz and 7, respectively) which results in significant improvements in the spectroscopic parameters determination. The present model is well constrained and allows a reliable calculation of the rotational spectrum of the radical over the entire microwave to submillimeter-wave domain. It can be used with confidence for future searches of CH3O in the laboratory and the interstellar medium.

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Production of linear alkanes via the solid-state hydrogenation of interstellar polyynes

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Context. Highly unsaturated carbon chains, including polyynes, have been detected in many astronomical regions and planetary systems. With the success of the QUIJOTE survey of the Taurus Molecular Cloud-1 (TMC-1), the community has seen a “boom” in the number of detected carbon chains. On the other hand, the Rosetta mission revealed the release of fully saturated hydrocarbons, C3H8, C4H10, C5H12, and (under specific conditions) C6H14 with C7H16, from the comet 67P/Churyumov-Gerasimenko. The detection of the latter two is attributed to dust-rich events. Similarly, the analysis of samples returned from asteroid Ryugu by Hayabusa2 mission indicates the presence of long saturated aliphatic chains in Ryugu’s organic matter. Aims. The surface chemistry of unsaturated carbon chains under conditions resembling those of molecular clouds can provide a possible link among these independent observations. However, laboratory-based investigations to validate such a chemistry is still lacking. In the present study, we aim to experimentally verify the formation of fully saturated hydrocarbons by the surface hydrogenation of C2nH2 (n > 1) polyynes under ultra-high vacuum conditions at 10 K. Methods. We undertook a two-step experimental technique. First, a thin layer of C2H2 ice was irradiated by UV-photons (≥121 nm) to achieve a partial conversion of C2H2 into larger polyynes: C4H2 and C6H2. Afterwards, the obtained photoprocessed ice was exposed to H atoms to verify the formation of various saturated hydrocarbons. Results. In addition to C2H6, which was investigated previously, the formation of larger alkanes, including C4H10 and (tentatively) C6H14, is confirmed by our study. A qualitative analysis of the obtained kinetic data indicates that hydrogenation of HCCH and HCCCCH triple bonds proceeds at comparable rates, given a surface temperature of 10 K. This can occur on the timescales typical for the dark cloud stage. A general pathway resulting in formation of other various aliphatic organic compounds by surface hydrogenation of N- and O-bearing polyynes is also proposed. We also discuss the astrobiological implications and the possibility of identifying alkanes with JWST.

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Announcements

PhD position in Laboratory Astrochemistry

Applications are invited for a PhD in Laboratory Astrochemistry in the group of Professor Wendy Brown at the University of Sussex, UK.
The PhD position is available as past of the UK EPSRC Doctoral Landscape awards at the University of Sussex. For more information, look at the brochure on the University website, and look for Chemistry projects. Alternatively contact Wendy Brown (w.a.brown@sussex.ac.uk) for further information.
Application deadline 14th February 2025. To apply, follow the instructions here.

PhD Position: 3D Astrochemical Modelling of Star-Forming Regions

The newly established Emmy Noether Junior Research Group “Towards the Next Generation in Cosmic Ray Astrophysics” at the University of Duisburg-Essen led by Dr. Brandt Gaches is looking for a PhD student for novel investigations of the chemistry of star-forming molecular clouds. The PhD position is funded for 3.5 years. The project will be of interest to post-graduates who are looking to work with state-of-the-art star formation simulations, astrochemical modelling tools and development, and the analysis of large astrochemical datasets. The position can start as early as April 2025.

The deadline for applications is February 19, 2025. For more details on the position and how to apply, please see the job advertisement: https://www.uni-due.de/karriere/stelle.php?kennziffer=023-25
Please contact Brandt Gaches if you are interested in the project, or if you have any questions about the position: brandt.gaches@chalmers.se

3rd COST NanoSpace Joint Scientific Meeting

The 3rd Joint Scientific Meeting of the COST Action NanoSpace (CA21126; https://research.iac.es/proyecto/nanospace/) will take place 13-15 May 2025, at Kaunas University of Technology, Kaunas, Lithuania. You can find all detailed information about the venue, registration (participation is free), abstract submission, etc., in the meeting website: https://nanospace.ktu.edu/. The event will bring together leading scientists, researchers, and innovators to explore the engaging role of carbon molecular nanostructures in space.
The 3rd Action Joint Meeting will be focussed on the fundamental and applied research of diverse carbon molecular nanostructures (fullerenes, graphene, carbon nanotubes, and their derivatives) in the context of space science and exploration. The meeting will attack key questions on the formation, properties, and potential applications of these nanocarbon materials under space conditions. Another key nanocarbon topics for discussion will include:
i) Formation and Characterization;
ii) Space Radiation and Stability;
iii) Astrobiology and Planetary Science;
iv) Applications in Space Technology; and
v) Laboratory Studies.

This is the third NanoSpace Joint Scientific Meeting (in person), which will consolidate the interaction and collaboration among the diversity of disciplines (laboratory astrophysics, theoretical chemistry and physics, astronomy, among others) and researchers present in the Action. The program will be composed by scientific sessions separated by topic, with special attention to the Action progress and scientific results.

The deadline for registration and abstract submission is 5th April 2025.

Please check the meeting website (https://nanospace.ktu.edu/) for news and updates about the final list of invited speakers, hotel registration links, etc. More detailed information will be given in a second announcement.