AstroChemical Newsletter #112

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Abstracts

Shock-induced HCNH+ abundance enhancement in the heart of the starburst galaxy NGC 253 unveiled by ALCHEMI

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Understanding the chemistry of molecular clouds is pivotal to elucidate star formation and galaxy evolution. As one of the important molecular ions, HCNH+ plays an important role in this chemistry. Yet, its behavior and significance under extreme conditions, such as in the CMZs of external galaxies, are still largely unexplored. We aim to reveal the physical and chemical properties of the CMZ in the starburst galaxy NGC253 with multiple HCNH+ transitions to shed light on the molecule's behavior under the extreme physical conditions of a starburst. We employ molecular line data including results for four rotational transitions of HCNH+ from the ALCHEMI large program to investigate underlying physical and chemical processes. Despite weak intensities, HCNH+ emission is widespread throughout NGC253's CMZ, which suggests that this molecular ion can effectively trace large-scale structures within molecular clouds. Using the quantum mechanical coupled states approximation, we computed rate coefficients for collisions of HCNH+ with para-H2 and ortho-H2 at kinetic temperatures up to 500 K. Using these coefficients in a non-LTE modeling framework and employing a Monte Carlo Markov chain analysis, we find that HCNH+ emission originates from regions with H2 number densities of ~10^2.80−10^3.55 cm-3, establishing HCNH+ as a tracer of low-density environments. Our analysis reveals that most of the HCNH+ abundances in the CMZ of NGC253 are higher than all reported values in the Milky Way. We performed static, PDR, and shock modeling, and found that recurrent shocks could potentially account for the elevated HCNH+ abundances observed in this CMZ. We propose that the unexpectedly high HCNH+ abundances may result from chemical enhancement, primarily driven by the elevated gas temperatures and cosmic ray ionization rates of shocked, low-density gas in the nuclear starburst regions of NGC253.

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PDRs4All XII. Far-ultraviolet-driven formation of simple hydrocarbon radicals and their relation with polycyclic aromatic hydrocarbons

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We present subarcsecond-resolution ALMA mosaics of the Orion Bar PDR in [CI] 609um, C2H (4-3), and C18O (3-2) emission lines complemented by JWST images of H2 and aromatic infrared band (AIB) emission. The rim of the Bar shows very corrugated structures made of small-scale H2 dissociation fronts (DFs). The [CI] 609 um emission peaks very close (~0.002 pc) to the main H2-emitting DFs, suggesting the presence of gas density gradients. These DFs are also bright and remarkably similar in C2H emission, which traces "hydrocarbon radical peaks" characterized by very high C2H abundances, reaching up to several x10^-7. The high abundance of C2H and of related hydrocarbon radicals, such as CH3, CH2, and CH, can be attributed to gas-phase reactions driven by elevated temperatures, the presence of C+ and C, and the reactivity of FUV-pumped H2. The hydrocarbon radical peaks roughly coincide with maxima of the 3.4/3.3 um AIB intensity ratio, a proxy for the aliphatic-to-aromatic content of PAHs. This implies that the conditions triggering the formation of simple hydrocarbons also favor the formation (and survival) of PAHs with aliphatic side groups, potentially via the contribution of bottom-up processes in which abundant hydrocarbon radicals react in situ with PAHs. Ahead of the DFs, in the atomic PDR zone (where [H]>>[H2]), the AIB emission is the brightest, but small PAHs and carbonaceous grains undergo photo-processing due to the stronger FUV field. Our detection of trace amounts of C2H in this zone may result from the photoerosion of these species. This study provides a spatially resolved view of the chemical stratification of key carbon carriers in a PDR. Overall, both bottom-up and top-down processes appear to link simple hydrocarbon molecules with PAHs in molecular clouds; however, the exact chemical pathways and their relative contributions remain to be quantified.

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Anharmonic Vibrational Frequencies and Spectroscopic Constants for the Six Conformers of 1,2-Diiminoethane: A Promising Prebiotic Molecule for Astronomical Detection

Megan McKissick and Ryan C. Fortenberry

The search for the molecular origins of life likely must go through polyimines, and this quantum chemical work shows that the anti-(E,Z)-1,2-diiminoethane molecule would be the next natural step as a detection target. This conformer exhibits a 2.78 D dipole moment and is the second-lowest-energy conformer after the nonpolar anti-(E,E) form. Additionally, the previously assigned N–H antisymmetric stretch of the lowest-energy anti-(E,E) conformer should likely be decreased in frequency to closer to 2930 cm–1. The full set of anharmonic, fundamental vibrational frequencies and spectroscopic constants of all six conformers are produced in this work and will aid in any possible, future characterization of 1,2-diiminoethane and its possible role in the buildup of prebiotic molecules where multiple C = N bonds are required.

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The hot corino-like chemistry of four FUor-like protostars

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Context: Compared to Class 0 protostars, the higher densities and lower temperatures of the disk midplanes of Class I young stellar objects (YSOs) limit the detectability of complex organic molecules (COMs). The elevated luminosities of eruptive YSOs increase disk temperatures sublimating frozen molecules and easing their detection. Aims: Our aim is to investigate the chemical composition of four FUor-like Class I YSOs: L1551 IRS 5, Haro 5a IRS, V346 Nor, and OO Ser, and to compare their abundances of COMs with other YSOs in the literature. Methods: We search for COMs line emission in ALMA Band 6 observations. We use the CASSIS software to determine their column densities (N) and excitation temperatures (Tex) assuming local thermodynamical equilibrium. Results: We detect 249 transitions from 12 COMs. In L1551 IRS 5 we identified CH3OH, 13CH3OH, CH318OH, CH2DOH, CH3CHO, CH3OCH3, CH3OCHO, CH3COCH3, C2H5OH, C2H5CN, 13CH3CN, and CH3C15)N. Haro 5a IRS and OO Ser have emission from CH3OH, CH3CHO, CH3OCH3, and CH3OCHO. CH3COCH3 is also detected in OO Ser. In V346 Nor we found CH3OH, CH2DOH, CH3CHO, CH3OCH3, CH3OCHO, and C2H5CN. The emission of COMs is compact in all targets. The analysis indicates their temperatures are above 100K. The abundance ratios of COMs derived for these eruptive YSOs, as well as for other protostars in the literature, span several orders of magnitude without any clear differentiation between the eruptive and quiescent YSOs. The column density of the main isotopologue of CH3OH should not be used as a reference, as most of the lines are optically thick. Conclusions: The hot and compact emission of COMs indicates that the four FUor-like targets are hot corino-like. Spectral studies of such objects can be useful to investigate the complex organic chemistry at later evolutionary stages than the usual Class 0 stage.

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More π, please: What drives the formation of unsaturated molecules in the interstellar medium?

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We present a computational investigation into the fragmentation pathways of ethanolamine (C2H7NO, EtA), propanol (C3H8O, PrO), butanenitrile (C4H7N, BuN), and glycolamide (C2H5NO2, GlA)—saturated organic molecules detected in the interstellar medium (ISM), particularly in the molecular cloud complex Sagittarius B2 (Sgr B2) and its molecular cloud G+0.693-0.027. Using electron-impact ionization data and Born–Oppenheimer molecular dynamics simulations, we investigate how cosmic rays, cosmic-ray-induced UV fields, and shock-induced heating can induce the fragmentation of these molecules, resulting in the formation of unsaturated species with extended π-bond networks. Despite the attenuation of external UV radiation in G+0.693-0.027, these energetic processes are capable of driving partial transformations of saturated into unsaturated molecules, supporting the coexistence of species like EtA and GlA alongside unsaturated nitriles such as cyanoacetylene (HC3N), cyanopropyne (CH3C3N), and cyanoallene (CH2CCHCN). Our findings underscore the significance of high-energy mechanisms in enhancing chemical complexity within molecular clouds and offer insights into the pathways that govern the evolution of organic molecules in the ISM.

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Chemistry and ro-vibrational excitation of HeH+ in the Planetary Nebula NGC 7027

Milan Sil, Alexandre Faure, Helmut Wiesemeyer, Pierre Hily-Blant, Jérôme Loreau, KD Pérez, Roman Čurík, François Lique

HeH+ belongs to the class of "reactive" ions that can be destroyed so quickly that chemical formation and destruction rates may compete with inelastic rates and should be considered when solving the statistical equilibrium equations. This so-called chemical "pumping" or "excitation" effect is investigated here for the first time in HeH+. The chemical evolution of HeH+ in NGC 7027 is modeled with the CLOUDY photoionization code using updated reaction rate coefficients. The non-LTE analysis of the three observed HeH+ emission lines is then performed with the CLOUDY and RADEX codes using an extensive set of spectroscopic and inelastic collisional data suitable for the specific high-temperature environment of NGC

7027. In a second approach, chemical formation and destruction rates of HeH+ are implemented in RADEX. This code is combined with MCMC sampling (performed on the RADEX-parameters space) to extract the best-fit HeH+ column density and physical conditions from the observed line fluxes. The CLOUDY and RADEX non-LTE results are found to be in good agreement, and the υ=1−0 P(2)/P(1) line ratio is better than 20%. Agreement to better than a factor of 2.3 is obtained when including the reaction between He(23S) and H as an additional source of HeH+. The RADEX-MCMC model with chemical pumping is found to reproduce both the observed line fluxes and the line ratio to 20%. Our results suggest that additional HeH+ lines must be detected in NGC 7027 to better constrain the physical conditions via non-LTE models. Uncertainties in collisional (reactive and inelastic) data of HeH+ have been largely reduced in this work. The three observed lines are not sensitive to chemical pumping while excited "short-lived" levels are significantly overpopulated with respect to a non-LTE model neglecting chemical excitation.

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Spectral Diversity of DiSCo's TNOs Revealed by JWST: Early Sculpting and Late Irradiation

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The spectral diversity of trans-Neptunian objects (TNOs) is crucial for understanding the processes that led to the formation and evolution of planetesimals in the outer solar system. Using near-IR (NIR) spectra obtained by the James Webb Space Telescope (JWST) as part of the DiSCo-TNOs large program, we report the detection of well-clustered subgroups of TNOs. A first subgroup has strong NIR features with contributions from H2O, CO2, CO, CH3OH, and other organic molecules. The 2.27 μm band area, commonly attributed to methanol, decreases with increasing eccentricity, which is compatible with a late destruction of CH3OH by cosmic ion irradiation at the edge of the heliosphere. The absence of the strongest CH3OH bands in the JWST spectra is compatible with an irradiation-induced surface stratification, with CH3OH abundance increasing with increasing depth. A second subgroup has much weaker NIR bands, and these cannot be explained by a late irradiation scenario. This group is further divided into two subgroups (cold classical TNOs and objects with low perihelion) that are spectrally very similar except for their CO2 band area. We propose two possible interpretations. In one scenario, the TNO subgroups sampled a similar molecular inventory in the protoplanetary disk, after which early surface processes, such as primordial sublimation or irradiation from the young Sun, sculpted the two groups before planetary migration occurred. In a second scenario, the subgroups formed in different locations of the disk where molecules were available in different abundances. A combination of both scenarios is also possible.

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Announcements

839. WE-Heraeus Seminar: Charting the Cosmos

We are pleased to announce the 839th WE-Heraeus Seminar titled "Charting the Cosmos: From Cosmic Stellar Nurseries to Evolved Stars using High Powered Telescopes," which will take place at Wasem Kloster, Engelthal, Germany, from August 18 to 22, 2025.

CALL FOR ABSTRACTS IS NOW OPEN!

Seminar Overview
Star formation and evolution are fundamental to cosmic structure, yet the processes driving them remain poorly understood. Key questions include how atomic clouds transition into molecular clouds to form stars, and how stars shape their environments on both local and global scales. The 839th WE-Heraeus Seminar aims to foster collaboration and showcase cutting-edge research in these areas, featuring new observations, as well as the latest theoretical and computational simulations. By uniting experts from the major fields of modern astronomy, we hope to address the complexities of star formation and stellar evolution more effectively.

We strongly encourage early-career researchers to apply and particularly welcome applications from women, in line with the Wilhelm and Else-Heraeus Foundation's commitment to equal opportunities.

Additionally, this seminar will honor the life and work of Prof. Dr. Karl M. Menten, our dear friend, mentor, and colleague, whose sudden passing has left us heartbroken. His legacy, however, lives on through his profound contributions over the past forty years, which continue to inspire countless researchers in Astronomy and Astrophysics.

Seminar Topics
The seminar will feature sessions on the following topics:
Cool Evolved Stars
Star Formation

Galactic Centre
Galactic Surveys
Interstellar Medium & Spectroscopy
Instrumentation Landscape

For more details, please visit our website (https://indico.mpifr-bonn.mpg.de/event/6/) or contact us via email at: charting2025@mpifr-bonn.mpg.de.