

AstroChemical Newsletter #74

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Abstracts

[Enlightening the chemistry of infalling envelopes and accretion disks around Sun-like protostars: the ALMA FAUST project](#)

C. Codella, C. Ceccarelli, C. Chandler, N. Sakai, S. Yamamoto, and the FAUST team

The huge variety of planetary systems discovered in recent decades likely depends on the early history of their formation. In this contribution we introduce the FAUST Large Program, which focuses specifically on the early history of Solar-like protostars and their chemical diversity at scales of ~ 50 au, where planets are expected to form. In particular, the goal of the project is to reveal and quantify the variety of chemical composition of the envelope/disk system at scales of 50 au in a sample of Class 0 and I protostars representative of the chemical diversity observed at larger scales. For each source, we propose a set of molecules able to: (1) disentangle the components of the 50-2000 au envelope/disk system; (2) characterise the organic complexity in each of them; (3) probe their ionization structure; (4) measure their molecular deuteration. The output will be a homogeneous database of thousands of images from different lines and species, i.e., an unprecedented source-survey of the chemical diversity of Solar-like protostars. FAUST will provide the community with a legacy dataset that will be a milestone for astrochemistry and star formation studies.

Frontiers Astronomy and Space Sciences, in press

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[The Role of Terahertz and Far-IR Spectroscopy in Understanding the Formation and Evolution of Interstellar Prebiotic Molecules](#)

Duncan V. Mifsud, Perry A. Hailey, Alejandra Traspas Muiña, Olivier Auriacombe, Nigel J. Mason, and Sergio Ioppolo

Stellar systems are often formed through the collapse of dense molecular clouds which, in turn, return copious amounts of atomic and molecular material to the interstellar medium. An in-depth understanding of chemical evolution during this cyclic interaction between the stars and the interstellar medium is at the heart of astrochemistry. Systematic chemical composition changes as interstellar clouds evolve from the diffuse stage to dense, quiescent molecular clouds to star-forming regions and proto-planetary disks further enrich the molecular diversity leading to the evolution of ever more complex molecules. In particular, the icy mantles formed on interstellar dust grains and their irradiation are thought to be the origin of many of the observed molecules, including those that are deemed to be “prebiotic”; that is those molecules necessary for the origin of life. This review will discuss both observational (e.g., ALMA, SOFIA, Herschel) and laboratory investigations using terahertz and far-IR (THz/F-IR) spectroscopy, as well as centimeter and millimeter spectroscopies, and the role that they play in contributing to our understanding of the formation of prebiotic molecules. Mid-IR spectroscopy has typically been the primary tool used in laboratory studies, particularly those concerned with interstellar ice analogues. However, THz/F-IR spectroscopy offers an additional and complementary approach in that it provides the ability to investigate intermolecular interactions compared to the intramolecular modes available in the mid-IR. THz/F-IR spectroscopy is still somewhat under-utilized, but with the additional capability it brings, its popularity is likely to significantly increase in the near future. This review will discuss the strengths and limitations of such methods, and will also provide some suggestions on future research areas that should be pursued in the coming decade exploiting both space-borne and laboratory facilities.

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[Laboratory observation and astronomical search of 1-cyano propargyl radical, HCCCHCN](#)

C. Cabezas, M. Nakajima, C. H. Chang, M. Agundez, Y. Endo, and J. Cernicharo

The reaction between carbon atoms and vinyl cyanide, CH_2CHCN , is a formation route to interstellar 3-cyano propargyl radical, $\text{CH}_2\text{C}_3\text{N}$, a species that has recently been discovered in space. The 1-cyano propargyl radical (HC_3HCN), an isomer of $\text{CH}_2\text{C}_3\text{N}$, is predicted to be produced in the same reaction at least twice more efficiently than $\text{CH}_2\text{C}_3\text{N}$. Hence, HC_3HCN is a plausible candidate to be observed in space as well. We aim to generate the HC_3HCN radical in the gas phase in order to investigate its rotational spectrum. The derived spectroscopic parameters for this species will be used to obtain reliable frequency predictions to support its detection in space. The HC_3HCN radical was produced by an electric discharge, and its rotational spectrum was characterized using a Balle-Flygare narrowband-type Fourier-transform microwave spectrometer operating in the frequency region of 4-40 GHz. The spectral analysis was supported by high-level

ab initio calculations. A total of 193 hyperfine components that originated from 12 rotational transitions, a- and b-type, were measured for the HC3HCN radical. The analysis allowed us to accurately determine 22 molecular constants, including rotational and centrifugal distortion constants as well as the fine and hyperfine constants. Transition frequency predictions were used to search for the HC3HCN radical in TMC-1 using the QUIJOTE survey between 30.1-50.4 GHz. We do not detect HC3HCN in TMC-1 and derive a 3 σ upper limit to its column density of 6.0e11 cm⁻².

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Photodesorption of Acetonitrile CH₃CN in UV-irradiated Regions of the Interstellar Medium: Experimental Evidence

R. Basalgète, A.J. Ocaña, G. Féraud, C. Romanzin, L. Philippe, X. Michaut, J.-H. Fillion, M. Bertin

Pure acetonitrile (CH₃CN) and mixed CO:CH₃CN and H₂O:CH₃CN ices have been irradiated at 15 K with vacuum ultraviolet (VUV) photons in the 7–13.6 eV range using synchrotron radiation. VUV photodesorption yields of CH₃CN and of photoproducts have been derived as a function of the incident photon energy. The coadsorption of CH₃CN with CO and H₂O molecules, which are expected to be among the main constituents of interstellar ices, is found to have no significant influence on the VUV photodesorption spectra of CH₃CN, CHCN, HCN, CN, and CH₃. Contrary to what has generally been evidenced for most of the condensed molecules, these findings point toward a desorption process for which the CH₃CN molecule that absorbs the VUV photon is the one desorbing. It can be ejected in the gas phase as intact CH₃CN or in the form of its photodissociation fragments. Astrophysical VUV photodesorption yields, applicable to different locations, are derived and can be incorporated into astrochemical modeling. They vary from 0.67(+/- 0.33)e⁻⁵ to 2.0(+/- 1.0)e⁻⁵ molecule photon⁻¹ for CH₃CN depending on the region considered, which is high compared to other organic molecules such as methanol. These results could explain the multiple detections of gas-phase CH₃CN in different regions of the interstellar medium and are well correlated to astrophysical observations of the Horsehead nebula and of protoplanetary disks (such as TW Hya and HD 163296).

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Quantifying the chemical desorption of H₂S and PH₃ from amorphous water ice surfaces

K. Furuya, Y. Oba, T. Shimonishi

Nonthermal desorption of molecules from icy grain surfaces is required to explain molecular line observations in the cold gas of star-forming regions. Chemical desorption is one of the nonthermal desorption processes and is driven by the energy released by chemical reactions. After an exothermic surface reaction, the excess energy is transferred to products' translational energy in the direction perpendicular to the surface, leading to desorption. The desorption probability of product species, especially that of product species from water ice surfaces, is not well understood. This uncertainty limits our understanding of the interplay between gas-phase and ice surface chemistry. In the present work, we constrain the desorption probability of H₂S and PH₃ per reaction event on porous amorphous solid water (ASW) by numerically simulating previous laboratory experiments. Adopting the microscopic kinetic Monte Carlo method, we find that the desorption probabilities of H₂S and PH₃ from porous ASW per hydrogen addition event of the precursor species are 3 ± 1.5 % and 4 ± 2 %, respectively. These probabilities are consistent with a theoretical model of chemical desorption proposed in the literature if ~7 % of energy released by the reactions is transferred to the translational excitation of the products. As a byproduct, we find that approximately 70 % (40 %) of adsorption sites for atomic H on porous ASW should have a binding energy lower than ~300 K (~200 K). The astrochemical implications of our findings are briefly discussed.

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Methanol Mapping in Cold Cores: Testing Model Predictions

Anna Punanova, Anton Vasyunin, Paola Caselli, Alexander Howard, Silvia Spezzano, Yancy Shirley, Samantha Scibelli, Jorma Harju

Chemical models predict that in cold cores gas-phase methanol is expected to be abundant at the outer edge of the CO depletion zone, where CO is actively adsorbed. CO adsorption correlates with volume density in cold cores, and, in nearby molecular clouds, the catastrophic CO freeze-out happens at volume densities above 1e4 cm⁻³. The methanol production rate is maximized there and its freeze-out rate does not overcome its production rate, while the molecules are shielded from UV destruction by gas and dust. Thus, in cold cores, methanol abundance should generally correlate with visual extinction that depends both on volume and column density. In this work, we test the most basic model prediction that maximum methanol abundance is associated with a local A_v=4 mag in dense cores and constrain the model parameters with the observational data. With the IRAM 30 m antenna, we mapped the CH₃OH (2-1) and (3-2) transitions toward seven dense cores in the L1495 filament in Taurus to measure the methanol abundance. We use the Herschel/SPIRE maps to estimate visual extinction, and the C18O(2-1) maps from Tafalla & Hacar (2015) to estimate CO depletion. We explored the observed and modeled correlations between the methanol abundances, CO depletion, and visual extinction varying the key model parameters. The modeling results show that hydrogen surface diffusion via tunneling is crucial to reproduce the observed

methanol abundances, and the needed reactive desorption efficiency matches the one deduced from laboratory experiments.

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Measurements of Ortho-to-para Nuclear Spin Conversion of H₂ on Low-temperature Carbonaceous Grain Analogs: Diamond-like Carbon and Graphite

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Hydrogen molecules have two nuclear spin isomers: ortho-H₂ and para-H₂. The ortho-to-para ratio (OPR) is known to affect chemical evolution as well as gas dynamics in space. Therefore, understanding the mechanism of OPR variation in astrophysical environments is important. In this work, the nuclear spin conversion (NSC) processes of H₂ molecules on diamond-like carbon and graphite surfaces are investigated experimentally by employing temperature-programmed desorption and resonance-enhanced multiphoton ionization methods. For the diamond-like carbon surface, the NSC time constants were determined at temperatures of 10–18 K and from 3900 ± 800 s at 10 K to 750 ± 40 s at 18 K. Similar NSC time constants and temperature dependence were observed for a graphite surface, indicating that bonding motifs (sp³ or sp² hybridization) have little effect on the NSC rates.

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Branching ratio for O + H₃⁺ forming OH⁺ + H₂ and H₂O⁺ + H

Pierre-Michel Hillenbrand, Nathalie de Ruelle, Xavier Urbain, Daniel W. Savin

The gas-phase reaction of O + H₃⁺ has two exothermic product channels, OH⁺ + H₂ and H₂O⁺ + H. In the present study, we analyze experimental data from a merged-beams measurement to derive thermal rate coefficients resolved by product channel for the temperature range from 10 to 1000 K. Published astrochemical models either ignore the second product channel or apply a temperature-independent branching ratio of 70% vs. 30% for the formation of OH⁺ + H₂ vs. H₂O⁺ + H, respectively, which originates from a single experimental data point measured at 295 K. Our results are consistent with this data point, but show a branching ratio that varies with temperature reaching 58% vs. 42% at 10 K. We provide recommended rate coefficients for the two product channels for two cases, one where the initial fine-structure population of the O(3P_J) reactant is in its J=2 ground state and the other one where it is in thermal equilibrium.

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