AstroChemical Newsletter #78

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Abstracts

Precursors of the RNA-world in space: Detection of (Z)-1,2-ethenediol in the interstellar medium, a key intermediate in sugar formation

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We present the first detection of (Z)-1,2-ethenediol, (CHOH)2, the enol form of glycolaldehyde, in the interstellar medium towards the G+0.693-0.027 molecular cloud located in the Galactic Center. We have derived a column density of (1.8±0.1)×10^13 cm^−2, which translates into a molecular abundance with respect to molecular hydrogen of 1.3×10^−10. The abundance ratio between glycolaldehyde and (Z)-1,2-ethenediol is ~5.2. We discuss several viable formation routes through chemical reactions from precursors such as HCO, H2CO, HCOH or CH2CHOH. We also propose that this species might be an important precursor in the formation of glyceraldehyde (HOCH2CHOHCHO) in the interstellar medium through combination with the hydroxymethylene (CHOH) radical.

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A new protonated molecule discovered in TMC-1: HCCNCH+

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In recent years we have seen an important increase in the number of protonated molecules detected in cold dense clouds. Here we report the detection in TMC-1 of HCCNCH+, the protonated form of HCCNC, which is a metastable isomer of HC3N. This is the first protonated form of a metastable isomer detected in a cold dense cloud. The detection was based on observations carried out with the Yebes 40m and IRAM 30m telescopes, which revealed four harmonically related lines. We derive a rotational constant B = 4664.431891 +/- 0.000692 MHz and a centrifugal distortion constant D = 519.14 +/- 4.14 Hz. From a high-level ab initio screening of potential carriers we confidently assign the series of lines to the ion HCCNCH+. We derive a column density of (3.0 +/- 0.5)e10 cm-2 for HCCNCH+, which results in a HCCNCH+/HCCNC abundance ratio of 0.010 +/- 0.002. This value is well reproduced by a state-of-the-art

chemical model, which however is subject to important uncertainties regarding the chemistry of HCCNCH+. The observational and theoretical status of protonated molecules in cold dense clouds indicate that there exists a global trend in which protonated-to-neutral abundance ratios MH+/M increase with increasing proton affinity of the neutral M, although if one restricts to species M with high proton affinities (>700 kJ/mol), MH+/M ratios fall in the range 0.001-0.1, with no apparent correlation with proton affinity. We suggest various protonated molecules that are good candidates for detection in cold dense clouds in the near future.

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Discovery of a new molecular ion, HC7NH+, in TMC-1

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We report the detection of the protonated form of HC7N in TMC-1. The discovery of the cation HC7NH+ was carried out via the observation of nine harmonically related lines in the Q-band using the Yebes 40m radiotelescope. The observed frequencies allowed us to obtain the rotational constants B_0=553.938802(160)MHz and D_0=3.6292(705) Hz. The identification of HC7NH+ is further supported by accurate ab initio calculations. We derived a column density of (5.5+/-0.7)e10 cm-2, which constitutes another piece of evidence for the identification of the carrier. In addition, we revised the HC7N column density and we derived a new value of (2.1+/-0.2)e13cm-2. Hence, the abundance ratio HC7N/HC7NH+ is 380, while those for HC3N/HC3NH+ and HC5N/HC5NH+ are 230 and 240, respectively. Here, we discuss these results within the framework of a chemical model for protonated molecules in cold dense clouds.

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Monte Carlo simulation of sugar synthesis on icy dust particles intermittently irradiated by UV in a protoplanetary disk

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Context. While synthesis of organic molecules in molecular clouds or protoplanetary disks is complex, observations of interstellar grains, analyses of carbonaceous chondrites, and UV photochemistry experiments are rapidly developing and are providing constraints on and clues to the complex organic molecule synthesis in space. This motivates us to construct a theoretical synthesis model. Aims. We developed a new code to simulate global reaction sequences of organic molecules and apply it to sugar synthesis by intermittent UV irradiation on the surface of icy particles in a protoplanetary disk. Here we show the first results of our new simulation. Methods. We applied a Monte Carlo method to select reaction sequences from all possible reactions, using the graph-theoretic matrix model for chemical reactions and modeling reactions on the icy particles during UV irradiation. Results. We obtain results consistent with the organic molecules in carbonaceous chondrites and obtained by experiments, albeit through a different pathway from the conventional formose reactions previously suggested. During UV irradiation, loosely bonded O-rich large molecules are

continuously created and destroyed. After UV irradiation is turned off, the ribose abundance rapidly increases through the decomposition of the large molecules via breakage of O-O bonds and replacements of C-OH by C-H to reach O/C = 1 for sugars. The sugar abundance is regulated mostly by the total atomic ratio H/O of starting materials, but not by their specific molecular forms. Deoxyribose is simultaneously synthesized, and most of the molecules end up in complexes with C-rich molecules.

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The ALMA-PILS survey: First tentative detection of 3-hydroxypropenal (HOCHCHCHO) in the interstellar medium and chemical modeling of the C3H4O2 isomers

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Characterizing the molecular composition of solar-type protostars is useful for improving our understanding of the physico-chemical conditions under which the Sun and its planets formed. In this work, we analyzed the Atacama Large Millimeter/submillimeter Array (ALMA) data of the Protostellar Interferometric Line Survey (PILS), an unbiased spectral survey of the solar-type protostar IRAS 16293–2422, and we tentatively detected 3-hydroxypropenal (HOCHCHCHO) for the first time in the interstellar medium towards source B. Based on the observed line intensities and assuming local thermodynamic equilibrium, its column density is constrained to be ~1e15 cm−2, corresponding to an abundance of 1e−4 relative to methanol, CH3OH. Additional spectroscopic studies are needed to constrain the excitation temperature of this molecule. We included HOCHCHCHO and five of its isomers in the chemical network presented in Manigand et al. (2021) and we predicted their chemical evolution with the Nautilus code. The model reproduces the abundance of HOCHCHCHO within the uncertainties. This species is mainly formed through the grain surface reaction CH2CHO + HCO → HCOCH2CHO, followed by the tautomerization of HCOCH2CHO into HOCHCHCHO. Two isomers, CH3COCHO and CH2COHCHO, are predicted to be even more abundant than HOCHCHCHO. Spectroscopic studies of these molecules are essential in searching for them in IRAS 16293–2422 and other astrophysical sources.

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Fevering Interstellar Ices Have More CH3OD

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Mono-deuterated methanol is thought to form during the prestellar core stage of star formation. Observed variations in the CH2DOH/CH3OD ratio suggest that its formation is strongly dependent on the surrounding cloud conditions. Thus, it is a potential tracer of the physical conditions before the onset of star formation. A single-point physical model representative of a typical prestellar core is coupled to chemical models to investigate potential formation pathways towards deuterated methanol at the prestellar stage. Simple addition reactions of H and D are not able to reproduce observed abundances. The implementation of an experimentally verified abstraction scheme leads to the efficient formation of methyl-deuterated methanol, but lacks sufficient formation

of hydroxy-deuterated methanol. CH3OD is most likely formed at a later evolutionarymstage, potentially from H-D exchange reactions in warm ices between HDO (and D2O) and CH3OH. The CH2DOH/CH3OD ratio is not an appropriate tracer of the physical conditions during the prestellar stage, but might be better suited as a tracer of ice heating.

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Gliding on ice in search of accurate and cost-effective computational methods for astrochemistry on grains: the puzzling case of the HCN isomerization

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The isomerization of hydrogen cyanide to hydrogen isocyanide on icy grain surfaces is investigated by an accurate composite method (jun-Cheap) rooted in the coupled cluster ansatz and by density functional approaches. After benchmarking density functional predictions of both geometries and reaction energies against jun-Cheap results for the relatively small model system HCN--(H2O)2 the best performing DFT methods are selected. A large cluster containing 20 water molecules is then employed within a QM/QM′ approach to include a realistic environment mimicking the surface of icy grains. Our results indicate that four water molecules are directly involved in a proton relay mechanism, which strongly reduces the activation energy with respect to the direct hydrogen transfer occurring in the isolated molecule. Further extension of the size of the cluster up to 192 water molecules in the framework of a three-layer QM/QM'/MM model has a negligible effect on the energy barrier ruling the isomerization. Computation of reaction rates by transition state theory indicates that on icy surfaces the isomerization of HNC to HCN could occur quite easily even at low temperatures thanks to the reduced activation energy that can be effectively overcome by tunneling.

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Vibrationally-excited Lines of HC3N Associated with the Molecular Disk around the G24.78+0.08 A1 Hyper-compact HII Region

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We have analyzed Atacama Large Millimeter/submillimeter Array Band 6 data of the hyper-compact HII region G24.78+0.08 A1 (G24 HC HII) and report the detection of vibrationally-excited lines of HC3N (v7=2, J=24−23). The spatial distribution and kinematics of a vibrationally-excited line of HC3N (v7=2, J=24−23, l=2e) are found to be similar to the CH3CN vibrationally-excited line (v8=1), which indicates that the HC3N emission is tracing the disk around the G24 HC HII region previously identified by the CH3CN lines. We derive the 13CH3CN/HC13CCN abundance ratios around G24 and compare them to the CH3CN/HC3N abundance ratios in disks around Herbig Ae and T Tauri stars. The 13CH3CN/HC13CCN ratios around G24 (~3.0−3.5) are higher than the CH3CN/HC3N ratios in the other disks (~0.03−0.11) by more than one order of magnitude. The higher CH3CN/HC3N ratios around G24 suggest that the thermal

desorption of CH3CN in the hot dense gas and efficient destruction of HC3N in the region irradiated by the strong UV radiation are occurring. Our results indicate that the vibrationally-excited HC3N lines can be used as a disk tracer of massive protostars at the HC HII region stage, and the combination of these nitrile species will provide information of not only chemistry but also physical conditions of the disk structures.

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Interstellar detection and chemical modeling of iso-propanol and its normal isomer

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The detection of a branched alkyl molecule in the high-mass star forming protocluster Sgr B2(N) permitted by the advent of ALMA revealed a new dimension of interstellar chemistry. Astrochemical simulations subsequently predicted that beyond a certain degree of molecular complexity, branched molecules could even dominate over their straight-chain isomers. More generally, we aim at probing further the presence in the ISM of complex organic molecules with the capacity to exhibit both a normal and iso form, via the attachment of a functional group to either a primary or secondary carbon atom. We used the imaging spectral line survey survey ReMoCA performed with ALMA and the results of a recent spectroscopic study of propanol to search for the iso and normal isomers of this molecule in the hot molecular core Sgr B2(N2). We expanded the network of the astrochemical model MAGICKAL to explore the formation routes of propanol. We report the first interstellar detection of iso-propanol toward a position of Sgr B2(N2) that shows narrow linewidths. We also report the first secure detection of normal-propanol in a hot core. i-Propanol is found to be nearly as abundant as n-propanol, with an abundance ratio of 0.6 similar to the ratio of 0.4 that we obtained previously for i- and n-propyl cyanide in Sgr B2(N2). The results are in good agreement with the outcomes of our astrochemical models, which indicate that OH-radical addition to propylene in dust-grain ice mantles, driven by water photodissociation, can produce appropriate quantities of n- and i-propanol. The n-to-i ratio in Sgr B2(N2) may be a direct inheritance of the branching ratio of this reaction process. The detection of n- and i-propanol and their ratio indicate that the modest preference toward the normal form of propyl cyanide determined previously may be a more general feature among similarly sized interstellar molecules. [abridged]

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Linking Characteristics of the Polycyclic Aromatic Hydrocarbon Population with Galaxy Properties: A Quantitative Approach Using the NASA Ames PAH IR Spectroscopic Database

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Utilizing the data and tools provided through the NASA Ames PAH IR Spectroscopic Database (PAHdb), we study the PAH component of over 900 Spitzer-IRS galaxy spectra. Employing a database-fitting approach, the average PAH size, the PAH size distribution, and PAH ionization fraction are deduced. In turn, we examine their connection with the properties of the host galaxy. We found that PAH population within galaxies consists of middle-sized PAHs with an average number of carbon atoms of Nc = 55, and a charge state distribution of ~ 40% ionized – 60% neutral. We describe a

correlation between the 6.2/11.2 μm PAH ratio with the ionization parameter (γ ≡ (G0 / ne)(Tgas / 1K)^0.5), a moderate correlation between the 8.6/11.2 μm PAH ratio and specific star-formation rate, and a weak anti-correlation between γ and M∗. From the PAHdb decomposition we provide estimates for the 3.3 μm PAH band, not covered by Spitzer observations, and establish a correlation between the 3.3/11.2 μm PAH ratio with Nc. We further deliver a library of mid-IR PAH template spectra parameterized on PAH size and ionization fraction, which can be used in galaxy spectral energy distribution fitting codes for the modeling of the mid-IR PAH emission component in galaxies.

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Acetone–Water Interactions in Crystalline and Amorphous Ice Environments

Michelle R. Brann, Stephen P. Hansknecht, Mark Muir, and S. J. Sibener

We present research that systematically examines acetone interacting with various D2O ices of terrestrial and astrophysical interest using time-resolved, in situ reflection absorption infrared spectroscopy (RAIRS). We examine acetone deposited on top of different D2O ice films: high-density, nonporous amorphous (np-ASW), and crystalline (CI) films as well as porous amorphous (p-ASW) with various pore morphologies. Analysis of RAIR spectra changes after acetone exposure, and we find that more hydrogen bonding occurs between acetone and p-ASW ices as compared to acetone and np-ASW or CI ices. Hydrogen bonding quantification occurred by two independent RAIR spectral changes: a greater relative intensity of the 1703 cm–1 feature at low acetone coverage as part of a 14 cm-1 shift in the C═O region and an ∼30% integrated dangling bond area reduction after acetone exposure. Interestingly, when changing the water structure to be more porous (deposited at 70° compared to 30°), there is a further reduction in the amount of hydrogen bonding that occurs. This suggests that there is a lack of access to surface sites with dangling bonds in the pores as initial layers of acetone block the pores and acetone is unable to diffuse within the structure at low temperatures. In general, these results offer a clearer picture of the mechanisms that can occur when small organic hydrocarbons interact with various icy interfaces; a quantitative understanding of these interactions is essential for the accurate modeling of many astrophysical processes occurring on the surface of icy dust particles.

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The young embedded disk L1527 IRS: constraints on the water snowline and cosmic ray ionization rate from HCO+ observations

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The water snowline in circumstellar disks is a crucial component in planet formation, but direct observational constraints on its location remain sparse due to the difficulty of observing water in both young embedded and mature protoplanetary disks. Chemical imaging provides an alternative route to locate the snowline, andHCO+ isotopologues have been shown to be good tracers in protostellar envelopes and Herbig disks. Here

we present ~0.5" resolution (~35 au radius) Atacama Large Millimeter/submillimeter Array (ALMA) observations of HCO+ J=4-3 and H13CO+ J=3-2 toward the young (Class 0/I) disk L1527 IRS. Using a source-specific physical model with the midplane snowline at 3.4 au and a small chemical network, we are able to reproduce the HCO+ and H13CO+ emission, but for HCO+ only when the cosmic ray ionization rate is lowered to 1e-18 s-1. Even though the observations are not sensitive to the expected HCO+ abundance drop across the snowline, the reduction in HCO+ above the snow surface and the global temperature structure allow us to constrain a snowline location between 1.8 and 4.1 au. Deep observations are required to eliminate the envelope contribution to the emission and to derive more stringent constraints on the snowline location. Locating the snowline in young disks directly with observations of H2O isotopologues may therefore still be an alternative option. With a direct snowline measurement, HCO+ will be able to provide constraints on the ionization rate.

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Lyα irradiation of solid-state formamide

T. Suhasaria and V. Mennella

Context. Formamide (NH2CHO) has been proposed as a potential prebiotic precursor in the scientific discourse on the origin of life. It has been observed in different environments in space, including protostellar regions and comets. The abundance and stability of NH2CHO in the early stages of star formation can be better understood by incorporating the formation and destruction data in astrochemical models. Aims. We carried out an experimental investigation to study the destruction of pure NH2CHO ice at 12 K as a result of the interaction with Lyα (121.6 nm) photons. Methods. We studied UV photo destruction of NH2CHO using Fourier-transform infrared spectroscopy. Results. After UV processing, the intensity of NH2CHO IR bands decreases and new bands corresponding to HCN, CO, NH4+, OCN−, HNCO, and CO2 appeared in the spectrum. We then derived the destruction and cumulative product formation cross-sections. Conclusions. A comparison of destruction rates derived from the cross-section in a cold and dense molecular cloud for different energetic processing agents reveals that UV photons induce NH2CHO destruction at a level that is one order of magnitude greater than that affected by cosmic rays; however, it is three orders of magnitude lower than that of H atoms.

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