

AstroChemical Newsletter #70

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Abstracts

The GUAPOS project II. A comprehensive study of peptide-like bond molecules

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Peptide-like bond molecules, which can take part to the formation of proteins in a primitive Earth environment, have been detected up to now only towards a few sources. We present a study of HNCO, HC(O)NH₂, CH₃NCO, CH₃C(O)NH₂, CH₃NHCHO, CH₃CH₂NCO, NH₂C(O)NH₂, NH₂C(O)CN, and HOCH₂C(O)NH₂ towards the hot core G31.41+0.31. We have used the spectrum obtained from the ALMA 3mm spectral survey GUAPOS, with an angular resolution of 1.2"×1.2" (about 4500 au), to derive column densities of all the molecular species, together with other 0.2"×0.2" (about 750 au) ALMA observations to study the morphology of HNCO, HC(O)NH₂ and CH₃C(O)NH₂. We have detected HNCO, HC(O)NH₂, CH₃NCO, CH₃C(O)NH₂, and CH₃NHCHO, for the first time all together outside the Galactic center. We have obtained molecular fractional abundances with respect to H₂ from 10⁻⁷ down to a few 10⁻⁹ and with respect to CH₃OH from 10⁻³ to about 4×10⁻². From the comparison with other sources, we find that regions in an earlier stage of evolution, such as pre-stellar cores, show abundances at least two orders of magnitude lower than those in hot cores, hot corinos or shocked regions. Moreover, molecular abundance ratios towards different sources are found to be consistent between them within about one order of magnitude, regardless of the physical properties (e.g. different masses and luminosities), or the source position throughout the Galaxy. New correlations between pairs of molecular abundances have also been found. These results suggest that all these species are formed on grain surfaces in early evolutionary stages of molecular clouds, and that they are subsequently released back to the gas-phase through thermal desorption or shock-triggered desorption.

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The impact of water vapor on the OH reactivity towards CH₃CHO at ultra-low temperatures (21.7-135.0 K): Experiments and Theory

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The role of water vapor (H₂O) and its hydrogen-bonded complexes in the gas-phase

reactivity of organic compounds with hydroxyl (OH) radicals has been the subject of many recent studies. Contradictory effects have been reported at temperatures between 200 and 400 K. For the OH + acetaldehyde reaction, a slight catalytic effect of H₂O was previously reported at temperatures between 60 and 118 K. In this work, we used Laval nozzle expansions to reinvestigate the impact of H₂O on the OH-reactivity with acetaldehyde between 21.7 and 135.0 K. The results of this comprehensive study demonstrate that water, instead, slows down the reaction by factors of ~3 (21.7 K) and ~2 (36.2–89.5 K), and almost no effect of added H₂O was observed at 135.0 K.

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Combined hydrodynamic and gas-grain chemical modeling of hot cores I. One-dimensional simulations

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Context. Gas-grain models have long been employed to simulate hot-core chemistry; however, these simulations have traditionally neglected to couple chemical evolution in tandem with a rigorous physical evolution of a source. This over-simplification particularly lacks an accurate treatment of temperature and spatial distribution, which are needed for realistic simulations of hot cores. Aims. We aim to combine radiation hydrodynamics (RHD) with hot-core chemical kinetics in one dimension to produce a set of astrochemical models that evolve according to explicitly calculated temperature, density, and spatial profiles. Methods. We solve radiation hydrodynamics for three mass-accretion-rate models using Athena++. We then simulate the chemistry using the hot-core chemical kinetic code MAGICKAL according to the physics derived from the RHD treatment. Results. We find that as the mass-accretion rate decreases, the overall gas density of the source decreases. In particular, the gas density for the lowest mass-accretion rate is low enough to restrict the proper formation of many complex organic molecules. We also compare our chemical results in the form of calculated column densities to those of observations toward Sgr B2(N2). We find a generally good agreement for oxygen-bearing species, particularly for the two highest mass-accretion rates. Conclusions. Although we introduce hot-core chemical modeling using a self-consistent physical treatment, the adoption of a twodimensional model may better reproduce chemistry and physics toward real sources and thus achieve better chemical comparisons with observations.

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The Beginning of HCN Polymerization: Iminoacetonitrile Formation and Its Implications in Astrochemical Environments

Hilda Sandström and Martin Rahm

Hydrogen cyanide (HCN) is known to react with complex organic materials and is a key reagent in the formation of various prebiotic building blocks, including amino acids and nucleobases. Here, we explore the possible first step in several such processes, the dimerization of HCN into iminoacetonitrile. Our study combines steered ab initio molecular dynamics and quantum chemistry to evaluate the kinetics and thermodynamics of base-catalyzed dimerization of HCN in the liquid state. Simulations predict a formation mechanism of iminoacetonitrile that is consistent with

experimentally observed time scales for HCN polymerization, suggesting that HCN dimerization may be the rate-determining step in the assembly of more complex reaction products. The predicted kinetics permits for iminoacetonitrile formation in a host of astrochemical environments, including on the early Earth, on periodically heated subsurfaces of comets, and following heating events on colder bodies, such as Saturn's moon Titan.

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HCN/HNC chemistry in shocks: a study of L1157-B1 with ASAI **B. Lefloch, G. Busquet, S. Viti, C. Vastel, E. Mendoza, M. Benedettini, C. Codella, L. Podio, A. Schutzer, P.R. Rivera-Ortiz, J.R.D. Lépine, R. Bachiller**

HCN and its isomer HNC play an important role in molecular cloud chemistry and the formation of more complex molecules. We investigate here the impact of protostellar shocks on the HCN and HNC abundances from high-sensitivity IRAM 30m observations of the prototypical shock region L1157-B1 and the envelope of the associated Class 0 protostar, as a proxy for the pre-shock gas. The isotopologues H₁₂CN, HN₁₂C, H₁₃CN, HN₁₃C, HC₁₅N, H₁₅NC, DCN and DNC were all detected towards both regions. Abundances and excitation conditions were obtained from radiative transfer analysis of molecular line emission under the assumption of Local Thermodynamical Equilibrium. In the pre-shock gas, the abundances of the HCN and HNC isotopologues are similar to those encountered in dark clouds, with a HCN/HNC abundance ratio ≈ 1 for all isotopologues. A strong D-enrichment ($D/H \approx 0.06$) is measured in the pre-shock gas. There is no evidence of ¹⁵N fractionation neither in the quiescent nor in the shocked gas. At the passage of the shock, the HCN and HNC abundances increase in the gas phase in different manners so that the HCN/HNC relative abundance ratio increases by a factor 20. The gas-grain chemical and shock model UCLCHEM allows us to reproduce the observed trends for a C-type shock with pre-shock density $n(H) = 10^5 \text{ cm}^{-3}$ and shock velocity $V_s = 40 \text{ km/s}$. We conclude that the HCN/HNC variations across the shock are mainly caused by the sputtering of the grain mantle material in relation with the history of the grain ices.

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The Ice Chamber for Astrophysics-Astrochemistry (ICA): A New Experimental Facility for Ion Impact Studies of Astrophysical Ice Analogs

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The Ice Chamber for Astrophysics-Astrochemistry (ICA) is a new laboratory end station located at the Institute for Nuclear Research (Atomki) in Debrecen, Hungary. The ICA has been specifically designed for the study of the physico-chemical properties of astrophysical ice analogs and their chemical evolution when subjected to ionizing radiation and thermal processing. The ICA is an ultra-high-vacuum compatible chamber containing a series of IR-transparent substrates mounted on a copper holder connected to a closed-cycle cryostat capable of being cooled down to 20 K, itself

mounted on a 360° rotation stage and a z-linear manipulator. Ices are deposited onto the substrates via background deposition of dosed gases. The ice structure and chemical composition are monitored by means of FTIR absorbance spectroscopy in transmission mode, although the use of reflectance mode is possible by using metallic substrates. Pre-prepared ices may be processed in a variety of ways. A 2 MV Tandatron accelerator is capable of delivering a wide variety of high-energy ions into the ICA, which simulates ice processing by cosmic rays, solar wind, or magnetospheric ions. The ICA is also equipped with an electron gun that may be used for electron impact radiolysis of ices. Thermal processing of both deposited and processed ices may be monitored by means of both FTIR spectroscopy and quadrupole mass spectrometry. In this paper, we provide a detailed description of the ICA setup as well as an overview of the preliminary results obtained and future plans.

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Dark cloud-type chemistry in PDRs with moderate UV field

Maria S. Kirsanova, Anna F. Punanova, Dmitry A. Semenov, Anton I. Vasyunin

We present a study of emission lines of small hydrocarbons C₂H and c-C₃H₂, and COMs precursors H₂CO and CH₃OH in order to better understand the possible chemical link between the molecular abundances and UV radiation field in photodissociation regions (PDRs). We study two PDRs around extended and compact HII regions with $G \leq 50$ Habings in the S235 star-forming complex. We find the highest abundances of both hydrocarbons on the edges of molecular clumps, while c-C₃H₂ is also abundant in the low-density expanding PDR around compact HII region S235A. We see the highest methanol column density towards the positions with the UV field $G \approx 20-30$ Habings and explain them by reactive desorption from the dust grains. The N(C₂H)/N(CH₃OH) ratio is lower by a factor of few or the order of magnitude in comparison with the Horsehead and Orion Bar PDRs. The ratio is similar to the value observed in hot corinos in the Perseus cloud. We conclude that ion-molecular and grain surface chemical routes rule the molecular abundances in the PDRs, and the PDRs inherit molecular abundances from the previous dark stage of molecular cloud evolution in spite of massive stars already emitting in optics.

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If you like C/O variations, you should have put a ring on it

Nienke van der Marel, Arthur Bosman, Sebastiaan Krijt, Gijs D. Mulders, Jennifer B. Bergner

The C/O-ratio as traced with C₂H emission in protoplanetary disks is fundamental for constraining the formation mechanisms of exoplanets and our understanding of volatile depletion in disks, but current C₂H observations show an apparent bimodal distribution which is not well understood, indicating that the C/O distribution is not described by a simple radial dependence. The transport of icy pebbles has been suggested to alter the local elemental abundances in protoplanetary disks, through settling, drift and trapping in pressure bumps resulting in a depletion of volatiles in the surface and an increase of the elemental C/O. We combine all disks with spatially resolved ALMA C₂H observations with high-resolution continuum images and constraints on the CO snowline to

determine if the C₂H emission is indeed related to the location of the icy pebbles. We report a possible correlation between the presence of a significant CO-icy dust reservoir and high C₂H emission, which is only found in disks with dust rings outside the CO snowline. In contrast, compact dust disks (without pressure bumps) and warm transition disks (with their dust ring inside the CO snowline) are not detected in C₂H, suggesting that such disks may never have contained a significant CO ice reservoir. This correlation provides evidence for the regulation of the C/O profile by the complex interplay of CO snowline and pressure bump locations in the disk. These results demonstrate the importance of including dust transport in chemical disk models, for a proper interpretation of exoplanet atmospheric compositions, and a better understanding of volatile depletion in disks, in particular the use of CO isotopologues to determine gas surface densities.

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Magnesium radicals MgC₅N and MgC₆H in IRC+10216

J. R. Pardo, C. Cabezas, J. P. Fonfría, M. Agúndez, B. Tercero, P. de Vicente, M. Guélin, J. Cernicharo

After the previous discovery of MgC₃N and MgC₄H in IRC+10216, a deeper Q-band (31.0-50.3 GHz) integration on this source had revealed two additional series of harmonically related doublets that we assigned on the basis of quantum mechanical calculations to the larger radicals MgC₅N and MgC₆H. The results presented here extend and confirm previous results on magnesium-bearing molecules in IRC+10216. We derived column densities of $(4.7 \pm 1.3) \times 10^{12}$ for MgC₅N and $(2.0 \pm 0.9) \times 10^{13}$ for MgC₆H, which imply that MgC₅N/MgC₃N=0.5 and MgC₆H/MgC₄H = 0.9. Therefore, MgC₅N and MgC₆H are present with column densities not so different from those of the immediately shorter analogs. The synthesis of these large magnesium cyanides and acetylides in IRC+10216 can be explained for their shorter counterparts by a two-step process initiated by the radiative association of Mg⁺ with large cyanopolynes and polyynes, which are still quite abundant in this source, followed by the dissociative recombination of the ionic complexes.

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Detection of deuterated methylcyanoacetylene, CH₂DC₃N, in TMC-1

C. Cabezas, E. Roueff, B. Tercero, M. Agúndez, N. Marcelino, P. de Vicente, J. Cernicharo

We report the first detection in space of the single deuterated isotopologue of methylcyanoacetylene, CH₂DC₃N. A total of fifteen rotational transitions, with J = 8-12 and K_a = 0 and 1, were identified for this species in TMC-1 in the 31.0-50.4 GHz range using the Yebes 40m radio telescope. The observed frequencies were used to derive for the first time the spectroscopic parameters of this deuterated isotopologue. We derive a column density of $(8.0 \pm 0.4) \times 10^{10}$ cm⁻². The abundance ratio between CH₃C₃N and CH₂DC₃N is ~22. We also theoretically computed the principal spectroscopic constants of ¹³C isotopologues of CH₃C₃N and CH₃C₄H and those of the deuterated isotopologues of CH₃C₄H for which we could expect a similar degree of deuteration enhancement. However, we have not detected either CH₂DC₄H nor

CH₃C₄D nor any ¹³C isotopologue. The different observed deuterium ratios in TMC-1 are reasonably accounted for by a gas phase chemical model where the low temperature conditions favor deuterium transfer through reactions with H₂D⁺.

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Interstellar detection of the simplest aminocarbyne, H₂NC: an ignored but abundant molecule

C. Cabezas, M. Agundez, N. Marcelino, B. Tercero, S. Cuadrado, J. Cernicharo

We report the first identification in space of H₂NC, a high-energy isomer of H₂CN that has been largely ignored in chemical and astrochemical studies. The observation of various unidentified lines around 72.2 GHz in the cold dark cloud L483 motivated the search for, and successful detection of, additional groups of lines in harmonic relation. After an exhaustive high-level ab initio screening of possible carriers, we confidently assign the unidentified lines to H₂NC based on the good agreement between astronomical and theoretical spectroscopic parameters and sound spectroscopic and astrochemical arguments. The observed frequencies are used to precisely characterize the rotational spectrum of H₂NC. This species is also detected in the cold dark cloud B1-b and the z=0.89 galaxy in front of the quasar PKS1830-211. We derive H₂NC/H₂CN abundance ratios of 1 in L483 and B1-b and 0.27 toward PKS1830-211. Neither H₂NC nor H₂CN are detected in the dark cloud TMC-1, which seriously questions a previous identification of H₂CN in this source. We suggest that the H₂NC/H₂CN ratio behaves as the HNC/HCN ratio, with values close to one in cold dense clouds and below one in diffuse clouds. The reactions N + CH₃ and C + NH₃ emerge as strong candidates to produce H₂NC in interstellar clouds. Further studies on these two reactions are needed to evaluate the yield of H₂NC. Due to the small number of atoms involved, it should be feasible to constrain the chemistry behind H₂NC and H₂CN, just as it has been done for HNC and HCN, as this could allow to use the H₂NC/H₂CN ratio as a probe of chemical or physical conditions of the host clouds.

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Discovery of benzyne, o-C₆H₄, in TMC-1 with the QUIJOTE line survey

J. Cernicharo, M. Agundez, R. I. Kaiser, C. Cabezas, B. Tercero, N. Marcelino, J. R. Pardo, P. de Vicente

We report the detection, for the first time in space, of a new non-functionalised hydrocarbon cycle in the direction of TMC-1: o-C₆H₄ (ortho-benzyne). We derive a column density for this hydrocarbon cycle of (5 ± 1)e¹¹ cm⁻². The abundance of this species is around 30 times lower than that of cyclopentadiene and indene. We compare the abundance of benzyne with that of other pure hydrocarbons, cycles or chains, and find that it could be formed from neutral-radical reactions such as C₂H + CH₂CHCCH and C + C₅H₅, and possibly through C₄H + C₂H₄, C₃H + CH₂CCH₂, and C₃H₂ + C₃H₃. Hence, the rich content of hydrocarbon cycles observed in TMC-1 could arise through a bottom-up scenario involving reactions of a few radicals with the abundant hydrocarbons recently revealed by the QUIJOTE line survey.

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Modeling accretion shocks at the disk-envelope interface - Sulfur chemistry

M. L. van Gelder, B. Tabone, E. F. van Dishoeck, B. Godard

As material from an infalling protostellar envelope hits the forming disk, an accretion shock may develop which could (partially) alter the envelope material entering the disk. Observations with the Atacama Large Millimeter/submillimeter Array (ALMA) indicate that emission originating from warm SO and SO₂ might be good tracers of such accretion shocks. The goal of this work is to test under what shock conditions the abundances of gas-phase SO and SO₂ increase in an accretion shock at the disk-envelope interface. Detailed shock models including gas dynamics are computed using the Paris-Durham shock code for non-magnetized J-type accretion shocks in typical inner envelope conditions. The effect of pre-shock density, shock velocity, and strength of the ultraviolet (UV) radiation field on the abundance of warm SO and SO₂ is explored. Warm gas-phase chemistry is efficient in forming SO under most J-type shock conditions considered. In lower-velocity (~3 km/s) shocks, the abundance of SO is increased through subsequent reactions starting from thermally desorbed CH₄ toward H₂CO and finally SO. In higher velocity (>4 km/s) shocks, both SO and SO₂ are formed through reactions of OH and atomic S. The strength of the UV radiation field is crucial for SO and in particular SO₂ formation through the photodissociation of H₂O. Thermal desorption of SO and SO₂ ice is only relevant in high-velocity (>5 km/s) shocks at high densities (>10⁷ cm⁻³). Warm emission from SO and SO₂ is a possible tracer of accretion shocks at the disk-envelope interface as long as a local UV field is present. Additional observations with ALMA at high-angular resolution could provide further constraints. Moreover, the James Webb Space Telescope will give access to other possible slow, dense shock tracers such as H₂, H₂O, and [S I] 25 μm.

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