AstroChemical Newsletter #70

September 2021

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Abstracts

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

L. Colzi, V. M. Rivilla, M. T. Beltrán, I. Jiménez-Serra, C. Mininni, M. Melosso, R. Cesaroni, F. Fontani, A. Lorenzani, A. Sánchez-Monge, S. Viti, P. Schilke, L. Testi, E. R. Alonso, L. Kolesniková

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.

Accepted for publication in A&A
DOI: 10.1051/0004-6361/202141573
Full-text URL: https://arxiv.org/abs/2107.11258

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

E. M. Neeman, D. González, S. Blázquez, B. Ballesteros, A. Canosa, L. Vereecken, M. Antiñolo, J. Albaladejo, E. Jiménez

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.

Journal of Chemical Physics 155 (3) 034306 (2021)
DOI: 10.1063/5.0054859
Full-text URL: https://aip.scitation.org/doi/full/10.1063/5.0054859

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

Barger, C. J., Lam, K. H., Li, Z.-Y., Davis, S. W., Herbst, E. & Garrod, R. T.

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.

Astronomy & Astrophysics, 2021, 651, A43
DOI: 10.1051/0004-6361/202039226
Full-text URL: https://ui.adsabs.harvard.edu/abs/2021A%26A...651A..43B/abstract

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.

Accepted in ACS Earth Space Chem.
DOI: 10.1021/acsearthspacechem.1c00195
Full-text URL: https://pubs.acs.org/doi/10.1021/acsearthspacechem.1c00195

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≈ 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 cm−3 and shock velocity Vs= 40 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.

Published in MNRAS
DOI: 10.1093/mnras/stab2134
Full-text URL: https://arxiv.org/abs/2107.10596

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

P. Herczku, D.V. Mifsud, S. Ioppolo, Z. Juhász, Z. Kanuchová, A. Traspas Muina, P.A. Hailey, I. Rajta, I. Vajda, N.J. Mason, R.W. McCullough, B. Paripás, B. Sulik

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 Tandetron 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.

Published in Rev. Sci. Instrum. (2021), 92, 084501
DOI: 10.1063/5.0050930
Full-text URL: https://aip.scitation.org/doi/10.1063/5.0050930

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<=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≈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.

accepted in MNRAS
DOI: 10.1093/mnras/stab2361
Full-text URL: https://arxiv.org/abs/2108.05387

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.

Accepted by A&A Letters
Full-text URL: https://arxiv.org/abs/2108.07679

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±1.3)×1012 for MgC5N and (2.0±0.9)×1013 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 cyanopolyynes and polyynes, which are still quite abundant in this source, followed by the dissociative recombination of the ionic complexes.

A&A Letters, accepted
DOI: 10.1051/0004-6361/202141671
Full-text URL: https://arxiv.org/abs/2108.01480

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 Ka = 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±0.4)×1010 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 deuteron transfer through reactions with H2D+.

Astronomy & Astrophysics, Volume 650, L15
DOI: [10.1051/0004-6361/202141371](https://doi.org/10.1051/0004-6361/202141371)
Full-text URL: https://arxiv.org/abs/2106.03404

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.

A&A, accepted.
DOI: [10.1051/0004-6361/202141491](https://doi.org/10.1051/0004-6361/202141491)
Full-text URL: https://arxiv.org/abs/2107.08389

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.

A&A, Volume 652, L9
DOI: [10.1051/0004-6361/202141660](https://doi.org/10.1051/0004-6361/202141660)
Full-text URL: https://arxiv.org/abs/2108.02308

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 (>10^7 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.

A&A, Forthcoming article
DOI: 10.1051/0004-6361/202141591
Full-text URL: https://arxiv.org/abs/2107.09750