

# AstroChemical Newsletter #56

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## Abstracts

### **DC3N observations towards high-mass star-forming regions**

**V. M. Rivilla, L. Colzi, F. Fontani, M. Melosso, P. Caselli, L. Bizzocchi, F. Tamassia, L. Dore**

We present the study of deuteration of cyanoacetylene (HC3N) towards a sample of 28 high-mass star-forming cores divided into different evolutionary stages, from starless to evolved protostellar cores. We report for the first time the detection of DC3N towards 15 high-mass cores. The abundance ratios of DC3N with respect HC3N range in the interval 0.003–0.022, lower than those found in low-mass protostars and dark clouds. No significant trend with the evolutionary stage, or with the kinetic temperature of the region, has been found. We compare the level of deuteration of HC3N with those of other molecules towards the same sample, finding weak correlation with species formed only or predominantly in gas-phase (N<sub>2</sub>H<sup>+</sup> and HNC, respectively), and no correlation with species formed only or predominantly on dust grains (CH<sub>3</sub>OH and NH<sub>3</sub>, respectively). We also present a single-dish map of DC3N towards the protocluster IRAS 05358+3543, which shows that DC3N traces an extended envelope (~0.37 pc) and peaks towards two cold condensations separated from the positions of the protostars and the dust continuum. The observations presented in this work suggest that deuteration of HC3N is produced in the gas of the cold outer parts of massive star-forming clumps, giving us an estimate of the deuteration factor prior to the formation of denser gas.

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### **Determination of accurate rest frequencies and hyperfine structure parameters of cyanobutadiyne, HC5N**

**Thomas F. Giesen, Michael E. Harding, Jürgen Gauss, Jens-Uwe Grabow, Holger S. P. Müller**

Very accurate transition frequencies of HC5N were determined between 5.3 and 21.4 GHz with a Fourier transform microwave spectrometer. The molecules were generated by passing a mixture of HC3N and C<sub>2</sub>H<sub>2</sub> highly diluted in neon through a discharge valve followed by supersonic expansion into the Fabry-Perot cavity of the spectrometer. The accuracies of the data permitted us to improve the experimental <sup>14</sup>N nuclear quadrupole coupling parameter considerably and the first experimental determination of the <sup>14</sup>N nuclear spin-rotation parameter. The transition frequencies are also well suited to determine in astronomical observations the local speed of rest

velocities in molecular clouds with high fidelity. The same setup was used to study HC7N, albeit with modest improvement of the experimental  $^{14}\text{N}$  nuclear quadrupole coupling parameter. Quantum chemical calculations were carried out to determine  $^{14}\text{N}$  nuclear quadrupole and spin-rotation coupling parameters of HC5N, HC7N, and related molecules. These calculations included evaluation of vibrational and relativistic corrections to the non-relativistic equilibrium quadrupole coupling parameters; their considerations improved the agreement between calculated and experimental values substantially.

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## The chemistry of cosmic dust analogues from from C, C<sub>2</sub>, and C<sub>2</sub>H<sub>2</sub> in C-rich Circumstellar Envelopes

**Gonzalo Santoro , Lidia Martínez, Koen Lauwaet, Mario Accolla , Guillermo Tajuelo-Castilla, Pablo Merino, Jesús M. Sobrado, Ramón J. Peláez, Víctor J. Herrero, Isabel Tanarro, Álvaro Mayoral, Marcelino Agúndez , Hassan Sabbah, Christine Joblin , José Cernicharo , and José Ángel Martín-Gago**

Interstellar carbonaceous dust is mainly formed in the innermost regions of circumstellar envelopes around carbon-rich asymptotic giant branch stars (AGBs). In these highly chemically stratified regions, atomic and diatomic carbon, along with acetylene, are the most abundant species after H<sub>2</sub> and CO. In a previous study, we addressed the chemistry of carbon (C and C<sub>2</sub>) with H<sub>2</sub> showing that acetylene and aliphatic species form efficiently in the dust formation region of carbon-rich AGBs whereas aromatics do not. Still, acetylene is known to be a key ingredient in the formation of linear polyacetylenic chains, benzene, and polycyclic aromatic hydrocarbons (PAHs), as shown by previous experiments. However, these experiments have not considered the chemistry of carbon (C and C<sub>2</sub>) with C<sub>2</sub>H<sub>2</sub>. In this work, by employing a sufficient amount of acetylene, we investigate its gas-phase interaction with atomic and diatomic carbon. We show that the chemistry involved produces linear polyacetylenic chains, benzene, and other PAHs, which are observed with high abundances in the early evolutionary phase of planetary nebulae. More importantly, we have found a nonnegligible amount of pure and hydrogenated carbon clusters as well as aromatics with aliphatic substitutions, both being a direct consequence of the addition of atomic carbon. The incorporation of alkyl substituents into aromatics can be rationalized by a mechanism involving hydrogen abstraction followed by methyl addition. All the species detected in the gas phase are incorporated into nanometric-sized dust analogs, which consist of a complex mixture of sp, sp<sup>2</sup>, and sp<sup>3</sup> hydrocarbons with amorphous morphology.

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## Chemical composition in the IRAS 16562-3959 high-mass star-forming region

**Kotomi Taniguchi, Andres E. Guzman, Liton Majumdar, Masao Saito, Kazuki Tokuda**

We have analyzed the Atacama Large Millimeter/submillimeter Array (ALMA) cycle 2 data of band 6 toward the G345.4938+01.4677 massive young protostellar object

(G345.5+1.47 MYSO) in the IRAS 16562–3959 high-mass star-forming region with an angular resolution of  $\sim 0.3$  arcsec, corresponding to  $\sim 760$  au. We spatially resolve the central region which consists of three prominent molecular emission cores. A hypercompact (HC) H II region (Core A) and two molecule-rich cores (Core B and Core C) are identified using the moment zero images of the H30 $\alpha$  line and a CH<sub>3</sub>OH line, respectively. Various oxygen-bearing complex organic molecules (COMs), such as (CH<sub>3</sub>)<sub>2</sub>CO and CH<sub>3</sub>OCHO, have been detected toward the positions of Core B and Core C, while nitrogen-bearing species, CH<sub>3</sub>CN, HC<sub>3</sub>N and its <sup>13</sup>C isotopologues, have been detected toward all of the cores. We discuss the formation mechanisms of H<sub>2</sub>CO by comparing the spatial distribution of C<sup>18</sup>O with that of H<sub>2</sub>CO. The <sup>33</sup>SO emission, on the other hand, shows a ring-like structure surrounding Core A, and it peaks on the outer edge of the H30 $\alpha$  emission region. These results imply that SO is enhanced in a shock produced by the expanding motion of the ionized region.

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## Carbon isotopic fractionation in molecular clouds

**L. Colzi, O. Sipilä, E. Roueff, P. Caselli, F. Fontani**

C-fractionation has been studied from a theoretical point of view with different models of time-dependent chemistry, including both isotope-selective photodissociation and low-temperature isotopic exchange reactions. Recent chemical models predict that the latter may lead to a depletion of <sup>13</sup>C in nitrile-bearing species, with <sup>12</sup>C/<sup>13</sup>C ratios two times higher than the elemental abundance ratio of 68 in the local interstellar medium. Since the carbon isotopic ratio is commonly used to evaluate the <sup>14</sup>N/<sup>15</sup>N ratios with the double-isotope method, it is important to study carbon fractionation in detail to avoid incorrect assumptions. In this work we implemented a gas-grain chemical model with new isotopic exchange reactions and investigated their introduction in the context of dense and cold molecular gas. In particular, we investigated the <sup>12</sup>C/<sup>13</sup>C ratios of HNC, HCN, and CN using a grid of models, with temperatures and densities ranging from 10 to 50 K and 2e<sup>3</sup> to 2e<sup>7</sup> cm<sup>-3</sup>, respectively. We suggest a possible <sup>13</sup>C exchange through the <sup>13</sup>C + C<sub>3</sub>  $\rightarrow$  <sup>12</sup>C + <sup>13</sup>CC<sub>2</sub> reaction, which does not result in dilution, but rather in <sup>13</sup>C enhancement, for molecules that are formed starting from atomic carbon. This effect is efficient in a range of time between the formation of CO and its freeze-out on grains. Furthermore, the parameter-space exploration shows, on average, that the <sup>12</sup>C/<sup>13</sup>C ratios of nitriles are predicted to be a factor 0.8–1.9 different from the local <sup>12</sup>C/<sup>13</sup>C of 68 for high-mass star-forming regions. This result also affects the <sup>14</sup>N/<sup>15</sup>N ratio: a value of 330 obtained with the double-isotope method is predicted to vary in the range 260–630, up to 1150, depending on the physical conditions. Finally, we studied the <sup>12</sup>C/<sup>13</sup>C ratios of nitriles by varying the cosmic-ray ionization rate: the <sup>12</sup>C/<sup>13</sup>C ratios increase with it because of secondary photons and cosmic-ray reactions.

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## Hot Corinos Chemical Diversity: Myth or Reality?

**Marta De Simone, Cecilia Ceccarelli, Claudio Codella, Brian E. Svoboda, Claire Chandler, Mathilde Bouvier, Satoshi Yamamoto, Nami Sakai, Paola Caselli, Cecile Favre, Laurent Loinard, Bertrand Lefloch, Hanyu Baobab Liu, Ana López-Sepulcre, Jaime E. Pineda, Vianney Taquet, Leonardo Testi**

After almost 20 years of hunting, only about a dozen hot corinos, hot regions enriched in interstellar complex organic molecules (iCOMs), are known. Of them, many are binary systems with the two components showing drastically different molecular spectra. Two obvious questions arise. Why are hot corinos so difficult to find and why do their binary components seem chemically different? The answer to both questions could be a high dust opacity that would hide the molecular lines. To test this hypothesis, we observed methanol lines at centimeter wavelengths, where dust opacity is negligible, using the Very Large Array interferometer. We targeted the NGC 1333 IRAS 4A binary system, for which one of the two components, 4A1, has a spectrum deprived of iCOMs lines when observed at millimeter wavelengths, while the other component, 4A2, is very rich in iCOMs. We found that centimeter methanol lines are similarly bright toward 4A1 and 4A2. Their non-LTE analysis indicates gas density and temperature ( $\geq 10^6 \text{ cm}^{-3}$  and 100-190 K), methanol column density ( $\sim 10^{19} \text{ cm}^{-2}$ ) and extent ( $\sim 35 \text{ au}$  in radius) similar in 4A1 and 4A2, proving that both are hot corinos. Furthermore, the comparison with previous methanol line millimeter observations allows us to estimate the optical depth of the dust in front of 4A1 and 4A2, respectively. The obtained values explain the absence of iCOMs line emission toward 4A1 at millimeter wavelengths and indicate that the abundances toward 4A2 are underestimated by  $\sim 30\%$ . Therefore, centimeter observations are crucial for the correct study of hot corinos, their census, and their molecular abundances.

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## Tracking the Evolutionary Stage of Protostars through the Abundances of Astrophysical Ices

**W. R. M. Rocha and S. Pilling**

The physical evolution of young stellar objects (YSOs) is accompanied by an enrichment of the molecular complexity, mainly triggered by the heating and energetic processing of astrophysical ices. In this paper, a study of how the ice column density varies across the protostellar evolution has been performed. Tabulated data of H<sub>2</sub>O, CO<sub>2</sub>, CH<sub>3</sub>OH, and HCOOH observed by ground- and space-based telescopes toward 27 early-stage YSOs were taken from the literature. The observational data show that ice column density and spectral index ( $\alpha$ ), used to classify the evolutionary stage, are well correlated. A 2D continuum radiative transfer simulation containing bare and ice-covered grains at different levels of cosmic-ray processing were used to calculate the spectral energy distributions in different angle inclinations between face-on and edge-on configurations. The H<sub>2</sub>O:CO<sub>2</sub> ice mixture was used to address the H<sub>2</sub>O and CO<sub>2</sub> column density variation, whereas CH<sub>3</sub>OH and HCOOH are by-products of the virgin ice after energetic processing. The simulated spectra were used to calculate the ice column densities of YSOs in an evolutionary sequence. As a result, the models show that the ice column density variation of HCOOH with  $\alpha$  can be justified by envelope dissipation and energetic processing of ice. On the other hand, the ice column densities are mostly overestimated in the cases of H<sub>2</sub>O, CO<sub>2</sub> and CH<sub>3</sub>OH, even though the physical and cosmic-ray processing effects are taken into account.

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## Astrochemistry During the Formation of Stars

Jes K. Jorgensen, Arnaud Belloche, Robin T. Garrod

Star-forming regions show a rich and varied chemistry, including the presence of complex organic molecules -- both in the cold gas distributed on large scales, and in the hot regions close to young stars where protoplanetary disks arise. Recent advances in observational techniques have opened new possibilities for studying this chemistry. In particular, the Atacama Large Millimeter/submillimeter Array (ALMA) has made it possible to study astrochemistry down to Solar System size scales, while also revealing molecules of increasing variety and complexity. In this review, we discuss recent observations of the chemistry of star-forming environments, with a particular focus on complex organic molecules, taking context from the laboratory experiments and chemical models that they have stimulated. The key takeaway points are: The physical evolution of individual sources plays a crucial role in their inferred chemical signatures, and remains an important area for observations and models to elucidate. Comparisons of the abundances measured toward different star-forming environments (high-mass versus low-mass, Galactic center versus Galactic disk) reveal a remarkable similarity, an indication that the underlying chemistry is relatively independent of variations in their physical conditions. Studies of molecular isotopologs in star-forming regions provide a link with measurements in our own Solar System, and thus may shed light on the chemical similarities and differences expected in other planetary systems.

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## Seeds of Life in Space (SOLIS). X. Interstellar Complex Organic Molecules in the NGC 1333 IRAS 4A outflows

**M. De Simone, C. Codella, C. Ceccarelli, A. López-Sepulcre, A. Witzel, R. Neri, N. Balucani, P. Caselli, C. Favre, F. Fontani, B. Lefloch, J. Ospina-Zamudio, J. E. Pineda, V. Taquet**

**Aims:** A unique environment to study how interstellar Complex Organic Molecules (iCOMs) can be formed is the shocked gas along low-mass protostellar outflows, as the dust mantles composition is sputtered into the gas phase. The chemical richness in these environments has been so far studied only in the L1157 blue shifted outflow.

**Methods:** To understand if the L1157-B1 case is unique, we imaged the NGC 1333 IRAS 4A outflows using the NOEMA (NOthern Extended Millimeter Array) interferometer as part of the IRAM SOLIS (Seeds Of Life in Space) Large Program and compared the observations with the GRAINOBLE+ gas phase astrochemical model. **Results:** Several iCOMs were detected in the IRAS 4A outflows: methanol (CH<sub>3</sub>OH), acetaldehyde (CH<sub>3</sub>CHO), formamide (NH<sub>2</sub>CHO) and dimethyl ether (CH<sub>3</sub>OCH<sub>3</sub>), all sampling upper excitation energy up to ~30 K. We found a significant chemical differentiation between the IRAS 4A1 outflow, showing a richer molecular content, and the IRAS 4A2 one. The CH<sub>3</sub>OH/CH<sub>3</sub>CHO abundance ratio is lower by a factor ~4 in the former; furthermore the ratio in both outflows is lower by a factor ~10 with respect to hot corinos values.

**Conclusions:** After L1157-B1, IRAS 4A outflow is now the second outflow to show an evident chemical complexity. Given that CH<sub>3</sub>OH is a grain surface species, GRAINOBLE+ reproduced our observations assuming acetaldehyde formation in gas phase by the reaction of ethyl radical (CH<sub>3</sub>CH<sub>2</sub>) with atomic oxygen. Moreover, the chemical differentiation between the two outflows suggests that the IRAS 4A1 outflow is likely younger than the IRAS 4A2 one. Further investigation is needed to constrain the age of the outflow and observations of even younger shocks are necessary and future spectroscopic studies on CH<sub>3</sub>CH<sub>2</sub> are needed to be able to observe this species and



provide strong constraints on the CH<sub>3</sub>CHO formation.

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## A Survey of High Mass Star Forming Regions in the Lines of Deuterated Molecules

**E. A. Trofimova, I. I. Zinchenko, P. M. Zemlyanukha, M. Thomasson**

A survey of massive star forming regions in the lines of the lowest transitions of deuterated molecules DCN, DNC, DCO<sup>+</sup>, N<sub>2</sub>D<sup>+</sup> in the 4 mm wavelength range was performed using the 20 m radio telescope of the Onsala Space Observatory. A total of about 60 sources was observed. Lines of the DCN, DNC, and DCO<sup>+</sup> molecules are registered in about a third of them, lines of the N<sub>2</sub>D<sup>+</sup> molecule only in two. Estimates of the relative abundances of the molecules and deuteration degree are derived. The dependencies of these parameters and also ratios of the abundances of different deuterated molecules on temperature and velocity dispersion are analyzed. We found that the relative abundances of DCN and DNC and the DCN/HCN ratio are approximately constant in the temperature range from ~15 K to ~55 K, while relative abundance of DCO<sup>+</sup> decreases with increasing temperature. Average ratio DCN/HCN is ~10<sup>-2</sup> for detected sources. A correlation was found between the ratios of abundances of some molecules and velocity dispersion. At the same time there are correlation between line width and temperature.

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## Formation of Complex Organic Molecules in Cold Interstellar Environments through non-diffusive grain-surface and ice-mantle chemistry

**Mihwa Jin, Robin T. Garrod**

A prevailing theory for the interstellar production of complex organic molecules (COMs) involves formation on warm dust-grain surfaces, via the diffusion and reaction of radicals produced through grain-surface photodissociation of stable molecules. However, some gas-phase O-bearing COMs, notably acetaldehyde (CH<sub>3</sub>CHO), methyl formate (CH<sub>3</sub>OCHO), and dimethyl ether (CH<sub>3</sub>OCH<sub>3</sub>), are now observed at very low temperatures, challenging the warm scenario. Here, we introduce a selection of new non-diffusive mechanisms into an astrochemical model, to account for the failure of the standard diffusive picture and to provide a more generalized scenario of COM formation on interstellar grains. New generic rate formulations are provided for cases where: (i) radicals are formed by reactions occurring close to another reactant, producing an immediate follow-on reaction; (ii) radicals are formed in an excited state, allowing them to overcome activation barriers to react with nearby stable molecules; (iii) radicals are formed through photo-dissociation close to a reaction partner, followed by immediate reaction. Each process occurs without the diffusion of large radicals. The new mechanisms significantly enhance cold COM abundances, successfully reproducing key observational results for prestellar core L1544. H-abstraction from grain-surface COMs, followed by recombination, plays a crucial role in amplifying chemical desorption into the gas phase. The UV-induced chemistry produces significant COM abundances in the bulk ices, which are retained on the grains and may persist to

later stages. O<sub>2</sub> is also formed strongly in the mantle through photolysis, suggesting cometary O<sub>2</sub> could indeed be interstellar.

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## Chemical Variation among Protostellar Cores: Dependence on Prestellar Core Conditions

Yuri Aikawa, Kenji Furuya, Satoshi Yamamoto, Nami Sakai

Hot corino chemistry and warm carbon chain chemistry (WCCC) are driven by gas-grain interactions in star-forming cores: radical-radical recombination reactions to form complex organic molecules (COMs) in the ice mantle, sublimation of CH<sub>4</sub> and COMs, and their subsequent gas-phase reactions. These chemical features are expected to depend on the composition of ice mantle which is set in the prestellar phase. We calculated the gas-grain chemical reaction network considering a layered ice-mantle structure in star-forming cores, to investigate how the hot corino chemistry and WCCC depend on the physical condition of the static phase before the onset of gravitational collapse. We found that WCCC becomes more active, if the temperature is lower, or the visual extinction is lower in the static phase, or the static phase is longer. Dependence of hot corino chemistry on the static-phase condition is more complex. While CH<sub>3</sub>OH is less abundant in the models with warmer static phase, some COMs are formed efficiently in those warm models, since there are various formation paths of COMs. If the visual extinction is lower, photolysis makes COMs less abundant in the static phase. Once the collapse starts and visual extinction increases, however, COMs can be formed efficiently. Duration of the static phase does not largely affect COM abundances. Chemical diversity between prototypical hot corinos and hybrid sources, in which both COMs and carbon chains are reasonably abundant, can be explained by the variation of prestellar conditions. Deficiency of gaseous COMs in prototypical WCCC sources is, however, hard to reproduce within our models.

accepted to ApJ

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## Announcements

### AGU session - Down the icy road: the journey of ices from interstellar clouds to planetary systems

We are accepting papers for the AGU session "Down the icy road: The journey of ices from interstellar clouds to planetary systems."

<https://agu.confex.com/agu/fm20/webprogrampreliminary/Session102214.html>

The AGU Fall Meeting 2020 will take place on December 7-11 2020 and will very likely be held online (TBC). The deadline for abstract submissions is Wednesday, 29 July, at 23:59 EDT. <https://www.agu.org/Fall-Meeting/2020/Present/Abstracts>

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