

# AstroChemical Newsletter #101

April 2024

You can access the full abstracts by clicking the paper titles. Submit your abstracts before the 25th of each month for inclusion in the following newsletter.

## Abstracts

### **ALMA-IMF XI: The sample of hot core candidates. A rich population of young high-mass proto-stars unveiled by the emission of methyl formate**

**M. Bonfand, T. Csengeri, S. Bontemps, N. Brouillet, F. Motte, F. Louvet, A. Ginsburg, N. Cunningham, R. Galván-Madrid, F. Herpin, F. Wyrowski, M. Vaille-Manet, A. M. Stutz, J. Di Francesco, A. Gusdorf, M. Fernández-López, B. Lefloch, H-L. Liu, P. Sanhueza, R. H. Álvarez-Gutiérrez, F. Olguin, T. Nony, A. Lopez-Sepulcre, P. Dell'Ova, Y. Pouteau, D. Jeff, H.-R. V. Chen, M. Armante, A. Towner, L. Bronfman, N. Kessler**

Sites associated with high-mass star and cluster formation exhibit a so-called hot core phase, characterized by high temperatures and column densities of complex organic molecules. We built a comprehensive census of hot core candidates towards the ALMA-IMF protoclusters based on the detection of two CH<sub>3</sub>OCHO emission lines at 216.1 GHz. We used the source extraction algorithm GExt2D to identify peaks of methyl formate (CH<sub>3</sub>OCHO) emission that is a complex species commonly observed towards sites of star formation. We built up a catalog of 76 hot core candidates with masses ranging from about 0.2 to 80 M<sub>sun</sub>, of which 56 are new detections. A large majority of these objects are compact, rather circular, with deconvolved FWHM sizes of about 2300 au on average. About 30% of our sample of methyl formate sources have core masses above 8 M<sub>sun</sub> within sizes ranging from about 1000 au to 13400 au, which well correspond to archetypical hot cores. The origin of the CH<sub>3</sub>OCHO emission toward the lower-mass cores can be explained by a mixture of contribution from shocks, or may correspond to objects in a more evolved state, i.e. beyond the hot core stage. We find that the fraction of hot core candidates increases with the core mass. The large fraction of hot core candidates towards the most massive cores suggests that they rapidly enter the hot core phase and feedback effects from the forming protostar(s) impact their environment on short time-scales.

Accepted for publication in A&A

Full-text URL: <https://arxiv.org/abs/2402.15023>

### **Unexpected and delayed fragmentation dynamics of the organometallic ferrocene induced by ion-collision**

**F. Aguilar-Galindo, V. T. T. Nguyen, R. Singh, A. Domaracka, B. A. Huber, S. Díaz-Tendero, P. Rousseau and S. Maclot**

We have investigated the fragmentation dynamics of the organometallic ferrocene molecule after interaction with multiply charged ions using multicoincidence mass spectrometry and quantum chemistry calculations. We observed unexpected fragmentation dynamics of the two-body breakup channels from ferrocene dications revealing a charge screening effect from the iron atom and delayed fragmentation

dynamics. These observations are rationalized through the population of a specific long-lived excited state, where one positive charge is located on each cyclopentadienyl ring.

Phys. Chem. Chem. Phys., 2024, 26, 7638-7646

DOI: [10.1039/D3CP05430F](https://doi.org/10.1039/D3CP05430F)

Full-text URL: <https://hal.science/hal-04445499>

## Rotational-state-selected Carbon Astrochemistry

**Jutta Toscano**

The addition of individual quanta of rotational excitation to a molecule has been shown to markedly change its reactivity by significantly modifying the intermolecular interactions. So far, it has only been possible to observe these rotational effects in a very limited number of systems due to lack of rotational selectivity in chemical reaction experiments. The recent development of rotationally controlled molecular beams now makes such investigations possible for a wide range of systems. This is particularly crucial in order to understand the chemistry occurring in the interstellar medium, such as exploring the formation of carbon-based astrochemical molecules and the emergence of molecular complexity in interstellar space from the reaction of small atomic and molecular fragments.

Chimia 78, 40-44 (2024)

DOI: [10.2533/chimia.2024.40](https://doi.org/10.2533/chimia.2024.40)

Full-text URL: <https://arxiv.org/abs/2403.02844>

## The GUAPOS project. V: The chemical ingredients of a massive stellar protocluster in the making

**Á. López-Gallifa, V. M. Rivilla, M. T. Beltrán, L. Colzi, C. Mininni, Á. Sánchez-Monge, F. Fontani, S. Viti, I. Jiménez-Serra, L. Testi, R. Cesaroni, A. Lorenzani**

Most stars, including the Sun, are born in rich stellar clusters containing massive stars. Therefore, the study of the chemical reservoir of massive star-forming regions is crucial to understand the basic chemical ingredients available at the dawn of planetary systems. We present a detailed study of the molecular inventory of the hot molecular core G31.41+0.31 from the project GUAPOS (G31.41+0.31 Unbiased ALMA sPectral Observational Survey). We analyze 34 species for the first time plus 20 species analyzed in previous GUAPOS works, including oxygen, nitrogen, sulfur, phosphorus, and chlorine species. We compare the abundances derived in G31.41+0.31 with those observed in other chemically-rich sources that represent the initial and last stages of the formation of stars and planets: the hot corino in the Solar-like protostar IRAS 16293-2422 B, and the comets 67P/Churyumov-Gerasimenko and 46P/Wirtanen. The comparative analysis reveals that the chemical feedstock of the two star-forming regions are similar. The abundances of oxygen- and nitrogen-bearing molecules exhibit a good correlation for all pair of sources, including the two comets, suggesting a chemical heritage of these species during the process of star formation, and hence an early phase formation of the molecules. However, sulfur- and phosphorus-bearing species present worse correlations, being more abundant in comets. This suggests that while sulfur- and phosphorus-bearing species are predominantly trapped on the surface of icy grains in the hot close surroundings of protostars, they could be more easily released into gas phase in comets, allowing their cosmic abundances to be almost recovered.

Accepted for publication in Monthly Notices of the Royal Astronomical Society (MNRAS)

## Hydrocarbon chemistry in the inner regions of planet-forming disks

**Jayatee Kanwar, Inga Kamp, Peter Woitke, Christian Rab, W.F. Thi**

Context. The analysis of the mid-infrared spectra helps understanding the composition of the gas in the inner, dense and warm terrestrial planet forming region of disks around young stars. ALMA has detected hydrocarbons in the outer regions of the planet forming disk and Spitzer detected C<sub>2</sub>H<sub>2</sub> in the inner regions. JWST-MIRI provides high spectral resolution observations of C<sub>2</sub>H<sub>2</sub> and a suite of more complex hydrocarbons are now reported. Interpreting the fluxes observed in the spectra is challenging and radiation thermo-chemical codes are needed to properly take into account the disk structure, radiative transfer, chemistry and thermal balance. Various disk physical parameters like the gas-to-dust ratio, dust evolution including radial drift, dust growth and settling can affect the fluxes observed in the mid-IR. Still, thermo-chemical disk models were not always successful in matching all observed molecular emission bands simultaneously. Aims: The goal of this project is two-fold. Firstly, we analyse the warm carbon chemistry in the inner regions of the disk, namely within 10 au, to find pathways forming C<sub>2</sub>H<sub>2</sub> potentially missing from the existing chemical networks. Secondly, we analyse the effect of the new chemistry on the line fluxes of acetylene. Methods: We used the radiative thermo-chemical disk code called PRODIMO to expand the hydrocarbon chemistry that occurs in a typical standard T Tauri disks. We used the UMIST and the KIDA rate databases for collecting reactions for the species. We included a number of three-body and thermal decomposition reactions from the STAND2020 network. We also included isotopomers for the species that were present in the databases. The chemistry was then analysed in the regions that produce observable features in the mid-infrared spectra. We studied the effect of expanding the hydrocarbon chemistry on the mid-infrared spectra. Results: Acetylene is formed via two pathways in the surface layers of disks: neutral-neutral and ion-neutral. They proceed via the hydrogenation of C or C<sup>+</sup>, respectively. Thus, the abundances of C, C<sup>+</sup>, H and H<sub>2</sub> affect the formation of C<sub>2</sub>H<sub>2</sub>. Therefore, also the formation of H<sub>2</sub> indirectly affects the abundance of acetylene. Chemisorbed H is more efficient in forming H<sub>2</sub> compared to physisorbed H at warm temperatures and hence increases the abundance of C<sub>2</sub>H<sub>2</sub>. Conclusions: We provide a new extended warm chemical network that considers up to eight carbon atom long species, while also taking into account different isotopomers and can form the building blocks of PAHs: C<sub>6</sub>H<sub>6</sub>. For a standard T Tauri disk with a canonical value of gas-to-dust mass, the line fluxes increase only by a factor of less than 2. JWST is now detecting hydrocarbons such as methane, acetylene, and C<sub>4</sub>H<sub>2</sub> in disks with a high C/O ratio. Hence, this new extended warm hydrocarbon network will aid in interpreting the observed mid-infrared fluxes.

Astronomy & Astrophysics, Volume 681, id.A22, 16 pp.

DOI: [10.1051/0004-6361/202346262](https://doi.org/10.1051/0004-6361/202346262)

Full-text URL: <https://pure.rug.nl/ws/portalfiles/portal/932872762/aa46262-23.pdf>

## The Reservoir of the Per-emb-2 Streamer

**Kotomi Taniguchi, Jaime E Pineda, Paola Caselli, Tomomi Shimoikura, Rachel K. Friesen, Dominique M. Segura-Cox, Anika Schmiedeke**

Streamers bring gas from outer regions to protostellar systems and could change the chemical composition around protostars and protoplanetary disks. We have carried out mapping observations of carbon-chain species (HC<sub>3</sub>N, HC<sub>5</sub>N, CCH, and CCS) in the 3mm and 7mm bands toward the streamer flowing to the Class 0 young stellar object

(YSO) Per-emb-2 with the Nobeyama 45m radio telescope. A region with a diameter of  $\sim 0.04$  pc is located north with a distance of  $\sim 20,500$  au from the YSO. The streamer connects to this north region which is the origin of the streamer. The reservoir has high density and low temperature ( $n_{\text{H}_2} \approx 1.9 \times 10^4 \text{ cm}^{-3}$ ,  $T_{\text{kin}} = 10$  K), which are similar to those of early stage starless cores. By comparisons with the observed abundance ratios of CCS/HC<sub>3</sub>N to the chemical simulations, the reservoir and streamer are found to be chemically young. The total mass available for the streamer is derived to be 24–34  $M_{\odot}$ . If all of the gas in the reservoir will accrete onto the Per-emb-2 protostellar system, the lifetime of the streamer has been estimated at  $(1.1-3.2) \times 10^5$  yr, suggesting that the mass accretion via the streamer would continue until the end of the Class I stage.

The Astrophysical Journal

Full-text URL: <https://arxiv.org/abs/2402.19099>

## Fractionation in young cores: Direct determinations of nitrogen and carbon fractionation in HCN

**S. S. Jensen, S. Spezzano, P. Caselli, O. Sipilä, E. Redaelli, K. Giers, J. Ferrer Asensio**

We aim to determine the  $^{14}\text{N}/^{15}\text{N}$  and  $^{12}\text{C}/^{13}\text{C}$  ratios for HCN in six starless and prestellar cores and compare the results between the direct method using radiative transfer modeling and the indirect double isotope method assuming a fixed  $^{12}\text{C}/^{13}\text{C}$  ratio. We present IRAM 30m observations of the HCN 1-0, HCN 3-2, HC<sub>15</sub>N 1-0 and H<sup>13</sup>CN 1-0 transitions toward six embedded cores. The  $^{14}\text{N}/^{15}\text{N}$  ratio was derived using both the indirect double isotope method and directly through non-local thermodynamic equilibrium (NLTE) 1D radiative transfer modeling of the HCN emission. The latter also provides the  $^{12}\text{C}/^{13}\text{C}$  ratio, which we compared to the local interstellar value. The derived  $^{14}\text{N}/^{15}\text{N}$  ratios using the indirect method are generally in the range of 300-550. This result could suggest an evolutionary trend in the nitrogen fractionation of HCN between starless cores and later stages of the star formation process. However, the direct method reveals lower fractionation ratios of around  $\sim 250$ , mainly resulting from a lower  $^{12}\text{C}/^{13}\text{C}$  ratio in the range  $\sim 20-40$ , as compared to the local interstellar medium value of 68. This study reveals a significant difference between the nitrogen fractionation ratio in HCN derived using direct and indirect methods. This can influence the interpretation of the chemical evolution and reveal the pitfalls of the indirect double isotope method for fractionation studies. However, the direct method is challenging, as it requires well-constrained source models to produce accurate results. No trend in the nitrogen fractionation of HCN between earlier and later stages of the star formation process is evident when the results of the direct method are considered.

A&A, Accepted 26 February 2024

DOI: [10.1051/0004-6361/202449344](https://doi.org/10.1051/0004-6361/202449344)

Full-text URL: <https://arxiv.org/abs/2403.04408>

## Carbon-Chain Chemistry in the Interstellar Medium

**Kotomi Taniguchi, Prasanta Gorai, Jonathan C. Tan**

The presence of carbon-chain molecules in the interstellar medium (ISM) has been known since the early 1970s and  $>130$  such species have been identified to date, making up  $\sim 43\%$  of the total of detected ISM molecules. They are prevalent not only in star-forming regions in our Galaxy but also in other galaxies. These molecules provide important information on physical conditions, gas dynamics, and evolutionary stages of star-forming regions. Larger species of polycyclic aromatic hydrocarbons (PAHs) and fullerenes (C<sub>60</sub> and C<sub>70</sub>), which may be related to the formation of the carbon-chain

molecules, have been detected in circumstellar envelopes around carbon-rich Asymptotic Giant Branch (AGB) stars and planetary nebulae, while PAHs are also known to be a widespread component of the ISM in most galaxies. Recently, two line survey projects toward Taurus Molecular Cloud-1 with large single-dish telescopes have detected many new carbon-chain species, including molecules containing benzene rings. These new findings raise fresh questions about carbon-bearing species in the Universe. This article reviews various aspects of carbon-chain molecules, including observational studies, chemical simulations, quantum calculations, and laboratory experiments, and discusses open questions and how future facilities may answer them.

Accepted for Astrophysics and Space Science

DOI: [10.1007/s10509-024-04292-9](https://doi.org/10.1007/s10509-024-04292-9)

Full-text URL: <https://arxiv.org/abs/2303.15769>

## **Ionic fragmentation products of benzonitrile as important intermediates in the growth of polycyclic aromatic hydrocarbons**

**D. B. Rap, J.G.M. Schrauwen, B. Redlich, S. Brünken**

In various astronomical environments such as the interstellar medium or (exo)planetary atmospheres, an interplay of bottom-up growth and top-down destruction processes of (polycyclic) aromatic hydrocarbons (PAHs) takes place. To get more insight into the interplay of both processes, we disentangle the fragmentation and formation processes that take place upon dissociative ionization of benzonitrile. We build on previous spectroscopic detections of the ionic fragmentation products of benzonitrile and use these as reactants for low-temperature bottom-up ion-molecule reactions with acetylene. By combining kinetics and infrared action spectroscopy, we reveal exothermic pathways to various (polycyclic) aromatic molecules, including the pentalene and phenylacetylene radical cations. We determine the reaction rate coefficients and unambiguously assign the structures of the reaction products. The data is supplemented by potential energy surface calculations and the analysis of non-covalent interactions. This study shows the unexpected formation of a linked four- and six-membered ring structure (phenylcyclobutadiene radical cation) with molecular formula  $C_{10}H_8^+$ , and not the commonly observed isomer naphthalene $^+$ . All observed reactions proceed via radiative association processes and are relevant for the chemistry in (cold) astrochemical environments.

Phys. Chem. Chem. Phys. 26 (2024) 7296-7307

DOI: [10.1039/D3CP05574D](https://doi.org/10.1039/D3CP05574D)

Full-text URL: <https://repository.ubn.ru.nl/handle/2066/303932>

## **Chemical differentiation and gas kinematics around massive young stellar objects in RCW 120**

**K. V. Plakitina, M. S. Kirsanova, S. V. Kalenskii, S. V. Salii, D. S. Wiebe**

We present results of a spectral survey towards a dense molecular condensation and young stellar objects (YSOs) projected on the border of the HII region RCW 120 and discuss emission of 20 molecules which produce the brightest lines. The survey was performed with the APEX telescope in the frequency range 200 -- 260 GHz. We provide evidences for two outflows in the dense gas. The first one is powered by the RCW 120 S2 YSO and oriented along the line of sight. The second outflow around RCW 120 S1 is aligned almost perpendicular to the line of sight. We show that area with bright emission of CH<sub>3</sub>OH, CH<sub>3</sub>CCH and CH<sub>3</sub>CN are organised into an onion-like structure where CH<sub>3</sub>CN traces warmer regions around the YSOs than the other molecules.

Methanol seems to be released to the gas phase by shock waves in the vicinity of the outflows while thermal evaporation still does not work towards the YSOs. We find only a single manifestation of the UV radiation to the molecules, namely, enhanced abundances of small hydrocarbons CCH and c-C<sub>3</sub>H<sub>2</sub> in the photo-dissociation region.

accepted by Astrophysical Bulletin

Full-text URL: <https://arxiv.org/abs/2403.12934>

## **Complex organic molecules uncover deeply embedded precursors of hot cores. An APEX unbiased spectral survey of infrared quiet massive clumps.**

**L. Bouscasse, T. Csengeri, F. Wyrowski, K. M. Menten, S. Bontemps**

During the process of star formation, the dense gas undergoes significant chemical evolution leading to the emergence of a rich variety of molecules associated with hot cores and hot corinos. However, the physical and chemical conditions involved in this evolution are poorly constrained. We provide here a full inventory of the emission from complex organic molecules (COMs) to investigate the physical structure and chemical composition of six high-mass protostellar envelopes. We aim to investigate the conditions for the emergence of COMs in hot cores. We performed an unbiased spectral survey towards six infrared-quiet massive clumps between 159 GHz and 374 GHz with the APEX 12 m telescope. We detect up to 11 COMs, of which at least five COMs are detected towards all sources. Towards all the objects, most of the COM emission is found to be cold, with respect to the typical temperatures at which COMs are found, with a temperature of 30 K and extended with a size of ~0.3 pc. Although for our sample of young massive clumps the bulk of the gas has a cold temperature, we also detect emission from COMs originating from the immediate vicinity of the protostar revealing a compact and hot component of the envelope. Only three out of the six sources exhibit a hot gas component. We find a gradual emergence of the warm component in terms of size and temperature, together with an increasing molecular complexity, allowing us to establish an evolutionary sequence for our sample based on COMs. Our findings confirm that our sample of infrared-quiet massive clumps are in an early evolutionary stage during which the bulk of the gas is cold. The presence of COMs is found to be characteristic of these early evolutionary stages. We suggest that the emergence of hot cores is preceded by a phase in which mostly O-bearing COMs appear first with similar abundances to hot corinos albeit with larger source sizes.

36 pages, 18 figures, accepted for publication in A&A

DOI: [10.1051/0004-6361/202348803](https://doi.org/10.1051/0004-6361/202348803)

Full-text URL: <https://arxiv.org/abs/2403.05237>

## **Announcements**

### **Webinar on 9 May 2024: What's Under the Hood of Astrochemistry?**

We wish to give everyone a warm welcome to our discussion of what's under the hood of astrochemistry. Speakers include Prof. Susanna Widicus Weaver of the University of Wisconsin-Madison and Dr. Vincent Esposito (recipient of the 2024 AAS LAD Dissertation prize) of the NASA Ames Research Center.

In many ways, chemistry is the fingerprint of astrophysics. Chemistry is the study of matter, and this matter interacts with light. This light is what we observe in telescopes

and even with space probes. Hence, the precepts of chemistry are essential for explaining how astronomical matter evolves and changes and how the physical conditions of an astronomical region affect the matter therein. Our presentations today will discuss vital molecules and chemical processes for understanding how different astronomical objects grow and evolve. This pertains to the molecular origins of life as well as how the universe continues to evolve and our ability to observe it.

Date: 9 May 2024 at 4:00 p.m. CEST | 10:00 a.m. EDT  
Webinar ID: 862 1065 5820

After registering, you will receive a confirmation email containing information on how to join the webinar. Registrations with academic institutional email addresses will be prioritized.

Unable to attend? Register anyway and we will let you know when the recording is available to watch. To register:

[https://us02web.zoom.us/webinar/register/2817095243052/WN\\_9Ja0Y8rjQsO\\_sLTdk4O1Ag](https://us02web.zoom.us/webinar/register/2817095243052/WN_9Ja0Y8rjQsO_sLTdk4O1Ag)  
For more information: <https://www.mdpi.com/journal/Chemistry/announcements/8100>