

# AstroChemical Newsletter #57

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## Abstracts

### Evolutionary study of complex organic molecules in high-mass star-forming regions

A. Coletta , F. Fontani, V. M. Rivilla, C. Mininni, L. Colzi , Á. Sánchez-Monge, M. T. Beltrán

We have studied four complex organic molecules (COMs), methyl formate ( $\text{CH}_3\text{OCHO}$ ), dimethyl ether ( $\text{CH}_3\text{OCH}_3$ ), formamide ( $\text{NH}_2\text{CHO}$ ), and ethyl cyanide ( $\text{C}_2\text{H}_5\text{CN}$ ), towards a large sample of 39 high-mass star-forming regions representing different evolutionary stages, from early to evolved phases. We aim to identify potential correlations between the molecules and to trace their evolutionary sequence through the star formation process. We analysed spectra obtained at 3, 2, and 0.9 mm with the IRAM-30m telescope. We derived the main physical parameters for each species by fitting the molecular lines. We compared them and evaluated their evolution, also taking several other interstellar environments into account. We report detections in 20 sources, revealing a clear dust absorption effect on column densities. Derived abundances are  $\sim 1\text{e-}10$ – $1\text{e-}7$  for  $\text{CH}_3\text{OCHO}$  and  $\text{CH}_3\text{OCH}_3$ ,  $\sim 1\text{e-}12$ – $1\text{e-}10$  for  $\text{NH}_2\text{CHO}$ , and  $\sim 1\text{e-}11$ – $1\text{e-}9$  for  $\text{C}_2\text{H}_5\text{CN}$ . The abundances of  $\text{CH}_3\text{OCHO}$ ,  $\text{CH}_3\text{OCH}_3$ , and  $\text{C}_2\text{H}_5\text{CN}$  are very strongly correlated ( $r > 0.92$ ) across  $\sim 4$  orders of magnitude.  $\text{CH}_3\text{OCHO}$  and  $\text{CH}_3\text{OCH}_3$  show the strongest correlations in most parameters, and a nearly constant ratio ( $\sim 1$ ) over a remarkable  $\sim 9$  orders of magnitude in luminosity for a wide variety of sources: pre-stellar to evolved cores, low- to high-mass objects, shocks, Galactic clouds, and comets. This indicates that COMs chemistry is likely early developed and then preserved through evolved phases. Moreover, the molecular abundances clearly increase with evolution. We consider  $\text{CH}_3\text{OCHO}$  and  $\text{CH}_3\text{OCH}_3$  to be most likely chemically linked: they could e.g. share a common precursor, or be formed one from the other. We propose a general scenario for all COMs, involving a formation in the cold, earliest phases of star formation and a following increasing desorption with the progressive heating of the evolving core.

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### Cosmic Ray Dissociation of Molecular Hydrogen and Dense Cloud Chemistry

Gargi Shaw, G. J. Ferland, and S. Ploeckinger

Dissociation of molecular hydrogen by secondary electrons produced by cosmic ray or X-ray ionization plays a crucial role in the chemistry of the densest part of molecular clouds. Here we study the effect of the mean kinetic energy of secondary electrons on this process. We compare predictions using a range of secondary electron energies and predictions of the cross sections with the values in the UMIST database. We find that the predicted column densities change by nearly one dex.

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### Constraints of the formation and abundances of methyl carbamate, a glycine isomer, in hot corinos

Dipen Sahu, Sheng-Yuan Liu, Ankan Das, Prasanta Gorai, Valentine Wakelam

Methyl carbamate  $\text{CH}_3\text{OC(O)NH}_2$  is an isomer of glycine. Quantum chemical analyses show that methyl carbamate is more stable isomer than glycine. Because of this, there could be a higher chance for methyl carbamate to exist in the interstellar medium as compared to glycine. Despite immense searches, till now glycine has not been detected in the ISM, therefore it is worthwhile to search its isomer methyl carbamate. In this paper, we present the constraints of methyl carbamate formation under the interstellar conditions. Large complex organic molecules are favorably produced in hot-corino environments of low mass protostars. We for the first time carried out astrochemical modeling focusing on the formation of methyl carbamate in physical conditions similar to hot-corino objects. Consequently, we examined ALMA archival data for existing spectral line observations toward hot corinos NGC1333 IRAS 4A2 and IRAS 16293B. Within the common spectral range towards these sources, we found three features are possibly related to the spectral transitions of methyl carbamate and consequently estimate the upper limit of column densities. Results of chemical modeling are consistent with the observational upper limit of estimated column density/abundance toward the sources. This may hint the validation of the proposed formation mechanism. Future observations using telescope like ngVLA may confirm the presence of MC toward the hot corinos.

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## Laboratory spectroscopy techniques to enable observations of interstellar ion chemistry

Brett A. McGuire, Oskar Asvany, Sandra Brünken & Stephan Schlemmer

Molecular ions have long been considered key intermediates in the evolution of molecular complexity in the interstellar medium. However, owing to their reactivity and transient nature, ions have historically proved challenging to study in terrestrial laboratory experiments. In turn, their detection and characterization in space is often contingent upon advances in the laboratory spectroscopic techniques used to measure their spectra. In this Review, we discuss the advances over the past 50 years in laboratory methodologies for producing molecular ions and probing their rotational, vibrational and electronic spectra. We largely focus this discussion around the widespread H<sub>3</sub><sup>+</sup> cation and the ionic products originating from its reaction with carbon atoms. Finally, we discuss the current frontiers in this research and the technical advances required to address the spectroscopic challenges that they represent.

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## First detection of <sup>13</sup>CH in the interstellar medium

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In recent years, a plethora of high spectral resolution observations of sub-mm and FIR transitions of methyldene (CH), have demonstrated this radical to be a valuable proxy for H<sub>2</sub>, that can be used for characterising molecular gas within the interstellar medium (ISM) on a Galactic scale, including the CO-dark component. Here we report the discovery of the <sup>13</sup>CH isotopologue in the ISM using the upGREAT receiver on board SOFIA. We have detected the three hyperfine structure components of the 2THz frequency transition from its ground-state toward four high-mass star-forming regions and determine <sup>13</sup>CH column densities. The ubiquity of molecules containing carbon in the ISM has turned the determination of the ratio between the abundances of carbon's two stable isotopes, <sup>12</sup>C/<sup>13</sup>C, into a cornerstone for Galactic chemical evolution studies. Whilst displaying a rising gradient with Galactocentric distance, this ratio, when measured using observations of different molecules (CO, H<sub>2</sub>CO, and others) shows systematic variations depending on the tracer used. These observed inconsistencies may arise from optical depth effects, chemical fractionation or isotope-selective photo-dissociation. Formed from C<sup>+</sup> either via UV-driven or turbulence-driven chemistry, CH reflects the fractionation of C<sup>+</sup>, and does not show any significant fractionation effects unlike other molecules previously used to determine the <sup>12</sup>C/<sup>13</sup>C isotopic ratio which make it an ideal tracer for the <sup>12</sup>C/<sup>13</sup>C ratio throughout the Galaxy. Therefore, by comparing the derived column densities of <sup>13</sup>CH with previously obtained SOFIA data of the corresponding transitions of the main isotopologue <sup>12</sup>CH, we derive <sup>12</sup>C/<sup>13</sup>C isotopic ratios toward Sgr B2(M), G34.26+0.15, W49(N) and W51E. Adding our values derived from <sup>12</sup>/<sup>13</sup>CH to previous calculations of the Galactic isotopic gradient, we derive a revised value of <sup>12</sup>C/<sup>13</sup>C = 5.87(0.45)<sub>R\_GC</sub> + 13.25(2.94).

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## Prebiotic Cytosine Synthesis from Urea in Interstellar Space: A Computational Mechanistic Study

Joong Chul Choe

The potential energy surfaces for the formation of cytosine (Cyt) and a protonated cytosine (CytH<sup>+</sup>) from reactions of urea with cyanoacetylene (CA), cyanoacetaldehyde (CAA), or their protonated ions, CAAH<sup>+</sup> and CAH<sup>+</sup> with or without H<sub>2</sub>O, have been determined from quantum chemical calculation using the CBS-QB3 method. The overall activation energies of the formation of Cyt or CytH<sup>+</sup> from urea + CA, urea + CAA and, urea + CAH<sup>+</sup> are 127, 211, and 31 kJ mol<sup>-1</sup>, respectively, which are too high for the thermal reactions to occur in the interstellar medium (ISM). The barrierless reaction pathways have been proposed for the formation of CytH<sup>+</sup> from urea + CAH<sup>++</sup> H<sub>2</sub>O and urea + CAAH<sup>+</sup>. A kinetic analysis shows that the synthesis of Cyt through the formation of CytH<sup>+</sup> from urea, CAH<sup>+</sup>, and H<sub>2</sub>O would be possible in the ISM.

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## FAUST I. The hot corino at the heart of the prototypical Class I protostar L1551 IRS5

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The study of hot corinos in Solar-like protostars has been so far mostly limited to the Class 0 phase, hampering our understanding of their origin and evolution. In addition, recent evidence suggests that planet formation starts already during

Class I phase, which, therefore, represents a crucial step in the future planetary system chemical composition. Hence, the study of hot corinos in Class I protostars has become of paramount importance. Here we report the discovery of a hot corino towards the prototypical Class I protostar L1551 IRS5, obtained within the ALMA Large Program FAUST. We detected several lines from methanol and its isotopologues ( $^{13}\text{CH}_3\text{OH}$  and  $\text{CH}_2\text{DOH}$ ), methyl formate and ethanol. Lines are bright toward the north component of the IRS5 binary system, and a possible second hot corino may be associated with the south component. The methanol lines non-LTE analysis constrains the gas temperature ( $\sim 100$  K), density ( $\geq 1.5 \times 10^8 \text{ cm}^{-3}$ ), and emitting size ( $\sim 10$  au in radius). All  $\text{CH}_3\text{OH}$  and  $^{13}\text{CH}_3\text{OH}$  lines are optically thick, preventing a reliable measure of the deuteration. The methyl formate and ethanol relative abundances are compatible with those measured in Class 0 hot corinos. Thus, based on the present work, little chemical evolution from Class 0 to I hot corinos occurs.

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