

AstroChemical Newsletter #23

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Abstracts

The interstellar chemistry of C₃H and C₃H₂ isomers

J-C Loison, M Agúndez, V Wakelam, E Roueff, P Gratier, N Marcelino, D N Reyes, J Cernicharo, M Gerin

We report the detection of linear and cyclic isomers of C₃H and C₃H₂ towards various starless cores and review the corresponding chemical pathways involving neutral (C₃H_x with $x=1,2$) and ionic (C₃H_x⁺ with $x = 1,2,3$) isomers. We highlight the role of the branching ratio of electronic Dissociative Recombination (DR) reactions of C₃H₂⁺ and C₃H₃⁺ isomers showing that the statistical treatment of the relaxation of C₃H^{*} and C₃H₂^{*} produced in these DR reactions may explain the relative c,l-C₃H and c,l-C₃H₂ abundances. We have also introduced in the model the third isomer of C₃H₂ (HCCCH). The observed cyclic-to-linear C₃H₂ ratio vary from 110 ± 30 for molecular clouds with a total density around 1×10^4 molecules.cm⁻³ to 30 ± 10 for molecular clouds with a total density around 4×10^5 molecules.cm⁻³, a trend well reproduced with our updated model. The higher ratio for low molecular cloud densities is mainly determined by the importance of the $H + l\text{-C}_3\text{H}_2 \rightarrow H + c\text{-C}_3\text{H}_2$ and $H + t\text{-C}_3\text{H}_2 \rightarrow H + c\text{-C}_3\text{H}_2$ isomerization reactions.

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¹³C isotopic fractionation of HC₃N in two starless cores: L1521B and L134N (L183)

Kotomi Taniguchi, Hiroyuki Ozeki, Masao Saito

We observed the J=5-4 rotational lines of the normal species and three ¹³C isotopologues of HC₃N at the 45 GHz band toward two low-mass starless cores, L1521B and L134N (L183), using the Nobeyama 45 m radio telescope in order to study the main formation pathways of HC₃N in each core. The abundance ratios of the three ¹³C isotopologues in L1521B are derived to be [H¹³CCCN]:[HC¹³CCN]:[HCC¹³CN] = 0.98 (0.14) : 1.00 : 1.52 (0.16) (1 sigma). The fractionation pattern is consistent with that at the cyanopolyyne peak in Taurus Molecular Cloud-1. This fractionation pattern suggests that the main formation pathway of HC₃N is the neutral-neutral reaction between C₂H₂ and CN. On the other hand, their abundance ratios in L134N are found to be [H¹³CCCN]:[HC¹³CCN]:[HCC¹³CN] = 1.5 (0.2) : 1.0 : 2.1 (0.4) (1 sigma), which are different from those in L1521B. From this fractionation pattern, we propose that the reaction between HNC and CCH is a possible main formation pathway of HC₃N in L134N. We find out that the main formation pathways of the same molecule are not common even in the similar physical conditions. We discuss the possible factors to

make a difference in fractionation pattern between L134N and L1521B/TMC-1.

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Detection of CH⁺, SH⁺, and their ¹³C- and ³⁴S- isotopologues toward PKS1830-211

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The $z=0.89$ molecular absorber toward PKS1830-211 provides us with the opportunity to probe the chemical and physical properties of the interstellar medium in the disk of a galaxy at a look-back time of half the present age of the Universe. Recent ALMA observations of hydrides have unveiled the multi-phase composition of this source's interstellar medium along two absorbing sightlines. Here, we report ALMA observations of CH⁺ and SH⁺, and of their ¹³C- and ³⁴S- isotopologues, as potential tracers of energetic processes in the interstellar medium. CH⁺ and ¹³CH⁺ are detected toward both images of PKS1830-211, CH⁺ showing the deepest and broadest absorption among all species observed so far. The [CH⁺]/[¹³CH⁺] abundance ratio is ~ 100 in the south-west line of sight. [...] Toward the north-east image, we find an even larger value of [CH⁺]/[¹³CH⁺], 146 ± 43 , although with a large uncertainty. This sightline intercepts the absorber at a larger galactocentric radius than the southwestern one, where material might be less processed in stellar nucleosynthesis. In contrast to CH⁺ and its ¹³C isotopologue, SH⁺ and ³⁴SH⁺ are only detected on the south-west sightline. These are the first detections of extragalactic SH⁺ and interstellar ³⁴SH⁺. The spectroscopic parameters of SH⁺ are reevaluated and improved rest frequencies of ³⁴SH⁺ are obtained. The [CH⁺]/[SH⁺] column density ratios show a large difference between the two lines of sight: ~ 25 and >600 toward the SW and NE image, respectively. We are not able to shed light on the formation process of CH⁺ and SH⁺ with these data, but the differences in the two sightlines toward PKS1830-211 suggest that their absorptions arise from gas with molecular fraction $\gtrsim 10\%$, with SH⁺ tracing significantly higher molecular fractions than CH⁺.

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Sensitivity analysis of grain surface chemistry to binding energies of ice species

E M Penteado, C Walsh, H M Cuppen

Advanced telescopes, such as ALMA and JWST, are likely to show that the chemical universe may be even more complex than currently observed, requiring astrochemical modelers to improve their models to account for the impact of new data. However, essential input information for gas-grain models, such as binding energies of molecules to the surface, have been derived experimentally only for a handful of species, leaving hundreds of species with highly uncertain estimates. We present in this paper a systematic study of the effect of uncertainties in the binding energies on an astrochemical two-phase model of a dark molecular cloud, using the rate equations approach. A list of recommended binding energy values based on a literature search of published data is presented. Thousands of simulations of dark cloud models were run,

and in each simulation a value for the binding energy of hundreds of species was randomly chosen from a normal distribution. Our results show that the binding energy of H₂ is critical for the surface chemistry. For high binding energy, H₂ freezes out on the grain forming an H₂ ice. This is not physically realistic and we suggest a change in the rate equations. The abundance ranges found are in reasonable agreement with astronomical ice observations. Pearson correlation coefficients revealed that the binding energy of HCO, HNO, CH₂, and C correlate most strongly with the abundance of dominant ice species. Finally, the formation route of complex organic molecules was found to be sensitive to the branching ratios of H₂CO hydrogenation.

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Organic molecules, ions, and rare isotopologues in the remnant of the stellar-merger candidate, CK Vulpeculae (Nova 1670)

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CK Vul is a star whose outburst was observed in 1670-72. A stellar-merger event was proposed to explain its ancient eruption. Aims: We aim to investigate the composition of the molecular gas recently discovered in the remnant of CK Vul. Methods: We observed millimeter and submillimeter-wave spectra of CK Vul using the IRAM 30m and APEX telescopes. Radiative-transfer modeling of the observed molecular features was performed to yield isotopic ratios for various elements. Results: The spectra of CK Vul reveal a very rich molecular environment of low excitation ($T_{\text{ex}} < 12$ K). Atomic carbon and twenty seven different molecules, including two ions, were identified. They range from simple diatomic to complex polyatomic species of up to 7 atoms large. The chemical composition of the molecular gas is indicative of carbon and nitrogen-driven chemistry but oxides are also present. Additionally, the abundance of F may be enhanced. The spectra are rich in isotopologues that are very rare in most known sources. All stable isotopes of C, N, O, Si, and S are observed and their isotopic ratios are derived. Conclusions: The composition of the remnant's molecular gas is most peculiar and gives rise to a very unique millimeter and submillimeter spectrum. The observation of ions and complex molecules suggests the presence of a photoionizing source but its nature (a central star or shocks) remains unknown. The elemental and isotopic composition of the gas cannot be easily reconciled with standard nucleosynthesis but processing in hot CNO cycles and partial He burning can explain most of the chemical peculiarities. The isotopic ratios of CK Vul are remarkably close to those of presolar nova grains but the link of Nova 1670 to objects responsible for these grains is unclear.

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Thermal desorption of astrophysically relevant molecules from forsterite(010)

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We present temperature programmed desorption (TPD) measurements of CO, CH₄, O₂ and CO₂ from the forsterite(010) surface in the sub-monolayer and multilayer coverage regimes. In the case of CO, CH₄ and O₂, multilayer growth begins prior to saturation of

the monolayer peak, resulting in two clearly distinguishable desorption peaks. On the other hand a single peak for CO₂ is observed which shifts from high temperature at low coverage to low temperature at high coverages, sharpening upon multilayer formation. The leading edges are aligned for all the molecules in the multilayer coverage regime indicating zero order desorption. We have extracted multilayer desorption energies for these molecules using an Arrhenius analysis. For sub-monolayer coverages, we observe an extended desorption tail to higher temperature. Inversion analysis has been used to extract the coverage dependent desorption energies in the sub-monolayer coverage regime, from which we obtain the desorption energy distribution. We found that owing to the presence of multiple adsorption energy sites on the crystalline surface the typical desorption energies of these small molecules are significantly larger than obtained in previous measurements for several other substrates. Therefore molecules bound to crystalline silicate surfaces may remain locked in the solid state for a longer period of time before desorption into the gas phase.

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Infrared study on the thermal evolution of solid state formamide

R. G. Urso, C. Scirè, G. A. Baratta, J. R. Brucato, G. Compagnini, Z. Kaňuchová, M. E. Palumbo, G. Strazzulla

Laboratory experiments have shown that the energetic processing, i.e. ion bombardment and UV photolysis, of interstellar grain mantles and cometary surfaces is efficient in the production of formamide. To explain its presence in the gas-phase in these astrophysical environments, a desorption mechanism has to be taken into account. In this work we show experimental results on the thermal evolution of formamide when deposited at 17 K as pure and in mixture with water or carbon monoxide. In these samples, we observed formamide desorption at 220 K. Moreover, we discuss its synthesis in a mixture containing molecular nitrogen, methane and water (N₂:CH₄:H₂O) deposited at 17 K and bombarded with 200 keV H⁺. Heating the sample, we observed that the newly formed formamide remains trapped in the refractory residue produced after the ion bombardment up to 296 K. To analyse the samples we used Fourier transform-infrared spectroscopy (FT-IR) that allowed us to study the infrared spectra between the deposition and the complete desorption of formamide. Here we discuss the experimental results in view of their astrophysical relevance.

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Isotope exchange involving HCO⁺ with CO: a theoretical approach

M. Mladenovic, E. Roueff

Aims. We aim to investigate fractionation reactions involved in the ¹²C/¹³C, ¹⁶O/¹⁸O, and ¹⁷O balance. **Methods.** Full-dimensional rovibrational calculations were used to compute numerically exact rovibrational energies and thermal equilibrium conditions to derive the reaction rate coefficients. A nonlinear least-squares method was employed to represent the rate coefficients by analytic functions. **Results.** New exothermicities are

derived for 30 isotopic exchange reactions of HCO^+ with CO. For each of the reactions, we provide the analytic three-parameter Arrhenius-Kooij formula for both the forward reaction and backward reaction rate coefficients, that can further be used in astrochemical kinetic models. Rotational constants derived here for the 170 containing forms of HCO^+ may assist detection of these cations in outer space.

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Seeds of Life in Space (SOLIS) III. Formamide in protostellar shocks: evidence for gas-phase formation

C. Codella, C. Ceccarelli, P. Caselli, N. Balucani, V. Barone, F. Fontani, B. Lefloch, L. Podio, S. Viti, S. Feng, R. Bachiller, E. Bianchi, F. Dulieu, I. Jimenez-Serra, J. Holdship, R. Neri, J. Pineda, A. Pon, I. Sims, S. Spezzano, A.I. Vasyunin, F. Alves, L. Bizzocchi, S. Bottinelli, E. Caux, A. Chacon-Tanarro, R. Choudhury, A. Coutens, C. Favre, P. Hily-Blant, C. Kahane, A. Jaber Al-Edhari, J. Laas, A. Lopez-Sepulcre, J. Ospina, Y. Oya, A. Punanova, C. Puzzarini, D. Quenard, A. Rimola, N. Sakai, D. Skouteris, V. Taquet, L. Testi, P. Theule, P. Ugliengo, C. Vastel, F. Vazart, L. Wiesenfeld, S. Yamamoto

Context: Modern versions of the Miller-Urey experiment claim that formamide (NH_2CHO) could be the starting point for the formation of metabolic and genetic macromolecules. Intriguingly, formamide is indeed observed in regions forming Solar-type stars as well as in external galaxies. Aims: How NH_2CHO is formed has been a puzzle for decades: our goal is to contribute to the hotly debated question of whether formamide is mostly formed via gas-phase or grain surface chemistry. Methods: We used the NOEMA interferometer to image NH_2CHO towards the L1157-B1 blue-shifted shock, a well known interstellar laboratory, to study how the components of dust mantles and cores released into the gas phase triggers the formation of formamide. Results: We report the first spatially resolved image (size $\sim 9''$, ~ 2300 AU) of formamide emission in a shocked region around a Sun-like protostar: the line profiles are blueshifted and have a FWHM ~ 5 km/s. A column density of $N(\text{NH}_2\text{CHO}) = 8 \times 10^{12} \text{ cm}^{-2}$, and an abundance (with respect to H-nuclei) of 4×10^{-9} are derived. We show a spatial segregation of formamide with respect to other organic species. Our observations, coupled with a chemical modelling analysis, indicate that the formamide observed in L1157-B1 is formed by gas-phase chemical process, and not on grain surfaces as previously suggested. Conclusions: The SOLIS interferometric observations of formamide provide direct evidence that this potentially crucial brick of life is efficiently formed in the gas-phase around Sun-like protostars.

A&A Letters, in press

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Announcements

Open PHD position in Astrochemistry

Subject: Sulphur-bearing molecules in star forming regions: Observational and laboratory investigations. Supervisors : L.E. Kristensen (Niels Bohr Institute & Natural History Museum of Denmark, University of Copenhagen), F. Dulieu (LERMA, University of Cergy-Pontoise & Paris Observatory) Thesis work: The thesis aims at tackle the

problem sulphur chemistry in star forming regions and in particular the of the origin of H₂S in ices, as well as its link with other observed forms in shocks. One half of the work will be devoted to laboratory astrophysics. Using the experimental set-ups located in Neuville-sur-Oise (FORMOLISM and VENUS), the synthesis of H₂S and the properties of the ice formed will be investigated. The experimental work will be done with the help of the team (<https://lerma.obspm.fr/spip.php?article48>). The other part will be devoted to the analysis of observations of sulphur bearing molecules in shocks, and will be mostly done in Copenhagen. More info: <https://www.u-cergy.fr/fr/laboratoires/lerma-cergy/actualite.html>

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