

# AstroChemical Newsletter #43

June 2019

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

### **A sensitive 3 mm line survey of L483: A broad view of the chemical composition of a core around a Class 0 object**

**M. Agundez, N. Marcelino, J. Cernicharo, E. Roueff, and M. Tafalla**

An exhaustive chemical characterization of dense cores is mandatory to understand how chemical composition changes from a starless to a protostellar stage. However, only a few sources have had their molecular composition characterized in detail. Here we present a 3 mm line survey of L483, a dense core around a Class 0 protostar, which was observed with the IRAM 30m telescope in the 80-116 GHz frequency range. We detected 71 molecules (140 including different isotopologues), most of which are present in the cold and quiescent ambient cloud according to their narrow lines (FWHM = 0.5 km/s) and low rotational temperatures (<10 K). Of particular interest among the detected molecules are the cis isomer of HCOOH, the complex organic molecules HCOOCH<sub>3</sub>, CH<sub>3</sub>OCH<sub>3</sub>, and C<sub>2</sub>H<sub>5</sub>OH, a wide variety of carbon chains, nitrogen oxides like N<sub>2</sub>O, and saturated molecules like CH<sub>3</sub>SH, apart from eight new interstellar molecules (HCCO, HCS, HSC, NCCNH<sup>+</sup>, CNCN, NCO, H<sub>2</sub>NCO<sup>+</sup>, and NS<sup>+</sup>), whose detection has been already reported. In general, fractional molecular abundances in L483 are systematically lower than in TMC-1 (especially for carbon chains), tend to be higher than in L1544 and B1-b, while they are similar to those in L1527. Apart from the overabundance of carbon chains in TMC-1, we find that L483 does not have a marked chemical differentiation with respect to starless/prestellar cores like TMC-1 and L1544, although it does chemically differentiate from Class 0 hot corino sources like IRAS 16293-2422. This fact suggests that the chemical composition of the ambient cloud of some Class 0 sources could be largely inherited from the dark cloud starless/prestellar phase. We explore the use of potential chemical evolutionary indicators, such as the HNCO/C<sub>3</sub>S, SO<sub>2</sub>/C<sub>2</sub>S, and CH<sub>3</sub>SH/C<sub>2</sub>S ratios, to trace the prestellar/protostellar transition. We also derived isotopic ratios for a variety of molecules, many of which show isotopic ratios close to the local interstellar medium values (remarkably all those involving <sup>34</sup>S and <sup>33</sup>S), while there are also several isotopic anomalies like an extreme depletion in <sup>13</sup>C for one of the two isotopologues of c-C<sub>3</sub>H<sub>2</sub>, a drastic enrichment in <sup>18</sup>O for SO and HNCO (SO being also largely enriched in <sup>17</sup>O), and different abundances for the two <sup>13</sup>C substituted species of C<sub>2</sub>H and the two <sup>15</sup>N substituted species of N<sub>2</sub>H<sup>+</sup>. We report the first detection in space of some minor isotopologues like c-C<sub>3</sub>D. The detailed chemical characterization of the dense core L483 presented here provides a piece, that together with similar exhaustive characterizations of other low-mass prestellar and protostellar sources, should allow us to understand which are the main factors that regulate the chemical composition of cores along the process of formation of low-mass protostars.

A&A (2019) 625, A147

DOI: [10.1051/0004-6361/201935164](https://doi.org/10.1051/0004-6361/201935164)

Full-text URL: <https://arxiv.org/abs/1904.06565>

## **Influence of galactic arm scale dynamics on the molecular composition of the cold and dense ISM II. Molecular oxygen abundance**

**V. Wakelam, M. Ruaud, P. Gratier, I. A. Bonnell**

Molecular oxygen has been the subject of many observational searches as chemical models predicted it to be a reservoir of oxygen. Although it has been detected in two regions of the interstellar medium, its rarity is a challenge for astrochemical models. In this paper, we have combined the physical conditions computed with smoothed particle hydrodynamics (SPH) simulations with our full gas-grain chemical model Nautilus, to study the predicted O<sub>2</sub> abundance in interstellar material forming cold cores. We thus follow the chemical evolution of gas and ices in parcels of material from the diffuse interstellar conditions to the cold dense cores. Most of our predicted O<sub>2</sub> abundances are below 1e-8 (with respect to the total proton density) and the predicted column densities in simulated cold cores is at maximum a few 1e14 cm<sup>-2</sup>, in agreement with the non detection limits. This low O<sub>2</sub> abundance can be explained by the fact that, in a large fraction of the interstellar material, the atomic oxygen is depleted onto the grain surface (and hydrogenated to form H<sub>2</sub>O) before O<sub>2</sub> can be formed in the gas-phase and protected from UV photo-dissociations. We could achieve this result only because we took into account the full history of the evolution of the physical conditions from the diffuse medium to the cold cores.

Accepted for publication in MNRAS

DOI: [10.1093/mnras/stz1122](https://doi.org/10.1093/mnras/stz1122)

Full-text URL: <https://arxiv.org/abs/1905.00800>

## **The Astrochemical Impact of Cosmic Rays in Protoclusters I: Molecular Cloud Chemistry**

**Brandt A.L. Gaches, Stella S.R. Offner, Thomas G. Bisbas**

We present astrochemical photo-dissociation region models in which cosmic ray attenuation has been fully coupled to the chemical evolution of the gas. We model the astrochemical impact of cosmic rays, including those accelerated by protostellar accretion shocks, on molecular clouds hosting protoclusters. Our models with embedded protostars reproduce observed ionization rates. We study the imprint of cosmic ray attenuation on ions for models with different surface cosmic ray spectra and different star formation efficiencies. We find that abundances, particularly ions, are sensitive to the treatment of cosmic rays. We show the column densities of ions are under predicted by the 'classic' treatment of cosmic rays by an order of magnitude. We also test two common chemistry approximations used to infer ionization rates. We conclude that the approximation based on the H<sub>3</sub><sup>+</sup> abundance under predicts the ionization rate except in regions where the cosmic rays dominate the chemistry. Our models suggest the chemistry in dense gas will be significantly impacted by the increased ionization rates, leading to a reduction in molecules such as NH<sub>3</sub> and causing H<sub>2</sub>-rich gas to become [C II] bright.

ApJ Accepted

Full-text URL: <https://arxiv.org/abs/1905.02232>

## **Alcohols on the Rocks: Solid-State Formation in a H<sub>3</sub>CC≡CH +**

## OH Cocktail under Dark Cloud Conditions

**Danna Qasim, Gleb Fedoseev, Thanja Lamberts, Ko-Ju Chuang, Jiao He, Sergio Ioppolo, Johannes Kästner, and Harold Linnartz**

A number of recent experimental studies have shown that solid-state complex organic molecules (COMs) can form under conditions that are relevant to the CO freeze-out stage in dense clouds. In this work, we show that alcohols can be formed well before the CO freeze-out stage (i.e., during the very early stage of the H<sub>2</sub>O-rich ice phase). This joint experimental and computational investigation shows that isomers n-propanol and isopropanol (H<sub>3</sub>CCH<sub>2</sub>CH<sub>2</sub>OH and H<sub>3</sub>CCHOHCH<sub>3</sub>) and n-propenol and isopropenol (H<sub>3</sub>CCH=CHOH and H<sub>3</sub>CCOH=CH<sub>2</sub>) can be formed in radical-addition reactions starting from propyne (H<sub>3</sub>CC≡CH) + OH at the low temperature of 10 K, where H<sub>3</sub>CC≡CH is one of the simplest representatives of stable carbon chains already identified in the interstellar medium (ISM). The resulting average abundance ratio of 1:1 for n-propanol:isopropanol is aligned with the conclusions from the computational work that the geometric orientation of strongly interacting species is influential to the extent of which “mechanism” is participating and that an assortment of geometries leads to an averaged-out effect. Three isomers of propanediol are also tentatively identified in the experiments. It is also shown that propene and propane (H<sub>3</sub>CCH=CH<sub>2</sub> and H<sub>3</sub>CCH<sub>2</sub>CH<sub>3</sub>) are formed from the hydrogenation of H<sub>3</sub>CC≡CH. This experimental finding falls in line with the lower activation barrier of hydrogenation of a C=C bond in comparison to a C≡C bond. Reactants and products are probed by temperature-programmed desorption–quadrupole mass spectrometry (TPD-QMS) and reflection absorption infrared spectroscopy (RAIRS). Product relative abundances are determined from TPD-QMS data. Computationally derived activation barriers give additional insight into what types of reactions and mechanisms are more likely to occur in the laboratory and in the ISM. Our findings not only suggest that the alcohols studied here share common chemical pathways and therefore can show up simultaneously in astronomical surveys but also that their extended counterparts that derive from polyynes containing H<sub>3</sub>C–(C≡C)<sub>n</sub>–H structures may exist in the ISM. Such larger species, such as fatty alcohols, are the possible constituents of simple lipids that primitive cell membranes on the early Earth are thought to be partially composed of.

ACS Earth and Space Chemistry, Complex Organic Molecules (COMs) in Star-Forming Regions special issue, published April 30 2019

DOI: [10.1021/acsearthspacechem.9b00062](https://doi.org/10.1021/acsearthspacechem.9b00062)

Full-text URL: <https://arxiv.org/abs/1905.05063>

## Physical and chemical fingerprint of protostellar disc formation

**E. Artur de la Villarmois, J. K. Jørgensen, L. E. Kristensen, E. A. Bergin, D. Harsono, N. Sakai, E. F. van Dishoeck and S. Yamamoto**

(Abridged) The purpose of this paper is to explore and compare the physical and chemical structure of Class I low-mass protostellar sources on protoplanetary disc scales. We present a study of the dust and gas emission towards a representative sample of 12 Class I protostars from the Ophiuchus molecular cloud with the Atacama Large Millimeter/submillimeter Array (ALMA). The continuum at 0.87 mm and molecular transitions from C<sub>17</sub>O, C<sub>34</sub>S, H<sub>13</sub>CO<sup>+</sup>, CH<sub>3</sub>OH, SO<sub>2</sub>, and C<sub>2</sub>H were observed at high angular resolution (0.4", ~60 au diameter) towards each source. Disc and stellar masses are estimated from the continuum flux and position-velocity diagrams, and six of the sources show disc-like structures. Towards the more luminous sources, compact emission and large line widths are seen for transitions of SO<sub>2</sub> that probe

warm gas (Eu  $\sim 200$  K). In contrast, C17O emission is detected towards the least evolved and less luminous systems. No emission of CH<sub>3</sub>OH is detected towards any of the continuum peaks, indicating an absence of warm CH<sub>3</sub>OH gas towards these sources. A power-law relation is seen between the stellar mass and the bolometric luminosity, corresponding to a mass accretion rate of  $(2.4 \pm 0.6) \times 10^{-7}$  M<sub>sun</sub>/year for the Class I sources. This mass accretion rate is lower than the expected value if the accretion is constant in time and rather points to a scenario of accretion occurring in bursts. The differentiation between C17O and SO<sub>2</sub> suggests that they trace different physical components: C17O traces the densest and colder regions of the disc-envelope system, while SO<sub>2</sub> may be associated with regions of higher temperature, such as accretion shocks. The lack of warm CH<sub>3</sub>OH emission suggests that there is no hot-core-like region around any of the sources and that the CH<sub>3</sub>OH column density averaged over the disc is low.

Accepted in A&A

DOI: [10.1051/0004-6361/201834877](https://doi.org/10.1051/0004-6361/201834877)

Full-text URL: <https://arxiv.org/abs/1904.13161>

## Why does ammonia not freeze out in the center of pre-stellar cores?

**O. Sipilä, P. Caselli, E. Redaelli, M. Juvela, and L. Bizzocchi**

We carried out a parameter-space exploration of the ammonia abundance in the pre-stellar core L1544, where it has been observed to increase toward the center of the core with no signs of freeze-out onto grain surfaces. We considered static and dynamical physical models coupled with elaborate chemical and radiative transfer calculations, and explored the effects of varying model parameters on the (ortho+para) ammonia abundance profile. None of our models are able to reproduce the inward-increasing tendency in the observed profile; ammonia depletion always occurs in the center of the core. In particular, our study shows that including the chemical desorption process, where exothermic association reactions on the grain surface can result in the immediate desorption of the product molecule, leads to ammonia abundances that are over an order of magnitude above the observed level in the innermost 15000 au of the core – at least when one employs a constant efficiency for the chemical desorption process irrespective of the ice composition. Our results seemingly constrain the chemical desorption efficiency of ammonia on water ice to below 1%. It is increasingly evident that time-dependent effects must be considered so that the results of chemical models can be reconciled with observations.

Accepted to MNRAS

DOI: [10.1093/mnras/stz1344](https://doi.org/10.1093/mnras/stz1344)

Full-text URL: <https://arxiv.org/abs/1905.02384>

## Formation of interstellar propanal and 1-propanol ice: a pathway involving solid-state CO hydrogenation

**D. Qasim, G. Fedoseev, K.-J. Chuang, V. Taquet, T. Lamberts, J. He, S. Ioppolo, E. F. van Dishoeck, and H. Linnartz**

1-propanol (CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>OH) is a three carbon-bearing representative of primary linear alcohols that may have its origin in the cold dark cores in interstellar space. To test this, we investigated in the laboratory whether 1-propanol ice can be formed along pathways possibly relevant to the prestellar core phase. We aim to show in a two-step approach that 1-propanol can be formed through reaction steps that are expected to take place

during the heavy CO freeze-out stage by adding C<sub>2</sub>H<sub>2</sub> into the CO + H hydrogenation network via the formation of propanal (CH<sub>3</sub>CH<sub>2</sub>CHO) as an intermediate and its subsequent hydrogenation. Temperature programmed desorption-quadrupole mass spectrometry (TPD-QMS) is used to identify the newly formed propanal and 1-propanol. Reflection absorption infrared spectroscopy (RAIRS) is used as a complementary diagnostic tool. The mechanisms that can contribute to the formation of solid-state propanal and 1-propanol, as well as other organic compounds, during the heavy CO freeze-out stage are constrained by both laboratory experiments and theoretical calculations. Here it is shown that recombination of HCO radicals, formed upon CO hydrogenation, with radicals formed upon C<sub>2</sub>H<sub>2</sub> processing - H<sub>2</sub>CCH and H<sub>3</sub>CCH<sub>2</sub> - offers possible reaction pathways to solid-state propanal and 1-propanol formation. This extends the already important role of the CO hydrogenation chain in the formation of larger COMs (complex organic molecules). The results are used to compare with ALMA observations. The resulting 1-propanol:propanal ratio concludes an upper limit of < 0:35-0:55, which is complemented by computationally-derived activation barriers in addition to the experimental results.

Accepted for publication in Astronomy and Astrophysics

DOI: [10.1051/0004-6361/201935217](https://doi.org/10.1051/0004-6361/201935217)

Full-text URL: <https://arxiv.org/abs/1905.07801>

## Vacuum Ultraviolet Photodesorption and Photofragmentation of Formaldehyde-Containing Ices

**Géraldine Féraud, Mathieu Bertin, Claire Romanzin, Rémi Dupuy, Franck Le Petit, Evelyne Roueff, Laurent Philippe, Xavier Michaut, Pascal Jeseck, and Jean-Hugues Fillion**

Nonthermal desorption from icy grains containing H<sub>2</sub>CO has been invoked to explain the observed H<sub>2</sub>CO gas phase abundances in protoplanetary disks (PPDs) and photon dominated regions (PDRs). Photodesorption is thought to play a key role; however, no absolute measurement of the photodesorption from H<sub>2</sub>CO ices was performed up to now, so that a default value is used in the current astrophysical models. As photodesorption yields differ from one molecule to the other, it is crucial to experimentally investigate photodesorption from H<sub>2</sub>CO ices. We measured absolute wavelength-resolved photodesorption yields from pure H<sub>2</sub>CO ices, H<sub>2</sub>CO on top of a CO ice (H<sub>2</sub>CO/CO), and H<sub>2</sub>CO mixed with CO ice (H<sub>2</sub>CO:CO) irradiated in the vacuum ultraviolet (VUV) range (7–13.6 eV). Photodesorption from a pure H<sub>2</sub>CO ice releases H<sub>2</sub>CO in the gas phase but also fragments, such as CO and H<sub>2</sub>. Energy-resolved photodesorption spectra, coupled with infrared (IR) and temperature-programmed desorption (TPD) diagnostics, showed the important role played by photodissociation and allowed discussion of photodesorption mechanisms. For the release of H<sub>2</sub>CO in the gas phase, they include desorption induced by electronic transitions (DIET), indirect DIET through CO-induced desorption of H<sub>2</sub>CO, and photochemical desorption. We found that H<sub>2</sub>CO photodesorbs with an average efficiency of  $\sim(4-10) \times 1e-4$  molecule/photon, in various astrophysical environments. H<sub>2</sub>CO and CO photodesorption yields and photodesorption mechanisms, involving photofragmentation of H<sub>2</sub>CO, can be implemented in astrochemical codes. The effects of photodesorption on gas/solid abundances of H<sub>2</sub>CO and all linked species from CO to complex organic molecules (COMs), and on the H<sub>2</sub>CO snowline location, are now on the verge of being unravelled.

ACS Earth Space Chem., Article ASAP

DOI: [10.1021/acsearthspacechem.9b00057](https://doi.org/10.1021/acsearthspacechem.9b00057)

## Electron-Induced Radiolysis of Astrochemically Relevant Ammonia Ices

**Katherine E. Shulenberger, Jane L. Zhu, Katherine Tran, Sebiha Abdullahi, Carina Belvin, Julia Lukens, Zoe Peeler, Ella Mullikin, Helen M. Cumberbatch, Jean Huang, Kathleen Regovich, Alice Zhou, Lauren Heller, Milica Markovic, Leslie Gates, Christina Buffo, Rhoda Tano-Menka, and Christopher R. Arumainayagam Esther Böhler and Petra Swiderek Sasan Esmaili, Andrew D. Bass, Michael Huels, and Léon Sanche**

We elucidate mechanisms of electron-induced radiolysis in cosmic (interstellar, planetary, and cometary) ice analogs of ammonia (NH<sub>3</sub>), likely the most abundant nitrogen-containing compound in the interstellar medium (ISM). Astrochemical processes were simulated under ultrahigh vacuum conditions by high-energy (1 keV) and low-energy (7 eV) electron-irradiation of nanoscale thin films of ammonia deposited on cryogenically cooled metal substrates. Irradiated films were analyzed by temperature-programmed desorption (TPD). Experiments with ammonia isotopologues provide convincing evidence for the electron-induced formation of hydrazine (N<sub>2</sub>H<sub>4</sub>) and diazene (N<sub>2</sub>H<sub>2</sub>) from condensed NH<sub>3</sub>. To understand the dynamics of ammonia radiolysis, the dependence of hydrazine and diazene yields on incident electron energy, electron flux, electron fluence, film thickness, and ice temperature were investigated. Radiolysis yield measurements versus (1) irradiation time and (2) film thickness are semiquantitatively consistent with a reaction mechanism that involves a bimolecular step for the formation of hydrazine and diazene from the dimerization of amidogen (NH<sub>2</sub>) and imine (NH) radicals, respectively. The apparent decrease in radiolysis yield of hydrazine and diazene with decreasing electron flux at constant fluence may be due to the competing desorption of these radicals at 90 K under low incident electron flux conditions. The production of hydrazine at electron energies as low as 7 eV and an ice temperature of 22 K is consistent with condensed phase radiolysis being mediated by low-energy secondary electrons produced by the interaction of high-energy radiation with matter. These results provide a basis from which we can begin to understand the mechanisms by which ammonia can form more complex species in cosmic ices.

ACS Earth Space Chem. 2019, 3, 800–810

DOI: [10.1021/acsearthspacechem.8b00169](https://doi.org/10.1021/acsearthspacechem.8b00169)

Full-text URL: <https://pubs.acs.org/doi/full/10.1021/acsearthspacechem.8b00169>

## Extension of the HCOOH and CO<sub>2</sub> solid-state reaction network during the CO freeze-out stage: inclusion of H<sub>2</sub>CO

**D. Qasim, T. Lamberts, J. He, K.-J. Chuang, G. Fedoseev, S. Ioppolo, A.C.A. Boogert, and H. Linnartz**

Formic acid (HCOOH) and carbon dioxide (CO<sub>2</sub>) are simple species that have been detected in the interstellar medium. The solid-state formation pathways of these species under experimental conditions relevant to prestellar cores are primarily based off of weak infrared transitions of the HOCO complex and usually pertain to the H<sub>2</sub>O-rich ice phase, and therefore more experimental data are desired. In this article, we present a new and additional solid-state reaction pathway that can form HCOOH and CO<sub>2</sub> ice at 10 K 'non-energetically' in the laboratory under conditions related to the "heavy" CO freeze-out stage in dense interstellar clouds, i.e., by the hydrogenation of an H<sub>2</sub>CO:O<sub>2</sub> ice mixture. This pathway is used to piece together the HCOOH and CO<sub>2</sub> formation routes when H<sub>2</sub>CO or CO reacts with H and OH radicals. Temperature

programmed desorption - quadrupole mass spectrometry (TPD-QMS) is used to confirm the formation and pathways of newly synthesized ice species as well as to provide information on relative molecular abundances. Reflection absorption infrared spectroscopy (RAIRS) is additionally employed to characterize reaction products and determine relative molecular abundances. We find that for the conditions investigated in conjunction with theoretical results from the literature, H+HOCO and HCO+OH lead to the formation of HCOOH ice in our experiments. Which reaction is more dominant can be determined if the H+HOCO branching ratio is more constrained by computational simulations, as the HCOOH:CO<sub>2</sub> abundance ratio is experimentally measured to be around 1.8:1. H+HOCO is more likely than OH+CO (without HOCO formation) to form CO<sub>2</sub>. Isotope experiments presented here further validate that H+HOCO is the dominant route for HCOOH ice formation in a CO-rich CO:O<sub>2</sub> ice mixture that is hydrogenated. These data will help in the search and positive identification of HCOOH ice in prestellar cores.

Accepted for publication in Astronomy and Astrophysics

DOI: [10.1051/0004-6361/201935068](https://doi.org/10.1051/0004-6361/201935068)

Full-text URL: <https://arxiv.org/abs/1905.06767>

## Detection of methoxymethanol as a photochemistry product of condensed methanol

**Hope Schneider, Anna Caldwell-Overdier, Sophie Coppieters 't Wallant, Lan Dau, Jean Huang, Ifunanya Nwolah, Muhammad Kasule, Christina Buffo, Ella Mullikin, Lily Widdup, Aury Hay, Si Tong Bao, Jeniffer Perea, Mayla Thompson, Rhoda Tano-Menka, Mileva Van Tuyl, Amy Wang, Sophia Bussey, Nina Sachdev, Christine Zhang, Michael C. Boyer and Christopher R. Arumainayagam**

We report the identification of methoxymethanol (CH<sub>3</sub>OCH<sub>2</sub>OH) as a photochemistry product of condensed methanol (CH<sub>3</sub>OH) based on temperature-programmed desorption studies conducted following photon irradiation at energies below the ionization threshold (9.8 eV) of condensed methanol. The first detection of methoxymethanol in the interstellar medium was reported in 2017 based on data from Bands 6 and 7 from the Atacama Large Millimeter/submillimeter Array (ALMA). The cosmic synthesis of 'complex' organic molecules such as methyl formate (HCOOCH<sub>3</sub>), dimethyl ether (CH<sub>3</sub>OCH<sub>3</sub>), acetic acid (CH<sub>3</sub>COOH), ethylene glycol (HOCH<sub>2</sub>CH<sub>2</sub>OH), and glycolaldehyde (HOCH<sub>2</sub>CHO) has been attributed to UV photolysis of condensed methanol found in interstellar ices. Experiments conducted in 1995 demonstrated that electron-induced radiolysis of methanol cosmic ice analogues yields methoxymethanol. In three recent publications (2016, 2017, and 2018), methoxymethanol was considered as a potential tracer for reactions induced by secondary electrons resulting from the interaction of cosmic rays with interstellar ices. However, the results presented in this study suggest that methoxymethanol can be formed from both radiation chemistry and photochemistry of condensed methanol.

MNRAS 485, L19–L23 (2019)

DOI: [10.1093/mnras/sz019](https://doi.org/10.1093/mnras/sz019)

Full-text URL: <https://academic.oup.com/mnras/article-abstract/485/1/L19/5319146>

## Experimental and Theoretical Studies of the Isotope Exchange Reaction $D + H_3^+ \rightarrow H_2D^+ + H$

**P.-M. Hillenbrand, K. P. Bowen, J. Liévin, X. Urbain, and D. W. Savin**

Deuterated molecules are important chemical tracers of prestellar and protostellar cores. Up to now, the titular reaction has been assumed to contribute to the generation of these deuterated molecules. We have measured the merged-beams rate coefficient for this reaction as a function of the relative collision energy in the range of about 10 meV to 10 eV. By varying the internal temperature of the reacting H<sub>3</sub><sup>+</sup> molecules, we found indications for the existence of a reaction barrier. We have performed detailed theoretical calculations for the zero-point-corrected energy profile of the reaction and determined a new value for the barrier height of  $\approx 68$  meV. Furthermore, we have calculated the tunneling probability through the barrier. Our experimental and theoretical results show that the reaction is essentially closed at astrochemically relevant temperatures. We derive a thermal rate coefficient of  $< 1 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$  for temperatures below 75 K with tunneling effects included and below 155 K without tunneling.

Astrophys. J. 877, 38 (2019)

DOI: [10.3847/1538-4357/ab16dc](https://doi.org/10.3847/1538-4357/ab16dc)

Full-text URL: <https://arxiv.org/abs/1904.02955>

## Extraterrestrial prebiotic molecules: photochemistry vs. radiation chemistry of interstellar ices

**Chris R. Arumainayagam, Robin T. Garrod, Michael C. Boyer, Aurland K. Hay, Si Tong Bao, Jyoti S. Campbell, Jingqiao Wang, Chris M. Nowak, Michael R. Arumainayagam and Peter J. Hodge**

In 2016, unambiguous evidence for the presence of the amino acid glycine, an important prebiotic molecule, was deduced based on in situ mass-spectral studies of the coma surrounding cometary ice. This finding is significant because comets are thought to have preserved the icy grains originally found in the interstellar medium prior to solar system formation. Energetic processing of cosmic ices via photochemistry and radiation chemistry is thought to be the dominant mechanism for the extraterrestrial synthesis of prebiotic molecules. Radiation chemistry is defined as the “study of the chemical changes produced by the absorption of radiation of sufficiently high energy to produce ionization.” Ionizing radiation in cosmic chemistry includes high-energy particles (e.g., cosmic rays) and high-energy photons (e.g., extreme-UV). In contrast, photochemistry is defined as chemical processes initiated by photon-induced electronic excitation not involving ionization. Vacuum-UV (6.2–12.4 eV) light may, in addition to photochemistry, initiate radiation chemistry because the threshold for producing secondary electrons is lower in the condensed phase than in the gas phase. Unique to radiation chemistry are four phenomena: (1) production of a cascade of low-energy ( $< 20$  eV) secondary electrons which are thought to be the dominant driving force for radiation chemistry, (2) reactions initiated by cations, (3) non-uniform distribution of reaction intermediates, and (4) non-selective chemistry leading to the production of multiple reaction products. The production of low-energy secondary electrons during radiation chemistry may also lead to new reaction pathways not available to photochemistry. In addition, low-energy electron-induced radiation chemistry may predominate over photochemistry because of the sheer number of low-energy secondary electrons. Moreover, reaction cross-sections can be several orders of magnitude larger for electrons than for photons. Discerning the role of photochemistry vs. radiation chemistry in astrochemistry is challenging because astrophysical photon-induced chemistry studies have almost exclusively used light sources that produce  $< 10$  eV photons. Because a primary objective of chemistry is to provide molecular-level mechanistic explanations for macroscopic phenomena, our ultimate goal in this review paper is to critically evaluate our current understanding of cosmic ice energetic



processing which likely leads to the synthesis of extraterrestrial prebiotic molecules.

Chem. Soc. Rev., 2019, 48, 2293

DOI: [10.1039/c7cs00443e](https://doi.org/10.1039/c7cs00443e)

Full-text URL:

<https://pubs.rsc.org/en/content/articlelanding/2019/cs/c7cs00443e#!divAbstract>

## Deuterated methanol toward NGC 7538-IRS1

J. Ospina-Zamudio, C. Favre, M. Kounkel, L-H. Xu, J. Neill, B. Lefloch, A. Faure, E. Bergin, D. Fedele, L. Hartmann

We investigate the deuteration of methanol towards the high-mass star forming region NGC 7538-IRS1. We have carried out a multitransition study of CH<sub>3</sub>OH, <sup>13</sup>CH<sub>3</sub>OH and of the deuterated flavors, CH<sub>2</sub>DOH and CH<sub>3</sub>OD, between 1.0–1.4 mm with the IRAM-30m antenna. In total, 34 <sup>13</sup>CH<sub>3</sub>OH, 13 CH<sub>2</sub>DOH lines and 20 CH<sub>3</sub>OD lines spanning a wide range of upper-state energies (E<sub>up</sub>) were detected. From the detected transitions, we estimate that the measured D/H does not exceed 1%, with a measured CH<sub>2</sub>DOH/CH<sub>3</sub>OH and CH<sub>3</sub>OD/CH<sub>3</sub>OH of about (32±8)×10<sup>-4</sup> and (10±4)×10<sup>-4</sup>, respectively. This finding is consistent with the hypothesis of a short-time scale formation during the pre-stellar phase. We find a relative abundance ratio CH<sub>2</sub>DOH/CH<sub>3</sub>OD of 3.2±1.5. This result is consistent with a statistical deuteration. We cannot exclude H/D exchanges between water and methanol if water deuteration is of the order 0.1%, as suggested by recent Herschel observations.

Accepted for publication in Astronomy & Astrophysics (See

<https://arxiv.org/abs/1905.09798>)

DOI: [10.1051/0004-6361/201834948](https://doi.org/10.1051/0004-6361/201834948)

Full-text URL: <https://arxiv.org/pdf/1905.09798.pdf>

## Announcements

### **Celebrating 40 years of Alexander Tielens' contribution to Science: the physics and chemistry of the ISM.**

September 2 - 6, 2019 at the Centre International du Congrès du Palais des Papes, Avignon, France

Xander Tielens has been driving research in the fields of interstellar physics and chemistry and the cosmic cycle of matter with outstanding contributions for 40 years. With this meeting, we wish to celebrate his scientific achievements and discuss future research directions opened up by his contributions. The meeting will focus on the fields strongly influenced by Xander involving the physical and chemical processes that control the interstellar medium and its life cycle: PDRs, interstellar and circumstellar dust, PAHs, ices and astrochemistry. We will especially emphasize future opportunities offered by the powerful telescopes at our disposal such as, for example, ALMA, SOFIA, IRAM and JWST.

Registration and abstract submission are open.

Oral contribution submission deadline: 1st June 2019

Conference website: <https://tielens2019.sciencesconf.org/>

### **Future Observations, Techniques and Methodology in Astrochemistry**

The Annual Meeting of the Astrophysical Chemistry Group of the RSC/RAS

June 24-25, 2019 at Queen Mary University of London, London, United Kingdom

The Astrophysical Chemistry Group is pleased to invite you to give a talk and/or present a poster at the Annual Meeting of the ApChem Group that will be held in the Lecture Theatre of the GO Jones building, Queen Mary University of London (QMUL) on June 24-25, 2019. The meeting, on the topic of 'Future Observations, Techniques and Methodology in Astrochemistry', will also incorporate the Annual General Meeting of the ApChem Group, which will be held at 5 pm on Monday 24th of June. The joint RSC/RAS meeting will consist of invited and contributed talks and poster presentations. Invited speakers for the event are Cecilia Ceccarelli (Observations), Catherine Walsh (Modelling), Sandra Brünken (Experiments) and Brian Ellison (Instrumentation). We wish to encourage early-career researchers (PDRAs and PhD students) to take the opportunity to inform the UK community of their work and research plans. Bursaries for early career researchers will be available. However, researchers will have to present a talk to qualify.

Registration and abstract submission are open.

Oral contribution submission deadline: 17th June 2019

Conference website: <http://www.rsc.org/events/detail/39676/future-observations-techniques-and-methodology-in-astrochemistry>

## **PHD announcement**

Prof P. Caselli (MPE, Garching, Germany) and prof F. Dulieu (LERMA, University of Cergy-Pontoise & Paris Observatory, France)

In the star formation cycle, the dark cloud phase precedes the birth of stars. Due to the high density and very low temperature conditions all species should a priori be trapped on the surface of the grains. This is not the case, and in particular the N<sub>2</sub> molecule (detected through N<sub>2</sub>H<sup>+</sup>) seems to be more resistant to freeze out. Molecules such as CN, CH<sub>3</sub>CN or HNCO are detected, and NH<sub>3</sub> maintains large abundances toward the center of dense cores, in disagreement with chemical models. Similarly, molecules containing an amine group (NH<sub>2</sub>CHO, NH<sub>2</sub>OH) are not detected, while their methylated counterparts (CH<sub>3</sub>CHO, CH<sub>3</sub>OH) are. The synthesis on dust grains of N-bearing molecules, particularly amines, is poorly understood and so models cannot explain if different N-bearing molecules have different chemical origins. The purpose of the PhD is to experimentally study the formation of N-molecules on cold surfaces and to model the chemistry of nitrogen in dense cores. The experimental part will be carried out in Neuville under the responsibility of F. Dulieu, while the modelling and comparison with observations will be carried out at the MPI in Garching under the supervision of P. Caselli.)

<https://www.u-cergy.fr/fr/laboratoires/lerma-cergy/actualite.html>

## **Whispers special session: Massive data processing and analysis in radioastronomy, Amsterdam, September 26, 2019**

First announcement and call for oral contributions and posters, deadline: Friday June 28th in the evening.

Datasets produced by the current and future generations of radio telescopes are becoming extremely large, due to the increase in sensitivity, instantaneous bandpass per pixel and number of pixels per receiver. This is true for the (sub)millimeter domain where the main instruments (IRAM-30m, NOEMA, ALMA, APEX, LMT, etc) now routinely process several tens of GHz with spectral resolutions of the order of 100 kHz (implying the measurements of about 500,000 frequencies simultaneously), as well as for the centimeter domain (VLA, FAST, LOFAR) and the foreseen SKA that will again represent a revolution in data rate. Data processing and analysis of these large volumes require the

development of innovative methods based on the most recent advances in signal processing.

To get the best out of such powerful telescopes, and answer key questions on a wide range of astrophysical topics (from the origin of stars and planets, to cosmic dawn), requires to build bridges between the astronomy community and the applied mathematics / signal processing communities. The proposed one-day session during the Whispers (Workshop on Hyperspectral Image and Signal Processing: Evolutions in Remote Sensing) workshop in Amsterdam aims at presenting the challenges encountered by the radio-astronomy community and the on-going activities to solve them. This event will be organized in 3 to 4 sessions of four to five 20-minutes contributed talks introduced by two invited presentations to set the field by Anna Scaife (Manchester, UK ): Radioastronomy challenges in cosmology and galaxy evolution studies

Susan Clark (Princeton, USA): Atomic and molecular line imaging as diagnostics for ISM and star formation

Posters will be presented during a flash session. The day will end with a round table to define directions for future collaborations. This table will be animated by Cyril Tasse (Obs. de Paris, France), Yves Wiaux (Heriot-Watt, UK, TBC), and the SOC members.

The themes of the workshop include

- \* Single dish and interferometer data processing
- \* Filtering of artifacts and denoising
- \* Structure identification with or without velocity information
- \* Clustering
- \* Identification and quantification of temporal variations
- \* Data - model comparisons

The astrophysics focus is put on the topics benefiting from advanced radioastronomy observations:

- \* The relationship between interstellar medium properties and star formation, from the local universe to distant galaxies.
- \* Observational constraints on Cosmic dawn and the epoch of reionization .

Registration is mandatory, with a reduced fee (190 euros) for the one day special session. The fee includes lunch and coffee breaks. Participants are invited to register and submit either an abstract, an already published paper, or an original paper for publication in IEEE.

Key dates:

- \* Submission deadline: 28 June 2019 (This is the actual deadline for this special session. Please disregard the website deadline.)
- \* Final program: 15 July 2019.
- \* End of registration: 10 September 2019.
- \* Special session: 26 September 2019.

SOC: Jérôme Bobin (CEA Saclay - IRFU/CosmoStat, France)

Chiara Ferrari (Observatoire de la Côte d'Azur, France)

Maryvonne Gerin (Observatoire de Paris, France)

Ralf Klessen (Heidelberg University, Germany)

Joshua E. G. Peek (Space Telescope Science Institute & Johns Hopkins University, USA)

Jérôme Pety (IRAM & Observatoire de Paris, France)

<http://www.ieee-whispers.com>

You have to create a login account and then submit an abstract. Please select the right session: "Massive data processing and analysis in radioastronomy".