# AstroChemical Newsletter #41

## April 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

### Theoretical study of the photodissociation reaction of methanol

**M. Kayanuma, M. Shoji, K. Furuya, Y. Aikawa, M. Umemura, Y. Shigeta**

The photodissociation of methanol, which is an important radical source on interstellar ices, was studied using quantum chemistry calculations. Surface hopping simulations using the time-dependent density functional theory were performed, and the potential energy curves of the low-lying excited states were analyzed using the second-order multireference perturbation theory to reveal the reaction mechanism in the gas phase. We showed that the generation of CH3O would more frequently occur than that of CH2OH on the S1 state in contrast to the ground state. We also discuss why the ratio of CH3O and CH2OH differs between the gas and solid phases.

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Full-text URL: https://www.sciencedirect.com/science/article/pii/S0009261418309084

### CO, H2O, H2O+ line and dust emission in a z = 3.63 strongly lensed starburst merger at sub-kiloparsec scales

**C. Yang, R. Gavazzi, A. Beelen, P. Cox, A. Omont, M. D. Lehnert, Y. Gao, R. J. Ivison, A. M. Swinbank, L. Barcos-Muñoz, R. Neri, A. Cooray, S. Dye, S. Eales, H. Fu, E. González-Alfonso, E. Ibar, M. J. Michałowski, H. Nayyeri, M. Negrello, J. Nightingale, I. Pérez-Fournon, D. A. Riechers, I. Smail, and P. van der Werf**

Using the Atacama Large Millimeter/submillimeter Array (ALMA), we report high angular-resolution observations of the redshift z=3.63 galaxy H-ATLAS J083051.0+013224 (G09v1.97), one of the most luminous strongly lensed galaxies discovered by the Herschel-Astrophysical Terahertz Large Area Survey (H-ATLAS). We present 0."2–0."4 resolution images of the rest-frame 188 and 419 μm dust continuum and the CO(6–5), H2O(211–202), and J_up = 2 H2O+ line emission. We also report the detection of H18O(211–202) in this source. The dust continuum and molecular gas emission are resolved into a nearly complete ~1."5 diameter Einstein ring plus a weaker image in the center, which is caused by a special dual deflector lensing configuration. The observed line profiles of the CO(6–5), H2O(211–202), and Jup = 2 H2O+ lines are strikingly similar. In the source plane, we reconstruct the dust continuum images and the spectral cubes of the CO, H2O, and H2O+ line emission at sub-kiloparsec scales. The reconstructed dust emission in the source plane is dominated by a compact disk with an effective radius of 0.7±0.1 kpc plus an overlapping extended disk with a radius twice as large. While the average magnification for the dust continuum is μ ∼ 10–11, the magnification of the line emission varies from 5 to 22 across different velocity components. The line emission of CO(6–5), H2O(211–202), and H2O+ have similar spatial and kinematic distributions. The molecular gas and dust content reveal that G09v1.97 is a gas-rich major merger in its pre-coalescence phase, with a total molecular gas mass of ∼10^11 M_sun. Both of the merging companions are intrinsically ultra-luminous infrared galaxies (ULIRGs) with infrared luminosities LIR reaching 4×10^12 L_sun, and the total LIR of G09v1.97 is (1.4±0.7)×10^13 L_sun. The approaching southern galaxy (dominating from V = -400 to -150 km s^-1 relative to the systemic velocity) shows no obvious kinematic structure with a semi-major half-light radius of a_s = 0.4 kpc, while the receding galaxy (0 to 350 km s^-1) resembles an a_s = 1.2 kpc rotating disk. The two galaxies are separated by a projected distance of 1.3 kpc, bridged by weak line emission (-150 to 0 km s^-1 ) that is co-spatially located with the cold dust emission peak, suggesting a large amount of cold interstellar medium (ISM) in the interacting region. As one of the most luminous star-forming dusty high-redshift galaxies, G09v1.97 is an exceptional source for understanding the ISM in gas-rich starbursting major merging systems at high redshift.

A&A in press
DOI: [10.1051/0004-6361/201833876](https://doi.org/10.1051/0004-6361/201833876)
Full-text URL: https://arxiv.org/abs/1903.00273

### Laboratory spectroscopic study of the 15N isotopomers of cyanamide, H2NCN, and a search for them toward IRAS 16293-2422 B

**A. Coutens, O. Zakharenko, F. Lewen, J. K. Jørgensen, S. Schlemmer, H. S. P. Müller**

Cyanamide is one of the few interstellar molecules containing two chemically different N atoms. It was detected recently toward the solar-type protostar IRAS 16293-2422 B together with H2N13CN and HDNCN in the course of the Atacama Large Millemeter/submillimeter Array (ALMA) Protostellar Interferometric Line Survey (PILS). The detection of the 15N isotopomers or the determination of upper limits to their column densities was hampered by the lack of accurate laboratory data at the frequencies of the survey. We wanted to determine spectroscopic parameters of the 15N isotopomers of

cyanamide that are accurate enough for predictions well into the submillimeter region and to search for them in the PILS data. We investigated the laboratory rotational spectra of H2-15NCN and H2NC15N in the selected region between 192 and 507 GHz employing a cyanamide sample in natural isotopic composition. Additionally, we recorded transitions of H2N13CN. We obtained new or improved spectroscopic parameters for the three isotopic species. Neither of the 15N isotopomers of cyanamide were detected unambiguously in the PILS data. Two relatively clean lines can be tentatively assigned to H2-15NCN. If confirmed, their column densities would imply a low 14N/15N ratio for cyanamide toward this source. The resulting line lists should be accurate enough for observations up to about 1 THz. More sensitive observations, potentially at different frequencies, may eventually lead to the astronomical detection of these isotopic species.

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## The ALMA-PILS survey: First detection of nitrous acid (HONO) in the interstellar medium

**A. Coutens, N. F. W. Ligterink, J.-C. Loison, V. Wakelam, H. Calcutt, M. N. Drozdovskaya, J. K. Jørgensen, H. S. P. Müller, E. F. van Dishoeck, S. F. Wampfler**

Nitrogen oxides are thought to play a significant role as a nitrogen reservoir and to potentially participate in the formation of more complex species. Until now, only NO, N2O and HNO have been detected in the interstellar medium. We report the first interstellar detection of nitrous acid (HONO). Twelve lines were identified towards component B of the low-mass protostellar binary IRAS 16293-2422 with the Atacama Large Millimeter/submillimeter Array, at the position where NO and N2O have previously been seen. A local thermodynamic equilibrium model was used to derive the column density (~ 9e14 cm-2 in a 0.5'' beam) and excitation temperature (~ 100 K) of this molecule. HNO, NO2, NO+, and HNO3 were also searched for in the data, but not detected. We simulated the HONO formation using an updated version of the chemical code Nautilus and compared the results with the observations. The chemical model is able to reproduce satisfactorily the HONO, N2O, and NO2 abundances, but not the NO, HNO, and NH2OH abundances. This could be due to some thermal desorption mechanisms being destructive and therefore limiting the amount of HNO and NH2OH present in the gas phase. Other options are UV photodestruction of these species in ices or missing reactions potentially relevant at protostellar temperatures.

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Full-text URL: https://arxiv.org/abs/1903.03378

## The challenges of modelling microphysics: ambipolar diffusion, chemistry, and cosmic rays in MHD shocks

**T. Grassi, M. Padovani, J. P. Ramsey, D. Galli, N. Vaytet, B. Ercolano, T. Haugboelle**

From molecular clouds to protoplanetary disks, non-ideal magnetic effects are important in many astrophysical environments. Indeed, in star and disk formation processes, it has become clear that these effects are critical to the evolution of the system. The efficacy of non-ideal effects are, however, determined by the complex interplay between magnetic fields, ionising radiation, cosmic rays, microphysics, and chemistry. In order to understand these key microphysical parameters, we present a one-dimensional non-ideal magnetohydrodynamics code and apply it to a model of a time-dependent, oblique, magnetic shock wave. By varying the microphysical ingredients of the model, we find that cosmic rays and dust play a major role, and that, despite the uncertainties, the inclusion of microphysics is essential to obtain a realistic outcome in magnetic astrophysical simulations.

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DOI: 10.1093/mnras/sty3519
Full-text URL: https://arxiv.org/abs/1901.00504

## The ALMA-PILS survey: the first detection of doubly-deuterated methyl formate (CHD2OCHO) in the ISM

**S. Manigand, H. Calcutt, J. K. Jørgensen, V. Taquet, H. S. P. Müller, A. Coutens, S. F. Wampfler, N. F. W. Ligterink, M. N. Drozdovskaya, L. E. Kristensen, M. H. D. van der Wiel, T. L. Bourke**

Studies of deuterated isotopologues of complex organic molecules can provide important constraints on their origin in star formation regions. In particular, the abundances of deuterated species are very sensitive to the physical conditions in the environment where they form. Because the temperatures in star formation regions are low, these isotopologues are enhanced to significant levels, which enables the detection of multiply deuterated species. However, for complex organic species, so far only the multiply deuterated variants of methanol and methyl cyanide have been reported. The aim of this paper is to initiate the characterisation of multiply deuterated variants of complex organic species with the first detection of doubly deuterated methyl formate, CHD2OCHO. We use ALMA observations from the Protostellar Interferometric Line Survey (PILS) of the protostellar binary IRAS 16293–2422 in the spectral range of 329.1 GHz to 362.9 GHz. Spectra towards each of the two protostars are extracted and analysed using a local thermal equilibrium model in order to derive the abundances of methyl formate and its deuterated variants. We report the first detection of doubly deuterated methyl formate CHD2OCHO in the ISM. The D-to-H ratio (D/H ratio) of CHD2OCHO is found to be 2–3 times higher than the D/H ratio of

CH2DOCHO for both sources, similar to the results for formaldehyde from the same dataset. The observations are compared to a gas-grain chemical network coupled to a dynamical physical model, tracing the evolution of a molecular cloud until the end of the Class 0 protostellar stage. The overall D/H ratio enhancements found in the observations are of about the same magnitude as the predictions from the model for the early stages of Class 0 protostars. However, that the D/H ratio of CHD2OCHO is higher than that of CH2DOCHO is still not predicted by the model. This suggests that a mechanism enhances the D/H ratio of singly and doubly deuterated methyl formate that is not in the model, for instance, mechanisms for H–D substitutions. This new detection provides an important constraint on the formation routes of methyl formate and outlines a path forward in terms of using these ratios to determine the formation of organic molecules through observations of differently deuterated isotopologues towards embedded protostars.

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## First interferometric study of enhanced N-fractionation in N2H+: the high-mass star-forming region IRAS 05358+3543

**L. Colzi, F. Fontani, P. Caselli, S. Leurini, L. Bizzocchi, G. Quaia**

Nitrogen (N) fractionation is used as a tool to search for a link between the chemical history of the Solar System and star-forming regions. A large variation of 14N/15N is observed towards different astrophysical sources, and current chemical models cannot reproduce it. With the advent of high angular resolution radiotelescopes it is now possible to search for N-fractionation at core scales. We present IRAM NOEMA observations of the J=1–0 transition of N2H+, 15NNH+ and N15NH+ towards the high-mass protocluster IRAS 05358+3543. We find 14N/15N ratios that span from about 100 up to about 220 and these values are lower or equal than those observed with single-dish observations towards the same source. Since N-fractionation changes across the studied region, this means that it is regulated by local environmental effects. We find also the possibility, for one of the four cores defined in the protocluster, to have a more abundant 15NNH+ with respect to N15NH+. This is another indication that current chemical models may be missing chemical reactions or may not take into account other mechanisms, like photodissociation or grain surface chemistry, that could be important.

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Full-text URL: https://arxiv.org/abs/1903.06567

## The complexity of Orion: an ALMA view. III. The explosion impact

**L. Pagani, E. Bergin, P.F. Goldsmith, G. Melnick, R. Snell, C. Favre.**

The chemistry of complex organic molecules in interstellar dark clouds is still highly uncertain due in part to the lack of constraining observations. Orion is the closest massive star-forming region, and observations making use of ALMA allow us to separate the emission regions of various Complex Organic Molecules (COMs) in both velocity and space. Orion also benefits from an exceptional situation, in that it is the site of a powerful explosive event that occured ∼500 years ago. We show that the closely surrounding Kleinmann-Low region has clearly been influenced by this explosion, with some molecular species having been pushed away from the densest parts while others have remained in close proximity. This dynamical segregation reveals the time dependence of the chemistry and, therefore allows us to better constrain the formation sequence of COMs and other species, including deuterated molecules.

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Full-text URL: http://aramis.obspm.fr/~pagani/lettre_explosion.pdf

## Spectroscopic Parameters of HTiCN/HTiNC: New Titanium Compounds of Astrochemical Interest

**P. Redondo, C. Barrientos, A. Largo**

A theoretical study of the [C, Ti, H, N] isomers, which are species of possible interstellar interest, has been carried out. We have employed different ab initio and density functional theory methodologies. Eleven isomers on the singlet, triplet, and quintet potential energy surfaces (PES) are characterized. The three most stable isomers of this system are obtained on the 3A" PES from the interaction of the titanium atom of TiH with the cyano radical, CN, giving the open chains hydro-titanium cyanide/isocyanide (HTiCN/HTiNC) and the cyclic arrangement HTi-CN. For the most stable isomers we apply a composite approach which considers the extrapolation to the complete basis set (CBS) limit, relativistic, and core-valence (CV) electron correlation corrections at the at the coupled cluster (CC) level including single and double excitations and a perturbative treatment of triple excitations (CCSD(T)). The lowest-lying isomer, HTiNC, is predicted to lie about 3.67 kcal/mol and 3.86 kcal/mol below HTiCN and the cyclic structure HTi-CN, respectively. Isomerization processes between these isomers show that the cyclic structure could easily isomerize into HTiNC (energy barrier is estimated to be only 0.48 kcal/mol). We report harmonic and anharmonic frequencies, infrared intensities and rotational constants that could help in their experimental characterization.

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Full-text URL: https://iopscience.iop.org/article/10.3847/1538-4357/aaf85b

# Announcements

## ERC Post-doctoral position in Astrochemistry at IPAG

Applications are invited for a Postdoctoral Research Position at IPAG in astrochemistry to begin on October 1st, 2019. The goal of the project is to perform observational and theoretical studies of the formation and evolution of complex organic molecules in star forming regions and their outflow shocks. The project will rely on the several observational Large programs led by the team with the IRAM instruments and the ALMA interferometer, and on the chemical modelling tools (both gas phase and grain surface chemistry) developed by our group at IPAG.
The project is funded by the ERC Advanced grant "Dawn of Organic Chemistry" (DOC; PI: C. Ceccarelli), the goal of which is to fully understand the organic chemistry during the first phases of a Solar-like planetary system formation. DOC involves observational work but also modelling and theoretical studies in quantum chemistry.
The ideal candidate will have background and experience in (sub)millimetre radioastronomy and/or shock modelling. He/she should have a PhD in Physics or Astronomy with broad interest in data processing and astrochemical modelling. The initial appointment will be for 2 years, with the possibility of further extension. Inquiries regarding this position can be directed to Dr. Bertrand Lefloch (bertrand.lefloch@univ-grenoble-alpes.fr).
To apply, please send a curriculum vitae and a research statement that includes your research experience to Dr. Bertrand Lefloch. Also, arrange for three letters of reference to be sent to the above e-mail address. The initial monthly net salary will be around 2000€ and is commensurate to experience. Social security is fully covered. The successful candidate will have a budget of about 4500€/year for travels and conferences. The closing date for the receipt of applications is June 15th, 2019.

## European Conference on Laboratory Astrophysics ECLA 2020: Linking dust, ice and gas in space

The interplay between ubiquitous dust, ice and gas in space knits an interesting tale from collapsing interstellar clouds to the formation of new stars, planets, moons and comets. Along this path the formation of complex organic molecules necessary to construct the building blocks of life brings us a step closer to the understanding of the evolution of life. The advancement in the understanding of these vast intricacies of space lies in the development of varied laboratory techniques together with astronomical observations and astrophysical modeling. The conference allows us an opportunity to ensure collaborations between scientists active in different research fields, which range from astronomy to geology and from chemistry to instrumentation. Further, new results will be discussed and ideas will be exchanged from interdisciplinary perspectives to address questions that will guide observations with the upcoming astronomical large-scale facilities, such as the James Webb Space Telescope.
http://frcongressi.net/ecla2020.meet

## Post-doctoral position in Evolved Stars research

A two-year post-doctoral position is available in the Evolved Stars group of the Department of Space, Earth and Environment at Chalmers University of Technology in Gothenburg, Sweden. The position will be hosted within the Galactic astronomy unit of the Astronomy and Plasma Physics division, in the research group of Dr. Elvire De Beck.
The project will make use of instruments such as ALMA, APEX, OSO 20m, and IRAM 30m in the millimeter/sub-millimeter, as well as the Herschel Space Observatory in the far-infrared. The research will focus on the physical and chemical properties of high- and low-mass stars in the late stages of their evolution, primarily through studies of molecular line observations. The successful applicant will be expected to lead the work in close collaboration with the other members of the group and partner institutes.
The group is active in observational astronomy at all wavelengths, with a focus on millimeter and submillimeter facilities, as well as radiative transfer modelling of molecular line emission and dust, and chemical modelling. The group has close connections to the Onsala Space Observatory, which is the Swedish national facility for Radio Astronomy. The observatory operates telescopes in Sweden, shares in the APEX telescope in Chile, and hosts the Nordic ALMA Regional Center (ARC). The research topics of the division cover a broad range of topics including formation and evolution of galaxies, the birth and death of stars, astrochemistry, and exoplanets.
Application details can be found via the online application submission form. http://www.chalmers.se/en/about-chalmers/Working-at-Chalmers/Vacancies/Pages/default.aspx?rmpage=job&rmjob=7284&rmlang=UK
Included Benefits: A competitive salary and benefits package are offered at Chalmers. Fellows are eligible for social security benefits, including health insurance, paid leave, and retirement benefits. The position also includes travel funds and opportunities for dissemination, networking, and international collaboration will be available.
Application Deadline: Wednesday, May 1, 2019
For further inquiries please contact elvire.debeck@chalmers.se.