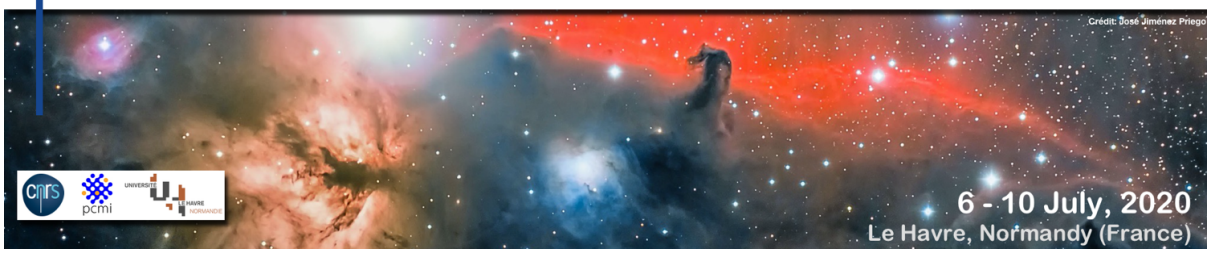
# Physique et Chimie du Milieu Interstellaire

# PCMI 2020 LE HAVRE




## Book of Abstracts

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# Non-thermal desorption of ice mantles: cosmic rays desorption of complex organic molecules

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Determining experimentally the magnitude of interstellar grain mantles accretion and desorption mechanisms is mandatory for astrophysical models to constrain and predict gas and solid phase chemical evolutions. Irradiation by cosmic rays have been simulated experimentally using high energy ions. The ice mantles phase transformation and sputtering yields for released species were monitored simultaneously by infrared spectroscopy and mass spectrometry. The dominant ice mantle species, can be effciently sputtered by cosmic rays. In this talk, the sputtering yield and its evolution as a function of ice mantle thickness for high-energy ions will be discussed in the context of astrophysical environments. Cosmic rays penetrating deep into dense clouds provide a major sputtering mechanism to desorb the observed complex organic molecules (COMs) built over the lifetime of dense clouds, when many other mechanisms fail at releasing them effciently from cold grains. We focused our study on the sputtering effciency of two complex organic molecules that are observed either in interstellar dense clouds ice mantles directly by infrared spectroscopy ($CH_3OH$), or observed in the gas phase by millimetre telescopes ($CH_3COOCH_3$). The sputtering was measured for different ice matrices dominated by water ice or carbon dioxide ices.

A large fraction of COMs desorbs as intact molecules with a proportion corresponding to the time dependent bulk composition of the ice mantles, the latter evolving with time due to the secondary photons VUV photolysis and CR ice mantle radiolysis. The astrophysical cases in relation with these experiments will be discussed.

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# The ISM of extreme dusty starbursts and normal galaxies at z>3 as seen by ALMA

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ALMA has opened a totally new window to explore the ISM of galaxies at z>3. It has proved the existence of very dusty and star-forming galaxies in the early Universe (up to z~8). The most extreme of them can form thousands of solar masses per year. Characterizing their ISM is essential to understand the origin of their impressive star formation rate. SPT SMG sample of lensed dusty star-forming galaxies is perfect to perform systematic surveys fine-structure ([CII], [CI], [NII], [OIII], [OI]) and molecular lines (CO, HCN, HNC, $HCO^+$, $H_2O$). I will present some findings from these studies: the high dense-gas fraction in the most extreme starburst correlates with their star formation efficiency [1], the far-infrared line ratios tend to indicate that these systems are PDR-dominated and have metallicities close from solar [2,3].

In addition, the unprecedented ALMA sensitivity also allows us to probe the ISM of normal galaxies at z>4 using the continuum and the very bright [CII] far-infrared line. The ALPINE ALMA large program targeted them in a sample of normal star-forming galaxies between z=4.4 and z=5.9. We detected 75 objects in [CII] and 23 in continuum [4]. Thanks to this first statistical sample at this epoch, we found that: about half of the star formation is still obscured at z~5 [5]; the SFR-[CII] relation does not evolve compared to the local Universe [4,6]; outflows and large [CII] halos are present around the most star-forming systems [7]; the morpho-dynamical analysis of these systems reveal a large fraction of mergers [8,9].

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# Chemical reactivity for formamide formation on and in ISM water ice grain

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The importance of on-grain processes towards reactivity in the interstellar medium (ISM) is a hot topic in the study of complex organic molecules synthesis. The role of water ice as catalyst may be manifold. Scenarios take place either at the surface of ice or inside cavity. One remarkable feature of water ice mantles is that it is subject to intense irradiation resulting in permanent destruction. We propose to take this into account.

Formamide is under intense research work as a prebiotic molecule, see for instance [1,2,3]. We propose a barrierless root for its formation starting with HCN or HNC. We take opportunity of this talk to show catalytic ability of the water ice also for HNC/HCN isomerization, a well-worn question, which might explain abundance ratios [4,5].

Different pathways are considered by means of quantum mechanics modeling. Both cluster and periodic approaches are used. Drawbacks and advantages of each approach are discussed in a pragmatic tone.

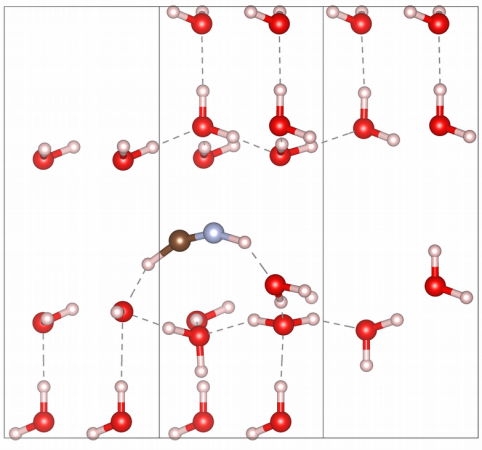

Figure 1 : HNC-HCN isomerization inside model cavity

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# Formation of $C_2$ and $C_3$ COMs in VUV processed interstellar ice analogs: a mechanistic study

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Ethylène glycol (EG) and glycolaldehyde (GA) are two of the largest COMs detected in the interstellar medium (ISM)[1,2]. These two species are ideal precursors for the formation of their $C_3$ analogs: glycerol (GCO) and the first sugar, namely glyceraldehyde (GCA)[3]. The former has been detected in meteorites[4]. In this contribution, we give new evidences for GCO and GCA formation in ice analogs composed of formaldehyde as a small fraction in water. Ices are VUV irradiated to generate radical precursors which induce COM formation during irradiation and warming processes. We were able to characterize and to quantify different sugars and polyols as a function of irradiation temperatures by using mass spectrometry during temperature programmed desorption (TPD) and *in-situ* IR spectroscopy. Results on irradiated ice analogs at different temperatures (from 15 K to 90 K) indicate a formation mechanism involving radical-formaldehyde reactions in the formation of GA (figure 1), EG, GCA and GCO rather than radical-radical recombination mechanisms. We also performed EPR experiments on astrochemically relevant ices as well as on rare gas matrix to detect radicals (H atoms, HCO, $CH_3$, $CH_2OH$, etc) that are precursors of observed COMs. Ultimately, we should be able to have a complete view on processes taking place in our ice analogs in order to describe more precisely what kind of mechanisms are involved in COMs formation.

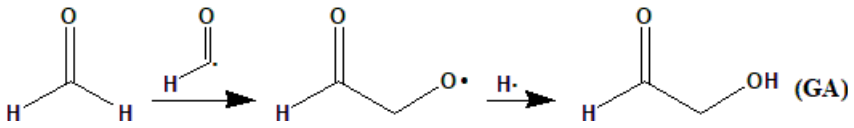


Figure 1: Alternative formation mechanism for GA in interstellar conditions.

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# Learning the 3D interstellar dust distribution of the Milky Way using CNNs

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Due to our observer position inside the Milky Way (MW), it is difficult to look at long distances inside the disk where the extinction rises following the interstellar dust density distribution. Therefore, mapping the MW extinction in 3D is useful not only to better understand the structure of the MW but also to improve any kind of observation that is affected by it.

3D extinction maps in the MW plane had previously been produced (Lallement et al. 2019 [1], Marshall et al. 2006 [2], …) using various methods that mainly rely on observed stellar population. In the case of Marshall et al., they only used 2MASS data, revealing distant structures thanks to the low extinction at infrared wavelengths. In contrast, Lallement et al. used the cross-matched Gaia - 2MASS catalog, taking advantage of Gaia parallaxes, but limited in distances by the strong visible extinction.

In this presentation we describe our method that uses Convolutional Neural Networks (CNN). They are noticeably able to deal with large amounts of data with a high dimensionality, allowing to efficiently combine information from 2MASS and Gaia in an heterogeneous way with no need of a cross-match. Indeed, the network is able to weight the influence of each catalog depending on the distance. Since such networks fall in the supervised machine learning category, we construct a suitable training sample based on a synthetic stellar population from the Besançon Galaxy Model [3] that makes use of a combination of 2MASS and Gaia observables. We will then present the long distance (up to 10 kpc) reconstructed maps from the trained network using observed data.

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# Chemical composition of comets

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For the last thirty years radio and infrared telescopes have enabled the investigation of the composition of the atmosphere of about 60 comets. About 30 molecules (Figure 1, [1,2,4,6]) have been identified in cometary atmosphere and their abundance relative to water, the main constituent, estimated. Isotopic ratios (D/H, $^{15}N/^{14}N$, $^{13}C/^{12}C$, $^{34}S/^{32}S$, $^{18}O/^{16}O$,…) have been measured in a few molecules in the brightest comets. In 2014-2016, the composition of comet 67P/Churyumov-Gerasimenko was monitored in-situ by the Rosetta spacecraft and over 60 different molecules have been identified [8]. I will review the diversity in composition we have measured within the comet family, with a recent extreme case enriched in CO and $N_2$ [3,7] and the possible connection with their dynamical origin. Short term (e.g. seasonal effect seen on comet 67P [5,8]) and long term evolution can also affect the observed abundances.

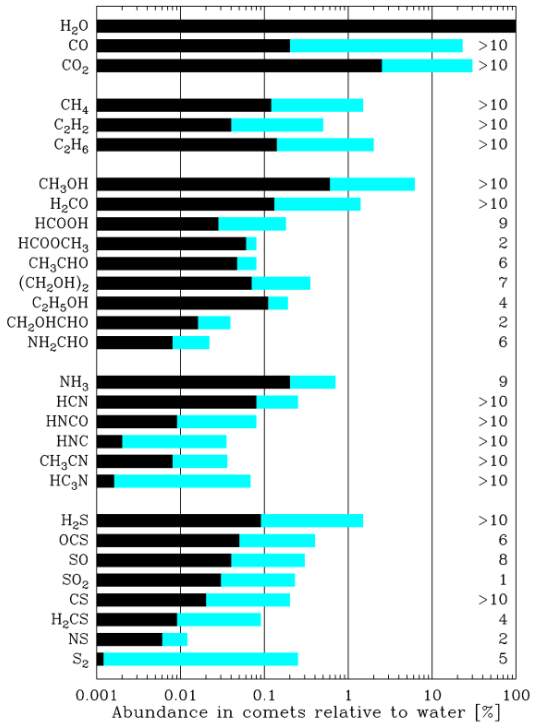


Figure 1 : Range of abundances relative to water of molecules detected remotely in comets (adapted from [4,6])

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# From Astrochemistry to Astrobiology: for a change in paradigm?

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It is generally proposed that astrochemistry in molecular clouds and then protoplanetary disks, leading to a semi-complex organic chemistry observed in radio astronomy, may represent a possible very early first step towards prebiotic chemistry. The frantically search for so called "prebiotic" molecules such as formamide, urea, glycine or glycolaldehyde, often referred as precursors of molecular bricks of life, seems indeed to be the sole goal to validate the hypothesis that links astrochemistry to astrobiology. In our scenario, interstellar ices photo/thermo chemistry, simulated in the laboratory since more than 30 years, leads to a very rich organic solid-state chemistry. The formation of complex organic soluble (and insoluble) materials presenting a large diversity of organic compounds, among them amino-acids, sugars (including ribose), nucleobases and most probably short peptides, is now well documented in the literature. Similarities with the organic matter in primitive carbonaceous chondrites are suggested by various analytical methods and this establishes a more convincing link toward the onset of prebiotic chemistry at the surface of telluric planets where minimal conditions could be met (presence of liquid water, seeding of organic materials and availability of a low entropy free energy source (UV-Visible photons)). A global scenario considering this possibility has been described in [1] and constitutes the basis of our now classical MICMOC experiment supported by the PCMI and the CNES. However, as suggested by ourselves in a recent paper [2], we propose that the true approach for the study of the transition from inert to living must focus not on the chemical compounds themselves but on the process by which auto-organization may take place in a far from equilibrium evolution of the organic matter that may have been delivered on the early Earth. This is the basis for the new MICMOC-LE experiment designed and in construction at PIIM. The goal is to observe the emergence of chemical (replicative) systems that are able to mimic natural selection, in the chemical world, a minimal requirement for any "living" system.

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# Laboratory measurements of gas-phase reactions between aromatic species and the CN radical at low temperatures

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The recent discovery of benzonitrile [1], the first aromatic molecule detected in the interstellar medium (ISM) using radio astronomy, has caused excitement due to the potential link between small aromatic molecules and polycyclic aromatic hydrocarbons (PAHs). Benzonitrile is thought to form via the reaction between the CN radical and benzene, and therefore may serve as a chemical proxy to determine the abundance of benzene which is invisible in the radio region due to its lack of dipole moment. The abundances of aromatic species in the ISM are not well understood due to a lack of experimental data. Most databases extrapolate the rate constants for production and destruction reactions of aromatic hydrocarbons from room temperature to low temperatures; an approximation that can break down in the case of reactions with submerged barriers and/or where quantum mechanical tunneling plays a significant role. Here, we have studied the reactions of benzene and toluene with the CN radical over the temperature range 15-296 K using the well-established CRESU technique (Cinétique de Réaction en Ecoulement Supersonique Uniforme, or Reaction Kinetics in Uniform Supersonic Flow) combined with the Pulsed Laser Photolysis-Laser-Induced Fluorescence method. Both these aromatic species have been detected in the atmosphere of Titan [2,3] and their reactions with the CN radical have been studied down to 105 K by Trevitt et al. [4]. I will also discuss our recent progress in combining chirped-pulse micro/mm-wave spectroscopy with the CRESU method and how we plan to employ this technique to measure product branching ratios for reactions of the CN radical with aromatics at low temperatures.

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# New investigation of the pure rotational spectrum of the $CH_2OH$ radical to enable its interstellar detection

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The hydroxymethyl radical ($CH_2OH$) is one of the two structural isomers, together with the methoxy radical ($CH_3O$), that can be produced by abstraction of a hydrogen atom from methanol ($CH_3OH$). In the interstellar medium (ISM), both $CH_2OH$ and $CH_3O$ are suspected to be intermediate species in many chemical reactions, including the reaction leading to the formation of methanol [1]. The determination of the $CH_3O/CH_2OH$ ratio in the ISM would bring important information concerning the formation processes of these species in the gas and solid phases [2]. Interestingly, while $CH_2OH$ is the most thermodynamically stable isomer, only $CH_3O$ has so far been detected in the ISM [3], despite the recent first laboratory detection of $CH_2OH$ pure rotational spectrum [4]. This lack of detection is possibly due to the non-observation in the laboratory of the most intense transitions at low temperature. To complete the spectroscopic knowledge on the CH2OH species, we thus led new high resolution studies in order to support a potential interstellar detection of the hydroxymethyl radical. We have recorded the pure rotational spectrum of $CH_2OH$ at room temperature in the millimeter-wave domain using a frequency multiplication chain spectrometer. In a similar technique as in Ref. [4], $CH_2OH$ was produced using H abstraction from $CH_3OH$ by halogen atoms. More than 100 new transitions were observed including the transitions involving the lowest $N$ and $K_a$ quantum numbers, predicted intense in astrophysical conditions. Using Pickett's symmetrically reduced axis system Hamiltonian, we fitted almost all infrared [5] and millimeter-wave lines available in the literature together with our new measurements, leading to a large improvement of the parameters values and allowing confident searches of the hydroxymethyl radical in cold environments of the ISM. In the presentation, I will describe all laboratory details as well as the current status of astrophysical searches.

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# Investigating the physical processes driving the evolution of gas, metals and dust in local and high-redshift low-metallicity galaxies

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The chemical enrichment in the interstellar medium (ISM) of galaxies is regulated by several physical processes: star birth and death, grain formation and destruction and galactic inflows and outflows. Understanding such processes and their relative importance is essential in order to follow galaxy evolution and the chemical enrichment through the cosmic epochs, and to interpret the available and future observations (from e.g. JWST and SPICA).

Despite the importance of such topics, the contribution of different stellar sources to the chemical enrichment of galaxies, e.g. massive stars exploding as Type II supernovae and low-mass stars, as well as the mechanisms driving the evolution of dust grains, e.g. grain growth in the ISM and destruction by SN shocks, remain controversial both on the observational and on the theoretical viewpoints.

In this talk I will revise our current knowledge on these physical processes and the observational challenges, and I will present what I have learned from a recent investigation focused on local low-metallicity galaxies and on Lyman Break Galaxies, often considered to be their high-redshift counterparts. In particular, I will discuss the role of stellar sources, galactic outflow and grain accretion/destruction in the ISM in the galaxy baryon cycle (see also Fig. 1).

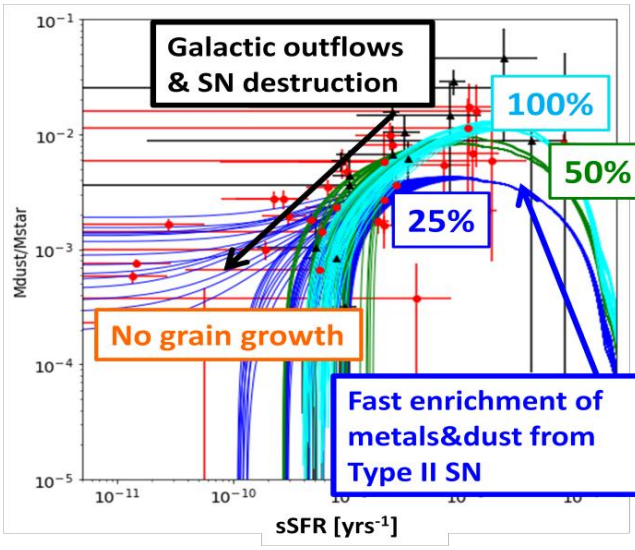


**Figure 1.** Specific mass of dust versus specific star formation rate for dwarf local galaxies (red dots) and Lyman Break Galaxies (black triangles) over plotted with three sets of models characterized by different condensation fraction of dust for supernovae, indicated with different colours. The various lines for the different sets are obtained with different inputs quantities in the chemical evolution models, e.g. mass of baryonic matter, galactic outflow efficiency and supernovae grain destruction efficiencies.

# 3D chemical evolution during the formation of a protoplanetary disk

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Significant physical changes occur during the star formation process from the cold core collapse until the formation of the disk in which planets can form. These physical changes can affect the chemistry and consequently the final composition of the disk. Cold cores are also known to show a diversity of chemical compositions (e.g., [1]). It remains to know if the initial abundances of the cold core can affect the final composition of the disk or if the physical evolution during the collapse and the disk formation play a major role in the disk composition.

To answer this question, we used 3D dense core collapse calculations performed with the adaptive-mesh-refinement RAMSES code. Among the $10^6$ tracer particles introduced in the simulations, 15,000 ended into the disk. We calculated the chemical evolution for these 15,000 particles for two different sets of initial abundances with the gas-grain code Nautilus ([2]) and compared the abundances of various molecules. Molecules can be classified into different categories, based on their dependence on the initial conditions. Spatial differences are also observed for different groups of molecules. In this presentation, I will summarize the main results of this study ([3]).

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# What do we know about Sulfur Astrochemistry?

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As of today, twenty-five different sulfur-bearing species have been observed in Space (i.e. ~10% of all the molecules detected in Space so far), from atomic (such as S and $S^+$) up to 9 atom molecules with $CH_3CH_2SH$. They are routinely observed in a wide variety of astrophysical objects from extra-galactic sources to our own Solar System, including different evolutionary stages along star formation processes. They are not only common tools to constrain the physical conditions (e.g. shock, infall, accretion tracers), but also, S-chemistry has recently been shown to play an important role in the formation of life building-blocks and planet habitability. However, in most of the astrophysical environments where S-bearing species are observed, the sum of observed S-species does not account for the sulfur cosmic abundance. The S-reservoir(s) question is still an unresolved important question. To date, it is not clear whether it is only an observation problem, or if it could also be due to critical physical and chemical aspects still missing in models. We recently compiled a review of our current knowledge and understanding of sulfur astrochemistry [1] that I will present in this talk. In particular, I will discuss some key aspects of the sulfur chemistry, such as the main uncertainties in current gas-grain chemical networks, which should stimulate new effort in experiments, calculations, and modeling.

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# Disks, gas kinematics, dust and complex organic molecules in the youngest protostars: an overview of CALYPSO results

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Class 0 protostars are the first protostars, experiencing such vigorous accretion that most of the final stellar mass will be accreted onto the central protostellar object in less than 0.1 Myrs. During this crucial star-building phase, the material from the circumstellar envelope must redistribute most of its initial angular momentum outward while being accreted, or centrifugal forces will prevent further star growth: this is the long-standing problem of angular momentum for star formation.

How this is done exactly remains poorly understood: several key questions tied to this angular momentum problem still remain open, such as the role of magnetic fields and envelope rotation for building protostellar disks and launching jets. Solving these questions is of paramount importance not only to better understand the origin of our own solar system, but also depicting the pristine conditions leading to the formation of most stars and planets. Ultimately, it relies on characterizing the physics at work in young accreting protostars.

CALYPSO (Continuum and Lines in Young Protostellar Objects -http://irfu.cea.fr/Projets/Calypso) is an IRAM Large Program tackling this long-standing angular momentum problem of star formation. We combined NOEMA and 30-m telescope observations to produce a comprehensive observational set of continuum and line emission in 16 of the nearest low-mass Class 0 protostars, probing the density, temperature, chemical and kinematic structure of these very young protostars down to 50 au scales.

We will present our statistical analysis of this ambitious observing program, with important results from a uniquely large sample regarding (i) the properties of the youngest circumstellar disks, (ii) the diversity of pristine chemical composition in star-forming cores, (iii) the angular momentum content of the youngest protostellar envelopes and (iv) some hints suggesting very early dust evolution towards planetesimals formation.

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# Size effects in dust polarized emission

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Dust polarized emission is now routinely used to trace the magnetic field associated to star formation. Modern facilities probe denser and denser environments, down to the scale of protoplanetary disks [PPDs] where dust grains have grains to (sub-)millimeter sizes [1]. Using the DUSTEM tool [2], I present how grain growth affects the spectral dependence of dust polarized emission. When the grains size approach the wavelength, the polarization fraction decreases until the direction of polarization flips by 90° ([3], Fig. 1). This particular regime of polarized emission may reconcile ALMA polarization observations of PPDs with standart dust alignment physics, and open the path to estimating grain size from polarized emission.

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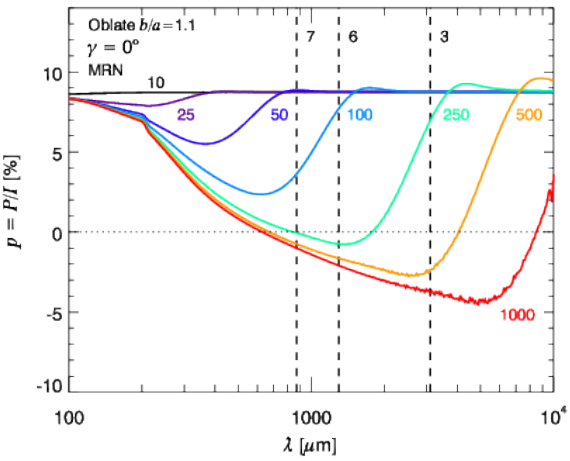


Figure 1 : Spectral dependence of the polarization fraction $p$, for various MRN-like size distributions. The maximal grains size (in microns) is indicated. A negative $p$ means that the polarization direction has flipped by 90° and is therefore parallel to the magnetic field [3].

# Collisional excitation of interstellar reactive molecules: towards a new statistical approach

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Our main knowledge about interstellar environments relies on molecular spectra. In such environments, the density is usually low and the frequency of collisions not large enough to maintain a local thermodynamical equilibrium (LTE). It is then necessary to take into account both collisional and radiative processes in order to properly interpret molecular spectra. State-to-state rate coefficients describing the collisional (de)excitation of interstellar species with the main collisional partners ($H_2$, H, He) are then essential. As for now, full quantum time-independent close-coupling calculations is the method of choice to obtain accurate collisional rate coefficients at typically low interstellar temperatures (< 100 K). However, in the case of reactive systems, i.e. open-shell molecules and ions that can undergo a reaction with the most dominant interstellar species H or $H_2$, this method is impractical due to its memory and CPU requirements. As a result, reliable collisional data is missing for many detected reactive molecules of key importance in astrochemistry (NH, $OH^+$, $CH^+$, $HCl^+$, $H_2O^+$, …), preventing a proper determination of their abundance.

Here, we present a new approach based on the statistical adiabatic channel model (SACM) to compute collisional rate coefficients in the case of reactive molecules. This efficient approach allows the determination of the rate coefficients with an accuracy meeting the needs of astrophysical applications while overcoming the memory and CPU limitations of the close-coupling method. This new approach was successfully validated on light triatomic systems for which full quantum time-independent close-coupling results were available such as $CH^+$ – H and $SH^+$ – H. The present statistical method should be considered as a useful alternative to prohibitive close-coupling calculations in order to provide the astrophysical community with accurate collisional data.

# Measuring the difference in collisional interaction of HCN/HNC with He at low temperatures using the CPUF technique

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HCN and HNC are commonly observed molecules in the interstellar medium (ISM) whose abundance ratios are sensitive to the physical conditions, especially in cold regions with active gas phase chemistry. In such regions, dissociative recombination reactions contributing to the production of both isomer are expected to lead to an HCN/HNC abundance ratio close to unity. However, the ratio derived from the observation is often found to be different. One possible explanation for this deviation lies in the fact that the excitation mechanism was the same for both species. Previous *ab initio* calculations of the collisions with He[1] and $H_2$[2], two of the most abundant colliders in the ISM, have shown that the rates for HNC with these colliders is much stronger, which could skew observational results. We have performed CPUF (Chirped Pulse in Uniform supersonic Flow) experiments[3] using a new setup to measure the difference in pressure-broadened linewidth of HCN and HNC at cold temperatures (down to 16 K) in He. A new E-band chirped pulse Fourier transform spectrometer was used to probe the $J$=1-0 transitions of HCN and HNC while the CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme) technique was used to produce cold flows of He. Pulsed laser photolysis of vinyl cyanide was used to generate HCN and HNC *in situ* under comparable conditions. The linewidth was found by fitting the free induction decay from these experiments recorded for each species at different temperatures. This was then compared against pressure broadening cross sections produced from close coupled scattering calculations performed on *ab initio* potential energy surfaces. We find that there is a difference in interaction of HCN and HNC with He at low temperatures and will discuss the impacts this may have for observing these species in the ISM.

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# Mapping the structural diversity of $C_{60}$ carbon clusters: modeling infrared and optical spectra

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The current debate about the nature of the carbonaceous material carrying the infrared (IR) emission spectra of planetary and protoplanetary nebulae, including the broad plateaus on the one hand, and the UV bump at 2175 Å observed in the interstellar medium extinction curve of galaxies on the other hand, calls for further studies on the interplay between structure and spectroscopy of carbon-based compounds of astrophysical interest. The recent observation of $C_{60}$ buckminsterfullerene in space suggests that carbon clusters of similar size may also be relevant. In the present work, broad statistical samples of $C_{60}$ isomers were computationally determined without any bias using a reactive force field. Structural analysis reveals four main structural families identified as cages, planar polycyclic aromatics, pretzels, and branched. Their IR spectra were subsequently obtained following local optimization with the density-functional-based tight-binding (DFTB) theory. Comparison with available astronomical spectra indicates that only the cage family could contribute to the plateau observed in the 6–9 μm region [1]. The optical spectra of the four populations were also computed at the Time Dependent-DFTB level. All families were found to display strong absorption in the 2–8 eV domain, mainly due to $\pi \rightarrow \pi^*$ transitions. The absorption features, however, differ from one family to another and finally, our quantum modeling indicates that the best candidates for the interstellar UV bump are cages and then flakes, while the opposite trend is found for the carbonaceous species formed in flame experiments [2].

The present framework shows great promise to explore and relate structural and spectroscopic features in more diverse and possibly hydrogenated carbonaceous compounds, in relation with astronomical observations.

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# Infrared OH emission as a diagnostic of the FUV field in disks and outflows from nascent sun-like stars

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Solar-type stars form by gravitational collapse of a rotating dense core and material with excess angular momentum forms a circumstellar disk that eventually gives birth to planets. The far-ultraviolet (FUV) radiation field is a key parameter that controls the chemical, physical and dynamical evolution of the dense gas around nascent stars, and in particular in disks and outflows: it regulates (i) the chemistry of disk upper layers and outflows, (ii) the thermal structure of disks, and (iii) the coupling between the gas and the magnetic field (by setting the charge of the grains and the ionization state of the gas) which regulates disk turbulence, accretion, and magneto-centrifugal ejection (Panoglou et al. 2012, Tabone et al. 2020). The upcoming JWST observations, together with ground-based infrared observatories (ELT, ELT) will allow a complete inventory of molecular and atomic emission from warm (~200-2000K) and irradiated gas and open unique diagnostics based on the excitation of these species. However, the local FUV radiation field incident on disks and outflows is poorly known, due to the complex sources of emission (the accreting nascent star and strong shocks along the jet) and the unknown level of dust and gas attenuation on the line of sight, severely limiting the diagnostic capabilities.

In this contribution, we present a new method to measure the local FUV field from the observation of rotationally excited (E>20000K) OH infrared lines in the mid-infrared domain. This method is based on our modeling effort to couple radiative transfer models to state-of-the-art quantum calculations of OH state-distribution following FUV photodissociation of $H_2O$. As a test case, our model has been successfully applied to Spitzer-IRS observations of tip of the HH211 bow-shock and suggests that protostellar jet shocks may have a decisive chemical and physical feedback on the circumstellar environment (Tabone et al. in prep). We will then discuss how to exploit the unique combination of high sensitivity and angular resolution offered by future (JWST-MIR, ELT-METIS) mid-infrared instruments to study the irradiation of disks from the observation of OH lines. Applications of our model to classical PDR regions (Le Petit et al. 2006) and interstellar shocks (Godard et al. 2019) will finally be discussed. This work constitutes also a decisive step toward a state-to-state chemistry of oxygen in photon-dominated environments.

# Isomerism Effects in the Collisional Excitation of Cyanoacetylene by Molecular Hydrogen

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Cyanopolyynes, known also as prebiotic molecules which likely preceded the presence of life on Earth, are present in space. For instance, cyanoacetylene ($HC_3N$) has been detected in a great variety of astronomical environments.[1] Due to its low rotational constant and large dipole moment, $HC_3N$ is considered as a very good thermometer and barometer in the interstellar medium (ISM). Furthermore, carbon chain molecules exhibit structural isomerism, the explicit study of which can lead to detailed information on the population of isomers. Regarding $HC_3N$, four of its isomers are stable according to laboratory experiments. Among them, only $HC_2NC$ and $HNC_3$ have been detected in the ISM and in the circumstellar envelope IRC+10216.[2,3] The precise determination of the abundance of the $HC_3N$ different isomers can lead to detailed information on the physical conditions and the feasibility of the isomerization processes in space. Therefore, rotational rate coefficients due to collision with the most abundant interstellar species ($H_2$) are crucial mainly when Local Thermodinamic Equilibrium (LTE) is not reach, which is very frequent in space.

New four-dimensional potential energy surfaces of the $HC_2NC$−$H_2$ and $HNC_3$−$H_2$ collisional systems were used to investigate the rotational excitation of $HC_2NC$ and $HNC_3$ by para- and ortho-$H_2$. In addition, we performed radiative transfer calculations to simulate the $HC_3N$, $HC_2NC$ and $HC_2NC$ emissions through a large velocity gradient (LVG) approach.

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# Astrochemistry of ices

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The elements C, H, O, and N, which are essential building blocks of life, are thought to be incorporated into planetesimals as ices and organic residues. These planetesimals arise in the 'protoplanetary disks' of gas and dust that are formed during the collapse of molecular cloud cores into newborn stars. Therefore, tracing the chemical evolution of ices from their origin in these molecular clouds to the planet-forming regions of protoplanetary disks is an essential part of the fields of cosmochemistry, astrochemistry, and astrobiology.

In this talk, I review some of the open questions in the astrochemistry of ices [1]. Then I highlight how recent laboratory experiments and chemical modeling open new avenues to explore these questions. Finally, I describe the observational opportunities presented by the Ice Age Early Release Science program on the soon-to-be launched James Webb Space Telescope ('JWST': ESA/NASA/CSA) to answer these questions. Ice Age is a publically available observing program to provide science-enhancing products to help the astrochemistry community prepare for JWST's Cycle 1 and 2. Proposals for JWST's Cycle 1 will likely be due in autumn 2020.

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# State-to-state chemistry

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Pressures are so low in the interstellar medium ($P < 10^{-10}$ mbar) that inelastic collisions cannot maintain a local thermodynamical equilibrium (LTE). Molecular populations thus do not follow a simple Maxwell-Boltzmann distribution and non-LTE spectra are the rule rather than the exception. A detailed knowledge of state-to-state processes, both radiative and inelastic, is thus crucial to properly analyze the observations. But in addition, reactive process can also play a role in the non-LTE distributions and vice-versa. This coupling between radiative, inelastic and reactive processes is difficult to model because, mainly, quantum state-selected collisional data are missing. We will present some recent examples of state-resolved rate coefficients for reactions of astrophysical interest (e.g. [1]). We will also present a state-to-state chemical model for $CH^+$ in the planetary nebula NGC 7027 [2] and for $H3^+$ in the Central Molecular Zone. Challenging perspectives in both theory and experiment will be finally discussed.

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# Hydrogenation of glyoxal in the interstellar medium: a potential precursor of glycolaldehyde and ethylene glycol?

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More than 70 complex organic molecules (COM) have been detected in the interstellar medium (ISM). Many of these complex molecules are chemically linked through energetic and non-energetic processing and may be involved in a complex prebiotic chemistry [1]. However, the formation reactions of numerous COMs remain unknown. Various astrophysical models propose mechanisms for the formation of these complex molecules based on the abundances of species already detected. This is the case of glycolaldehyde ($CHOCH_2OH$) and ethylene glycol ($HOCH_2CH_2OH$), two COMs detected in the ISM. Astrophysical models often proposed that the formation of these compounds would be directly linked to the hydrogenation of glyoxal (CHOCHO), a potential precursor which is not yet detected in the ISM [2].

In the context of explaining the formation of COMs in the ISM, we have performed, in this work, surface and bulk hydrogenations of solid CHOCHO at 3 and 10 K under ISM conditions in order to confirm or invalidate the astrophysical models [3]. Our results show that the hydrogenation of glyoxal does not lead to the formation of detectable amounts of heavier organic molecules such as glycolaldehyde and ethylene glycol but rather to lighter CO-bearing species such as CO, $H_2CO$, and CO–$H_2CO$, a reaction intermediate resulting from an H-addition–elimination process on CHOCHO. The solid phase formation of such a reaction intermediate has been confirmed through the neon matrix isolation of CO–$H_2CO$ species. Consequently, the hydrogenation of glyoxal under ISM conditions would lead to molecular fragmentations through H-addition-abstraction processing, more efficient than the H-addition reaction to form glycolaldehyde or ethylene glycol.

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# Chemical diversity toward high-mass star forming regions

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The high temperatures that prevail in high-mass star forming regions boost their gas-phase chemical complexity via thermal desorption of the complex organic molecules (COMs) trapped in dust-grain ice-mantles. These COMs are excellent diagnostic tools of the physical conditions of their environment. The high sensitivity and angular resolution provided by the Atacama Large Millimeter/submillimeter Array (ALMA) is a strong asset to investigate the physical and chemical structure of the envelope of high-mass protostars. I will present results from two ALMA projects, the imaging line survey Exploring Molecular Complexity with ALMA (EMoCA, [1]) which targets the galactic center molecular cloud Sagittarius B2, and the Search for high-mass Protostars with ALMA up to Kiloparsec Scales (SPARKS, [2]) toward 35 massive clumps. The analysis of the data shows that high-mass star forming cores exhibit a great diversity in their chemical composition (Fig. 1, left panel) and physical structure. By combining observations with astrochemical models we can study the building-up of chemical complexity and probe the environmental conditions (cosmic-ray ionization rate, UV radiation field) of the investigated sources (Fig. 1, right panel).

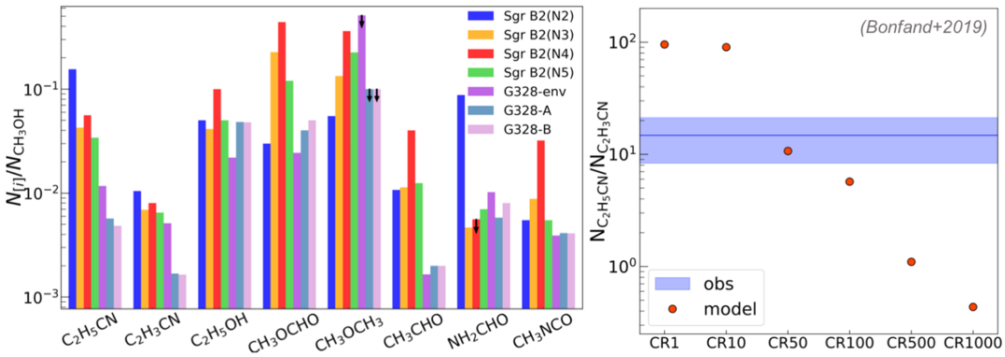


Figure 1: *(left)* Chemical abundances of selected COMs with respect to methanol, measured toward Sgr B2(N)'s hot cores [3] and G328.2551, a source from the SPARKS project [4]. *(right)* Abundance ratio of ethyl/vinyl cyanide calculated by the chemical model run for Sgr B2(N2), as a function of the cosmic-ray ionization rate (CRX means CRIR=X*1.3×$10^{-17}$ $s^{-1}$).

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# Porosity and micro-structure of interstellar ices: insights from neutron scattering experiments and molecular dynamics simulations.

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Interstellar ices are main molecular reservoirs of the interstellar medium and are assumed to be responsible for a large part of the observed molecular diversity. In particular, their surface act as a catalyst for surface reactions, but is also constantly affected by processes of exchanges with the gas phase, and thermal or energetic processing. Studying the surface properties and porosity of these ices and especially their porosity is therefore crucial to constrain the physical and chemical evolution of the ISM. In order to treat these questions, we developed a mixed theoretical and experimental approach to constrain the ice microstructure during both its deposition and heating upon desorption. Small-angle neutron scattering experiments have been conducted at the ISIS facility [1]; this allow a study of the ices at two angle ranges probing both the ice crystallinity but also its microstructure in terms of porosity and surface area. Secondly, classical molecular dynamics simulations have been implemented to study both deposition and heating of a water ice on a model surface [2]. Results from both methods are finally gathered to draw a reasonable scenario about ice microstructural evolution in the interstellar medium and how it drives the molecular exchanges between solid and gas phase.

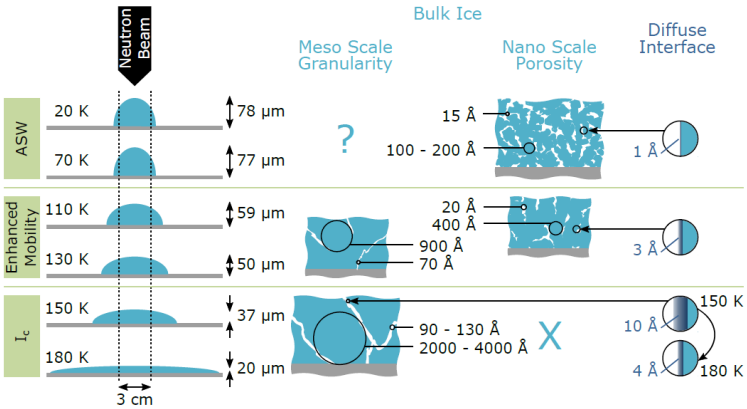


Figure 1 : Cartoon describing ice evolution (Gaertner et al *in prep*)

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# Effects of substrate porosity on the desorption characteristics of ices condensed on dust grains.

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Molecular ices condensed on the cold surface of dust grains undergo multiple interaction with cosmic rays, electrons and photons. These, together with thermal processes, are thought to be responsible for the presence of complex gas molecules in Interstellar Medium (ISM) through desorption events.

To examine the effects of the desorption processes, a number of laboratory studies are at place to mimic the astronomical conditions. Energetic constraints and ice compositions, as close as possible to the realistic ones, are usually taken into account. However, the possibility that the morphology of the dust grains may play a role in conveying thermal and non-thermal phenomena has been poorly explored. Such grains are not expected to be flat and uniform. On the contrary, very porous and inhomogeneous features may characterise their morphology.

Here we want to single out the role of substrate morphology in defining the thermal desorption characteristics of ices condensed on dust grains. In particular, we report a Thermal Programmed Desorption (TPD) study of different gas species (Ar, CO, $CH_4$, $H_2$) on a prototypical porous material obtained by laser ablation of a copper substrate. In all the TPD spectra, a broad desorption component is observed, at higher temperature in respect to the desorption of the same species condensed on a flat substrate. This finding could imply the co-existence of condensed species on porous dust grains at temperatures higher than those usually considered. In addition, porous materials may show photon and electron yields different from those reported for their flat counterpart.

# Rotational excitation of $H_3O^+$ cations by $H_2$: towards new insight into water chemistry

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The hydronium cation ($H_3O^+$) has been detected in both dense and diffuse interstellar medium (ISM) [1]. It was shown by Sternberg *et al*. [2] that the $H_3O^+$ ion is one of the backbones of oxygen and water chemistry in the ISM. Accurate determination of hydronium in astrophysical media requires to model its excitation through radiations and collisions. While the spectroscopy of the $H_3O^+$ was intensively studied [3], there are only limited works devoted to its collisional excitation. The interaction of $H_3O^+$ with He atoms (as a template for $H_2$) was recently studied [4], while for modelling the collisions involving hydronium ions the corresponding data of the isoelectronic $NH_3$ were also used [5]. Nevertheless, accurate rate coefficients for the $H_3O^+$ – $H_2$ collision are obviously required.

We have studied the rotational excitation of hydronium by $H_2$ molecules. For first, we present an accurate 5D potential energy surface for this system. Then the calculated rotational state-to-state cross sections and rate coefficients will be presented in a wide collision energy and temperature range.

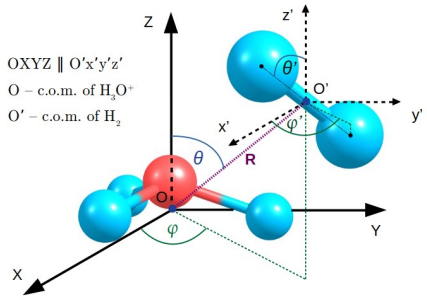


Figure 1 : The coordinate system used to study the $H_3O^+$ – $H_2$ collision

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# Dust evolution in the Horsehead Nebula

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Dust plays a crucial role in numerous physical and chemical processes in the interstellar medium (ISM). Variations of physical conditions in the ISM (i.e. particle density and radiation field) trigger evolution of the dust properties (i.e optical properties, abundances, size distribution, composition) which strongly impact the gas. It is therefore important to understand how dust evolves with the local environment.

We study dust evolution, through its emission and scattering properties, in nearby photon-dominated regions (PDRs) where the physical conditions vary widely but can be spatially resolved. We focus on the Horsehead Nebula a well-known PDR, which has been extensively studied. This moderately excited PDR (radiation field intensity corresponding to G0 ~100) has a nearly edge on geometry well suited to follow the impact of photons on dust grains, while the density increases towards the interior of the cloud. Furthermore, observations from the Herschel Space Observatory together with those from the Spitzer Space Telescope and the Hubble Space Telescope are available and provide us with a wealth of spatial and spectral information of dust and gas emission from the mid-IR to the submillimeter spectral ranges. To model the dust emission and scattering across this PDR, we use the THEMIS dust model [1], included in the dust physics numerical tool DustEM [2]. A 3D continuum radiative transfer code, SOC [3], is then used to assess dust emission and scattering at different positions inside the PDR. Considering first dust populations from the diffuse interstellar medium [1] with fixed abundances across the cloud we show that the short and long wavelength dust emission cannot be simultaneously matched [4].

We propose the following scenario. In the Inner part of the Horsehead, the grains are aggregates with or without ice mantles and are grains typical of dense clouds environment [5]. The radiative feedback of the binary stars on the Horsehead edge photo-processes the coagulated grains into smaller grains, similar to those of the diffuse ISM. However, the typical time-scale during which grains are photo-processed must be shorter than the typical time-scale associated with the photo-fragmentation of aggregates into smaller grains. Hence, small grains containing aromatic cycles does not have time to form which explains why the abundance of these grains is lower than in the diffuse ISM. Also, the increase in the minimum size of these grains may suggest that the smallest of these grains are photo-destructed and/or they don't have time to form from photo-fragmentation of larger grains. The slope steepening of the power-law size distribution of these grains may suggest that photo-fragmentation of aggregates leads to the creation of small grains instead of large grains [4].

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# Complex organic molecules in accretion shocks around a high-mass protostar

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The process of star formation gives rise to an increased molecular richness of the collapsing dense gas which sets both the physical and the chemical initial conditions for planet formation. While a large variety of molecules have been observed towards hot molecular cores surrounding emerging high-mass (proto)stars, the origin of the observed molecular composition and diversity is poorly constrained.

High angular resolution observations with ALMA revolutionize our understanding on where and how complex organic molecules emerge in the vicinity of stellar embryos. At the same time, large bandwidth observations immediately reveal the molecular composition of the gas. I will present results on the molecular composition of high-mass protostellar envelopes from the SPARKS project, which reveal in great detail the structure of the envelope surrounding a precursor of an O4-O5 type star. Detailed studies with ALMA and APEX allow us to study the structure of the envelope, determine its molecular composition and pin down the origin of various molecules, including COMs, within the different components of the envelope. Using LTE modelling we identify molecules, including 10 COMs towards two positions of accretion shocks and a position representing the bulk emission of the inner envelope. A quantitative comparison of molecular abundances shows a significant difference in their distribution: O-bearing COMs show a higher abundance towards the accretion shocks with a kinetic temperature $\sim$180 K, while N-bearing COMs with a CN group peak toward the central position, thus on the protostar and the accretion disk. The molecular composition seems to be significantly different towards the inner envelope suggesting an increase in abundance of O-bearing COMs towards the accretion shocks. The larger sample of young high-mass protostars revealed by the SPARKS project suggests that the observed accretion induced changes in the molecular composition of the gas may not be unique to this object.

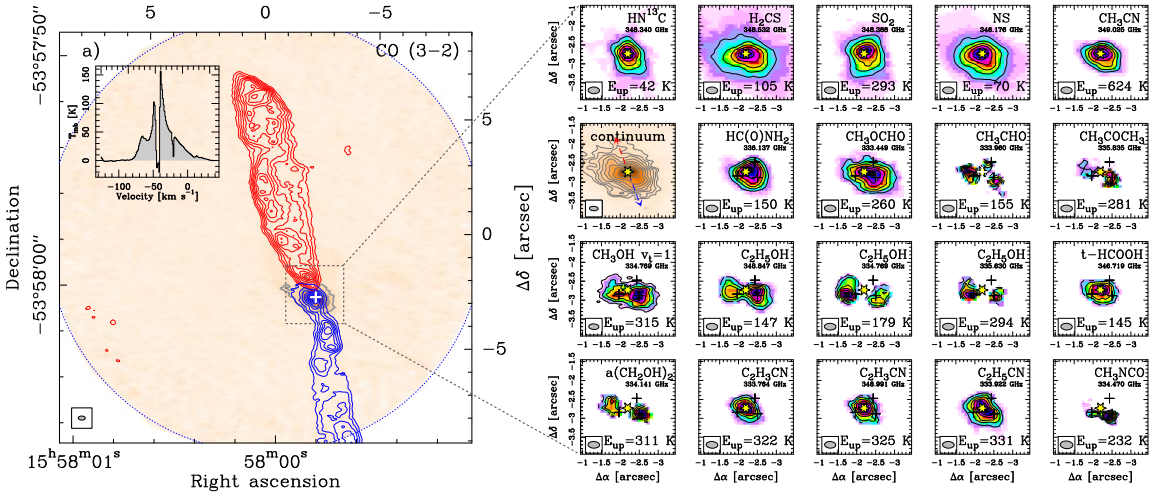


Figure **1** : View on the protostar embedded in the G328.25 clump. The left panel shows the 345 GHz continuum emission with ALMA and the molecular outflow is shown in blue and red contours. The inset shows the integrated CO (3-2) emission. The right panel shows a zoom on the inner region of the envelope, where several molecules are detected. Of particular interest is the different spatial distribution of O- versus N-bearing COMs.

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# A statistical analysis of dust polarization properties in ALMA observations of protostellar cores

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With the aim of characterizing the role played by magnetic fields in the formation of young protostars, several recent studies have revealed unprecedented features toward high angular resolution ALMA dust polarization observations of Class 0 protostellar cores. Especially, the dust polarization has been found to be interestingly enhanced along the cavity walls of bipolar outflows, which are subject to high irradiation from the reprocessed radiation field emanating from the central protostar. In addition, highly polarized dust thermal emission has been detected in region most likely linked with the infalling envelope within the equatorial plane, in the form of filamentary structure being potential magnetized accretion streamer. These observations allow us to investigate the different physical processes involved in the Radiative Alignment Torques (RATs) acting on dust grains from the core to disk scales. Notably, we propose that the polarized emission we see at millimeter wavelengths along the irradiated cavity walls can be reconciled with the expectations of RAT theory if the aligned grains present at < 500 au scales in Class 0 envelopes have grown larger than what is typically expected in young protostellar cores. To improve our understanding of the physical processes involved in the efficiency of dust alignment in a protostar, we gathered all the available ALMA dust polarization observations of Class 0 protostars, and performed a statistical analysis examining the trend between the dispersion of polarization position angles and the fractional polarization. Our results allow us to constraint the characteristics of the magnetic field at the protostellar core scales via comparisons performed with respect to previous results that Planck presented for the diffuse ISM and molecular clouds. We find a robust correlation allowing us to investigate a potential variation of the grain alignment efficiency toward a prototypical Class 0 protostellar core. Moreover, we compare these results with synthetic observations of POLARIS onto non-ideal MHD simulations of collapsing protostars. We compare the correlations derived from the simulations and detailed the impact that both, filtering and the dust grain alignment characteristics put into POLARIS, have on the statistics we developed. Our recent work, that makes use of statistics derived from ALMA dust polarization observations and synthetic observations of numerical simulations, allows us to better characterize the principal causes responsible for the grain alignment characteristics within a protostellar core.

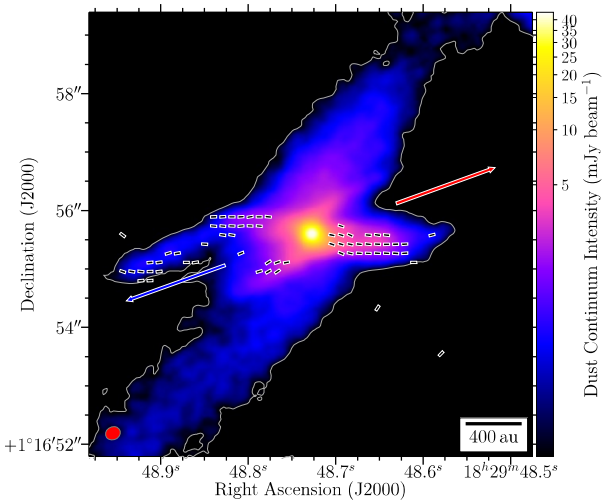


Figure 1: Magnetic field around Serpens Emb 8(N). Line segments represent the magnetic field orientation. The color scale is the total intensity (Stokes I) of the thermal dust emission. The blue and red arrows represent the directions of the blueshifted and redshifted lobes of the bipolar outflow, respectively. The polarized emission is clearly enhanced along the outflow cavity walls visible in the dust thermal emission.

# **Electron induced reactivity of molecular cations:** from mechanisms to new state-to-state cross sections and rate coefficients

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Electron-impact dissociative recombination, rovibrational (de)excitation and dissociative excitation of molecular cations are at the heart of molecular reactivity in the interstellar media and early Universe [1], being a major charge destruction path, and producing often atomic species in metastable states un-accessible through optical excitations.

These processes involve super-excited molecular states undergoing predissociation and autoionization, having thus strong resonant character. We use methods based on the Multichannel Quantum Defect Theory [2] and R-matrix theory [3], capable to account for the strong mixing between ionization and dissociative channels, open - direct mechanism - and closed - indirect mechanism, via capture into prominent Rydberg resonances [3] correlating to the ground and excited ionic states, and for rotational effects. These features will be illustrated and extensive data will be shown for several cations of high astrophysical and planetary relevance such as $H_2^+$ and $HD^+$[4], $CO^+$ [5], $SH^+$ [6], $CH^+$ [2,7], $N_2^+$ [8], $ArH^+$[9], and polyatomic systems like $HCO^+$, $N_2H^+$ [2], $CH_2NH_2^+$ [10] and $NH_2CH_2O^+$ [11]. Comparisons with other existing theoretical and experimental results will be given, and perspectives on the advancement in the theoretical treatment - addressing polyatomic systems, predicting branching ratios - will be outlined.

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# The chemical complexity of the solar-type protostar IRAS 16293-2422

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Star-forming regions are known to be chemically rich. A lot of complex organic molecules are detected in these objects. Some of these molecules could have played a role in the emergence of life. Indeed, they could have been incorporated into comets and asteroids before being delivered into Earth through impacts. Large unbiased spectral surveys are ideal to fully characterize the molecular content of star-forming regions. With the arrival of the Atacama Large Millimeter/submillimeter Array (ALMA), the sensitivity has significantly improved and many new species have been detected. These new detections provide important constraints on the chemistry of the early stages of the star formation process.

The solar-type protostar IRAS 16293-2422 is considered as a reference for astrochemical studies. It has been the target of a large spectral survey with ALMA in the framework of the PILS program ([1]), which led to important results, with for example, the first determination of isotopic ratios of several complex molecules (D, $^{15}$N, $^{13}$C) (e.g., [1], [2]). This presentation will focus on some of the most recent results obtained with the ALMA/PILS survey: the first detection of nitrous acid (HONO) in the interstellar medium ([3]) and the first detection of the 3-carbon molecules propenal ($C_2H_3CHO$) and propene ($C_3H_6$) towards a low-mass protostar ([4]). These observations were compared with a gas-grain chemical model developed in Bordeaux in order to determine the formation mechanisms of these species.

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# Organic molecules in the disks surrounding Fu-Ori objects

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One of the major problem in Astrochemistry is whether the organic chemistry during the star and planet formation process is inherited by planets and small bodies of the final planetary system. The formation of planets and comets occurs through the combination of dust and gas lying within the disks surrounding young stars. Among the molecules found in comets, some of them have also been detected in the interstellar medium (ISM). Although expected to be present in protoplanetary disks, the so-called prebiotic molecules have not been detected in those objects yet. This leads one to ask whether these molecules were altered or formed in the protosolar nebulae or whether they are of direct ISM heritage.

In that context, there is a specific class of disks, the ones surrounding Fu-Ori objects [see e.g. 1]. These objects are subject to episodic outbursts, a phenomenon which leads ices to sublimate and, therefore, make it possible the observation of the grain mantle molecular content [see e.g. 2] . The recent progress in the (sub-)millimeter instrumentation (high angular resolution, high sensitivity and large bandwidth), such as with ALMA and IRAM/NOEMA, has lead to an unprecedented capacity to study Fu-Ori objects. I will review and present some notable results on the detection of organic molecules towards the disk surrounding V883, in particular those recently obtain through observations performed with IRAM/NOEMA [3].

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# Rate coefficients for the CO + OH reaction at low temperatures – implications for interstellar chemistry

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The reaction between CO and OH, to form $CO_2$ and atomic H, has long been studied at higher temperatures due to its importance in atmospheric and combustion chemistry. While both CO and OH are abundant in the cold interstellar medium, the gas-phase reaction is assumed to be too slow [1] to be an important source of interstellar $CO_2$. Recent work [2] has shown that reactions involving the OH radical can become faster at low temperatures thanks to the formation of pre-reactive hydrogen bonded complexes, which are known to exist in this reaction. In addition, $CO_2$ ice is one of the most abundant ice components after $H_2O$ and its abundance cannot be explained by gas-phase $CO_2$ formation and freeze-out. Infrared ice observations in star-forming regions indicate that $CO_2$ is primarily found embedded in $H_2O$ ice [3]. The coincidence of $CO_2$ and $H_2O$ ices can be explained if $CO_2$ ice is primarily formed via the reaction between CO and OH [4]; however, the efficiency of this reaction in ices strongly depends on the magnitude of its multiple reaction barriers, and gas-phase measurements at low temperatures enable strong constraints to be placed on these important quantities [5]. Here, we report low temperature rate coefficients for the CO + OH ($v$ = 0, 1) reactions down to ~30 K, which are measured using the CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme) technique coupled with pulsed laser photolytic generation and laser induced fluorescence (LIF) detection of the OH ($v$ = 0, 1) radicals. Implications of these results for the potential energy surface of the CO + OH reaction, and its role in the interstellar gas-phase and surface chemistry will be discussed.

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# The gas composition, excitation and physical state in the debris disk surrounding 51 Oph

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If a central star is hot enough to provide a spectrum in the ultraviolet, an opportunity is presented to detect with great sensitivity various atomic and molecular constituents in the circumstellar medium. I will present our analysis of 305 absorption features from 25 different elements in a total of 108 energy levels in the UV and visible spectra of 51 Oph, a Herbig B9.5 star which is known to have a debris disk with a high inclination.

We interprete the relative populations of atoms in excited fine-structure and metastable levels in terms of optical pumping and collisional excitation by electrons in the disk and we found that most of the gas is situated at about 6 AU from the star, with an electron density of $[10^5 – 3\ 10^6]$ $cm^{-3}$ and a temperature T = 8000 K. The gas has N(H I) = $10^{21}$ $cm^{-2}$, it is partly ionized and has a composition similar to a mildly depleted ISM.

With a broader team and the development of new tools supported by PCMI, we are undertaking the analysis of absorption spectra of a couple of other stars presenting debris disks. I will present preliminary results of their gaseous constituents.

# Deuteration of glycolaldehyde via gas-phase reactions: A computational approach.

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The question of the formation mechanisms of interstellar Complex Organic Molecules (iCOMs) in the interstellar medium (ISM) is a main issue in the field of prebiotic chemistry. More particularly, glycolaldehyde is an important species, especially because it is the simplest sugar-related compound, and detected in Solar-like star forming regions.

In this context, the deuteration ratio between a mother and daughter species can be a powerful tool to confirm or disprove a type of reactivity and a reaction path [1]. In the case of gas-phase reactions, the reactivity and kinetics involving deuterated species can be very different than the one involving the same undeuterated compounds. It is therefore important to study the deuterated reactions themselves, since no parallel can be made with their undeuterated counterparts, as shown in Skouteris et al. 2017 [2] for the case of formamide.

The recent detection of deuterated glycolaldehyde in IRAS 16293-2422 [3] makes it another iCOM for which observations can be used to discriminate its chemical origin. Specifically, Skouteris et al. 2018 [4] proposed that glycolaldehyde is formed via gas-phase reactions starting from ethanol. In this contribution, we report a composite density functional theory (DFT) and ab-initio quantum chemistry study of the "ethanol-to-glycolaldehyde" gas-phase reaction involving the respective deuterated isotopologues. The comparison of our predictions based on the new theoretical rates with the observations favors a gas-phase synthesis of glycolaldehyde starting from ethanol.

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# Collisional excitation in CO-CO system

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Accurate determination of the physical conditions in comets can be inferred from the modeling of molecular spectra. In such environments, density can be so low ($n << 10^{10}$ cm$^{-3}$) that we cannot maintain Local Thermodynamical Equilibrium (LTE) [1]. Because of that, we need radiative and collisional properties of molecules to correctly interpret molecular spectra. Usually, in coma of the comets, the dominant species are water and the collisional excitation of molecules is mainly due to $H_2O$ molecules. However, in the case of the comets at large heliocentric distances, production of the CO gas is much larger than production rate of $H_2O$ and so that collisional excitation of molecules is mostly induced by CO molecules. Accurate collisional data implying the CO projectile is still missing because they are highly challenging to compute. Here, we present new accurate rate coefficients for the collisional excitation induced by CO molecule. The collisional system studied is the prototypical CO-CO van der Waals complex. Accurate determination of the rates coefficients will allow us to precisely define abundance of the CO in the comets.

We present a new calculation of the CO-CO system using an existing potential energy surface. Even with extremely developed computing techniques in recent years, it was unrealistic to perform exact calculations for this system. We combine approximate quantum treatment with innovative statistical methods in order to generate a reliable sets of collisional data. Collisional rate coefficients are provided for rotational levels up to $j = 10$ and for temperatures up to 200K. While the new results were compared with the partially converged results of Ndengue et al. [2], significant differences were found, especially for the dominant transitions. The impact of these new data of the astrophysical modeling is also discussed.

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# Combination of Ka band chirped pulse spectrometer with uniform supersonic flows for cold reaction dynamics studies

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Numerous chemical processes taking place in the interstellar medium, specifically in molecular clouds where the temperature ranges from 5 to 100 K, are being studied in the Institut de Physique de Rennes. The CRESUCHIRP project is an ERC research programme to combine the CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme, or Reaction Kinetics in Uniform Supersonic Flow) technique for studying collisional processes in the gas phase at very low temperatures with the chirped pulse Fourier transform micro/mm-wave (CPFTMW) spectroscopic technique[1] in order conduct kinetics measurements (rate constants and branching ratios) of cold chemical reactions in a system termed CPUF[2] (chirped pulse in uniform supersonic flow). For this project, a new CPFTMW spectrometer has been built to operate over the Ka-band (26.5-40 GHz). The performance of the spectrometer has been benchmarked with studies of the astrochemically relevant molecules carbonyl sulfide, vinyl cyanide and benzonitrile at room temperature and in cold CRESU flows down to 16 K. Although CPFTMW is very well suited for studying cold chemical reactions, the sensitivity of the technique is reduced by collisional broadening induced by the high density CRESU flows, therefore, reducing the collisional frequency rate is critical. Two different methods are being developed to achieve this, first is the use of a pulsed Laval nozzle to increase the effective pumping capacity of the system, the second is via molecular beam sampling with the use of a skimmer to create a secondary expansion at lower pressures. The latest results from these experiments will be presented.

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# The astrochemical link between Sun-like protostars and Solar System comets

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How the chemical complexity evolves during the process leading to the formation of a Sun and its planetary system? Is the chemical richness of a Solar-like planetary system (partially) inherited from the earliest stages or there is a complete chemical reset? A powerful way to start answering these questions is by comparing the observed astrochemical content in young protostars with that in comets, i.e. with the most pristine known material from which our Solar System formed. Protoplanetary disks observations suggest that planets and comets could start to form earlier than previously thought. For this reason evolved Class I protostars are the perfect laboratory where to study the initial conditions and the chemical content of planetesimal formation.

I will present a chemical systematic study of a few Class I sources obtained in the framework of three IRAM and ALMA Large Programs: ASAI [4], SOLIS [5] and FAUST (stars.riken.jp/faust/fausthome.html). The different datasets offer the opportunity to sample the different spatial scales, from the infalling envelope (~ 10000 au) down to the planet formation region (~ 50 au). The derived molecular abundances will be compared with those measured in younger Class 0 protostars as well as with those obtained by the ROSETTA mission for the comet 67P (see Fig. 1). These new observations represent a first test of the inheritance scenario from the protostellar phase.

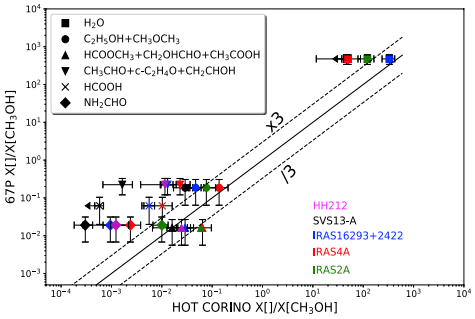


Figure 1 : Preliminary comparison between the chemical complexity of Class 0 and Class I protostars and the comet 67P (adapted from [2]). The present results will be updated in the light of the new SOLIS and FAUST observations.

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# The hunt for hot corinos and WCCC objects in the OMC-2/3 filament

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The protostellar stage is known to be chemically rich. Hot corinos, enriched in interstellar Complex Organic Molecules (iCOMs; e.g. - $CH_3OH$, $CH_3OCH_3$) [1][2], and Warm Carbon Chain Chemistry (WCCC) objects, enriched in hydrocarbons (e.g. CCH, c-$C_3H_2$) [3], are two extreme chemically distinct types of solar-mass protostars and are witnesses of this chemical diversity. Our Sun having been formerly a protostar, an obvious question is whether it experienced a hot corino phase, a WCCC phase or neither during its youth. In this context, we searched for hot corinos and/or WCCC objects in the OMC-2/3 filament, the nearest high- and low- mass star formation region, and the best-known analogue of our Sun's birth environment [4][5].

We first used single-dish observations of $CH_3OH$ and CCH, two species enhanced in hot corinos and WCCC objects respectively [3][6], to determine the chemical nature of nine protostars in OMC-2/3 and get a first census of hot corinos and WCCC objects in this region. Remarkably, we found that the molecular emission is dominated by the surrounding cloud/PDR, preventing us to determine whether hot corinos and/or WCCC objects are present in OMC-2/3. We are now investigating ALMA data allowing us to get rid of the external molecular emission. In this contribution, we will present our first results showing more robust indications about the chemical differentiation of the OMC-2/3 protostars.

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# Origin of the IMF and massive star binaries in W43

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W43-Main has been qualified as a "mini-starburst" region because of its high mass and exceptionnal star formation activity (Louvet et al. 2014). This extreme environment is an excellent laboratory to test star formation theories. Our group observed it with the world's largest submillimeter interferometer, ALMA (Motte, Nony, Louvet et al. 2018; ALMA-IMF Large Program). We showed that the mass distribution of cores (CMF) forming in one of its cloud, W43-MM1, does not follow the shape of the canonical IMF (Kroupa 2013). In contrast, in a more evolved W43 cloud we recently measured a CMF which is getting closer to the IMF shape. Our result suggests that the evolution of cloud structures strongly affects its core content and thus its CMF shape. The origin of the IMF could thus depend on the star formation environment, including cloud density and kinematics, more than we originally assumed.

In W43-MM1, we also discovered a clump harboring a binary system of protostars with masses ~50-100 M⊙ each. We speculate that we witness the formation of one of the most massive star binaries of our Galaxy.

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# Non-enzymatic metabolic reactions and life's origins

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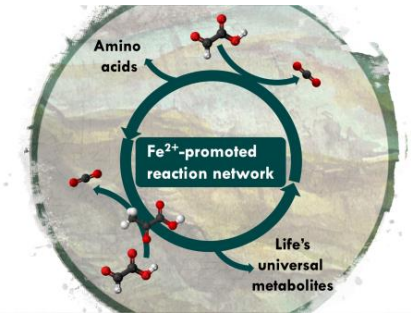
Life is governed by an intricate network of chemical reactions that make up metabolism. How the biochemistry of life as we know it came to be is studied by prebiotic chemistry. Lots of efforts in this area have focused on life's building blocks, often obtained in multi-step chemical syntheses [1]. However, focusing only on the molecular building blocks, rather than the processes that produce them, may have caused us to overlook what might be a fundamental feature of life. Why does life use the molecules, reactions, pathways and overall organization that it does? In this talk, I will present how the chemistry that led to life could have begun as a primitive non-enzymatic version of the biochemistry we know today, initially promoted by naturally occurring catalysts, for example geologically abundant iron-rich minerals and salts [2]. If it existed, such a reaction network would have built up and broken down life's chemical building blocks in much the same way as the pathways that do it today. The knowledge of processes and mechanisms that may have led to the emergence of life's core biochemical machinery is of paramount importance not only to the origins studies of life on Earth, but also to the search for life-like systems beyond our planet.

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# Absorption Spectroscopy of $C_{60}$ Fullerene at 1.7 μm

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Fullerenes have been discovered in various astrophysical objects first through their mid-infrared emission [1,2]. Their presence in diffuse clouds, under an ionized form, was later revealed through their electronic absorption signature. To date five DIBs have been assigned to $C_{60}^{+}$ [3,4]. Hints of fullerene and derivatives in the diffuse medium may be also lie in the near infrared region which corresponds to transitions involving several quanta of vibrations.

In this work we provide the first absorption spectra of neutral $C_{60}$ at 1.7 μm with tentative assignments [5]. This is the preparatory work of our low-temperature gas-phase NIR spectroscopy of $C_{60}$ that we intend to perform using a cavity ringdown spectrometer coupled to a hypersonic flow [6]. Only the comparison of astronomical data with gas-phase spectra can decisively identify the carriers of diffuse interstellar bands.

Absorption spectra of neutral $C_{60}$ have been recorded over the 1.65-2.78 μm wavelength range in the solid-phase by embedding in KBr pellet from 11 to 300 K using the ESPOIRs setup in Toulouse [7]. Observed bands were assigned to various 4 quanta combination modes using scaled harmonic force field analysis. Complete group theoretical analysis was performed to find the symmetry of all combination modes.

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# Cross sections for vibronic excitation and dissociative recombination of $CH^+$ by low-energy electron impact

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A theoretical approach for the electron-impact vibronic (de-)excitation and dissociative recombination of molecular ions with low-lying excited electronic states is described. In this approach, the fixed-nuclear R-matrix method is employed to compute electron-ion scattering matrices in the Born-Oppenheimer approximation. A vibronic frame transformation and the closed-channel elimination procedure in a spirit of molecular quantum defect theory are employed to construct an energy-dependent scattering matrix describing interactions between vibronic channels of the target ion induced by the incident electron. The obtained scattering matrix accounts for Rydberg series of vibronic resonances in the collisional spectrum. The approach is applied to $CH^+$ ion of an astrophysical and technological interest. Cross sections for vibronic (de-)excitation for different combinations of initial and final vibronic states (see figure 1) and dissociative recombination are computed. A good agreement between electronic-excitation cross sections, obtained using the quantum defect theory and in a direct R-matrix calculation, demonstrates that the present approach provides a reliable tool for determination of vibronic (de-)excitation and dissociative recombination cross sections for targets with low-energy electronic resonances. Such targets were difficult to treat theoretically using earlier methods.

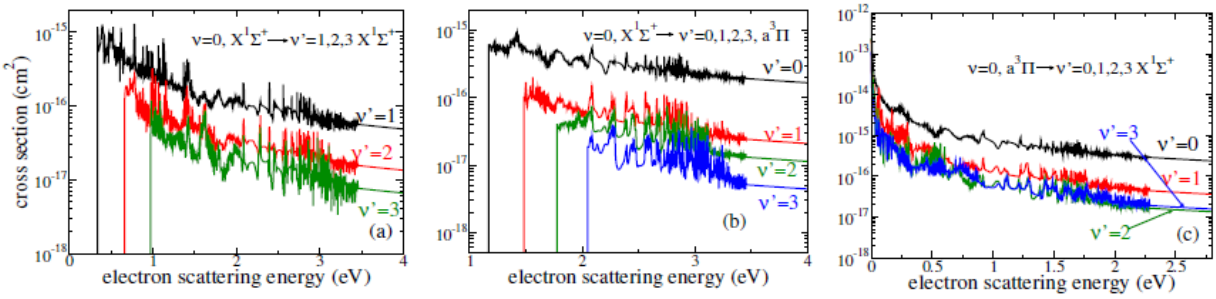


Figure 1 : Cross sections for vibronic excitations of $CH^+$ from the ground vibrational level v = 0 of the $X^1\Sigma^+$ state to v = 1, 2, 3 of the $X^1\Sigma^+$ state (left panel) , to v = 0, 1, 2, 3 of the $a^3\Pi$ state (middle panel), and for vibronic de-excitations from the ground vibrational level v = 0 of $a^3\Pi$ to v = 0, 1, 2, 3 of the $X^1\Sigma^+$ state (right panel).

# Determination of branching ratios for chemical reactions of astrophysical interest at cold temperatures using the Chirped Pulse in Uniform Flow (CPUF) technique

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The CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme, or Reaction Kinetics in Uniform Supersonic Flow) technique, combined with laser photolysis methods, has been used for years to the measure gas-phase chemical kinetics at low temperatures, related to astrophysical environments [1]. While overall rate constants have been measured at cold temperatures, product branching remain difficult to determine experimentally. To address this, the CPUF (Chirped Pulse in Uniform supersonic Flow) technique was recently developed [2] combining CRESU flows with chirped pulse Fourier transform spectroscopy, in order to measure the branching ratios of chemical reactions at cold temperatures.

We have designed and built a new E-band microwave spectrometer operating between 60-90 GHz to study product formation within the Rennes CRESU apparatus. This uses chirped pulse microwave (millimeter wave) spectroscopy to detect a wide variety of molecules toward measuring branching ratio of reaction of astrophysical interest. The experimental setup and challenges of these experiments will be discussed. Initial results towards measuring reaction product between CN radicals and simple hydrocarbon at cold temperatures (down to 16K) will be presented, as well as study of photolysis products from vinyl cyanide photodissociation. Future development and directions of the instrument will be discussed.

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# From filaments to dense cores with Herschel, ArTéMiS, ALMA

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The origin of the stellar initial mass function (IMF) is one of the most debated issues in astrophysics. I will discuss new insights into this problem based on a systematic census of prestellar cores and molecular filaments in nearby clouds taken as part of the Herschel Gould Belt survey, as well as higher-resolution observations with APEX/ArTéMiS and ALMA. Our Herschel findings support a filament paradigm for solar-type star formation, whereby Jeans-type fragmentation of 0.1-pc wide « supercritical » filaments produces < 0.1 pc prestellar cores, which subsequently collapse to "core-fed" protostars [1,2,3,4]. They suggest that the dense cores making up the peak of the prestellar core mass function (CMF) - and indirectly the peak of the IMF - result from gravitational fragmentation of molecular filaments near the critical mass per unit length [5]. The origin of the Salpeter power-law tail of the CMF/IMF is more uncertain. On one hand, our ArTéMiS and ALMA results suggest that denser filaments form more massive cores, thus probably more massive protostars, and that the high-mass end of the CMF/IMF may be directly inherited from the Salpeter-like power-law distribution of filament masses per unit length observed with Herschel [5,6]. On the other hand, there is a growing body of evidence that massive prestellar cores may not exist and that high-mass protostars may be "clump-fed'', gathering mass from parsec-scale "hub-filament" structures [7]. In an effort to clarify where and how the transition between a "core-fed" and a "clump-fed" regime of protostellar mass growth occurs, we have initiated a large program (CAFFEINE) with ArTéMiS on APEX, whose current status will be briefly described.

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# Extrema of dissipation in MHD turbulence

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Turbulence is known to play a fundamental role (star formation process, molecular abundances, self-similarity of molecular cloud...) in the interstellar medium. The lack of exact mathematical description and the impossibility of simulations to reproduce the full inertial range, between injection and dissipation scale makes its role hard to grasp. Although we know turbulence is ubiquitous.

In the present study, we choose to probe the turbulent dissipation with compressible isothermal simulations of decaying MHD turbulence, that take unprecedented care at resolving and controlling dissipation. An essential facet of turbulence is the intermittency of the cascade that leads to coherent structures of high dissipation. We found these structures correspond to nearly planar regions, i.e. density, velocity and magnetic fields vary mostly across one direction. The orientation of these planar structures seems to be strongly correlated with the direction of the local magnetic field. We link these highly dissipative regions to fast/slow shocks and magnetic discontinuities (Parker sheets, rotational discontinuity...). Our results show that most structures we find in simulations correspond to these classes. The relative dissipative weights of these processes strongly depend on the initial flow until one turnover time.

# Planck/Herschel analysis of correlations between filamentary structures and magnetic fields in star forming regions

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Pre-stellar cores form in the dense interstellar medium, mostly within filamentary structures. Magnetic fields are believed to play a key, albeit poorly understood, role in the whole sequence of structure formation, from interstellar filaments down to stars. It is, therefore, instructive to study the correlation between magnetic fields and filaments hosting cold cores in star forming regions under various conditions (ambient density, star formation efficiency, and core evolutionary stage). This can be investigated by combining column density maps from Herschel with magnetic field orientation maps from Planck. For this purpose, we have developed a method, based on an improvement of the Rolling Hough Transform code[1], for the detection and extraction of filamentary structures. This new method allows us to analyse the relative orientation[2] between filaments and the local magnetic field over a broad range of density, from striations to dense filaments. We present the results obtained for a sample[3] of Herschel fields from the 'Galactic Cold Cores' project, probing different Galactic environments. In order to separate the different emitting components in a given field and locate them along the line of sight, we use $^{12}$CO[4] and HI[5] (l, b, v) cubes, as well as dust extinction[6] (l, b, d) cubes. We also investigate whether the star formation efficiency is linked to the relative orientation between filaments and the local magnetic field.

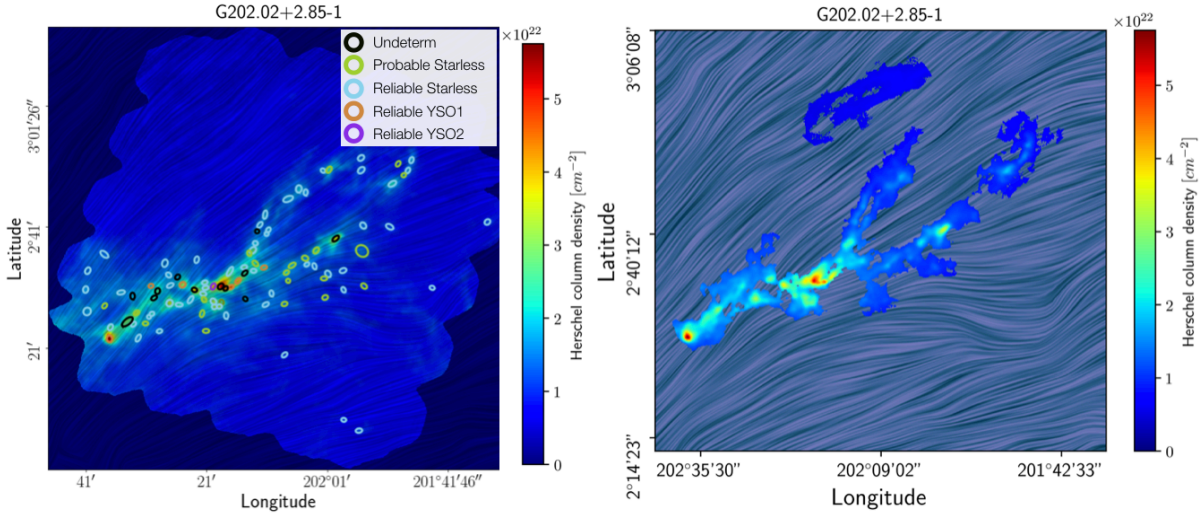


*Figure 1 : Example of the G202 field showing the Herschel column density together with the Planck magnetic field orientation. Left: cores at different evolutionary stages[7]. Right: filaments extracted with our new method.*

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# Ionization fractions in the local diffuse ISM

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We have combined the particularly comprehensive collection of interstellar absorption features observed in the far-UV spectrum of the closest (d=24 pc) B star alpha Leo with a model for the partial ionization of various atomic species in diffuse gas, to describe the ionization fraction of atoms in the local ISM (Gry & Jenkins 2017).

The electron density ($n(e) = 0.11 \pm 0.03$ cm$^{-3}$) and the temperature ($T = 6500 \pm 700$ K) are derived from the combined observation of two equilibria: Mg ionization and $C^+$ fine-structure excitation.

The equilibrium ionization fractions result from balancing the effects of radiative and dielectronic recombination with free electrons against ionization rates due to the EUV and X-ray radiation fields and charge exchange reactions, following equations outlined by Jenkins (2013).

The partition of $N(H_{tot})$ into 2/3 $N(H^0)$ and 1/3 $N(H^+)$ is derived from the observed ionization fraction of nitrogen $N(N^0)/N(N_{tot}) = 0.6$ combined with our photoionization model for hydrogen and our knowledge of n(e). This yields a total hydrogen density of $n(H_{tot}) = 0.3$ cm$^{-3}$ and $n(H^0) = 0.2$ cm$^{-3}$.

From the ionization model, we compute the ion fractions for 10 atomic species:

| | $Log(X^0/X_{tot})$ | $Log(X^+/X_{tot})$ | $Log(X^{++}/X_{tot})$ | $Log(X^{3+}/X_{tot})$ |
|---|---|---|---|---|
| H | −0.17 | −0.48 | | |
| He | −0.28 | −0.33 | −1.75 | |
| C | | −0.15 | −1.46 | −6.02 |
| N | −0.22 | −0.40 | −3.54 | |
| O | −0.15 | −0.52 | −3.77 | |
| Mg | | −0.16 | −0.52 | −5.56 |
| Si | | 0.00 | −4.60 | −8.36 |
| S | | −0.05 | −1.00 | −5.33 |
| Ar | −0.81 | −0.07 | −4.29 | |
| Fe | | 0.00 | −3.03 | −6.43 |

The elements Si, S, and Fe have ion fractions near unity for their preferred stages of ionization. The elements C, N, O, Mg and Ar in contrast have significant concentrations in higher ionization levels. We note that He is always more ionized than H.

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# Empirical Constraints on Cosmic Dust Evolution Parameters

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Understanding how dust is formed from the heavy elements ejected by evolved stars, and subsequently processed in the interstellar medium (ISM), through successive waves of star formation, is a key to deciphering galaxy evolution. It is also necessary in order to design accurate diagnostics, as a changing dust composition biases our estimates of the extinction, photoelectric yield and chemical surface area, at a given time. The modeling of cosmic dust evolution, at the scale of a galaxy, relies on several uncertain parameters: (i) the average dust condensation e ciency in stellar ejecta; (ii) the average grain growth e ciency in the ISM; (iii) the average dust destruction rate by supernova shock waves. Both theoretical and observational attempts at constraining these parameters from detailed studies of each isolated processes have led to inconsistent estimates that can span several orders of magnitude.

I will present a study tackling this problem empirically, with a statistical approach. We have used the recent estimates of the dust, gas and stellar masses, as well as the star formation rates and metallicities of 900 nearby galaxies, covering a large range of evolutionary stages. These estimates were derived with the hierarchical Bayesian dust SED model HerBIE [1], applied to the homogeneous DustPedia sample [2]. From these estimates, we have consistently inferred the star formation history (SFH) of each object, as well as the three parameters discussed above, using a dust evolution code [3]. We have provided not only a reliable estimate of these global dust evolution parameters, but also their uncertainties and correlations, and their dependency on the assumed initial mass function and on the functional form of the SFH. We are currently extending this analysis to a sub-sample of spatially-resolved objects with addition of NIKA2 millimeter observations, in preparation to SPICA.

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# The heating of the Interstellar Medium : Contribution of Polycyclic Aromatic Hydrocarbons Photoionization

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The role of photoelectrons resulting from the photoionzation of very small graphitic grains or PAHs, has been put forward since the early paper by B.T. Draine [1]. A number of other contributions discussing the photoelectric heating followed, among which: Verstraete et al [2], Bakes & Tielens [3], Weingartner et al [4], E. Habart et al [5]. These processes are also discussed in the context of the global dust spectral energy distribution (see Compiègne et al [6])

The ionization potentials (IP) of PAHs differ from a specific molecule to another, but their values remain in a limited range: from ~7 eV (for Nc > 40 Carbon atoms) to ~8 eV for Naphthalene (Nc=10). These values, remaining significantly below the Lyman cut-off at 13.6 eV, leave the possibility to create energetic photoelectrons. On the other hand the PAHs photoionization cross sections (usually considered to be proportional to the number of carbon atoms) get quite large near their maximum value (around 17 eV *id est* ~ 33 Megabarn per C-atom, see Verstraete et al [2]), so that a significant part of these species must be present in cationic forms. Consequently, an equivalent number of photoelectrons are created as a result from the photoionization events, the kinetic energy of which being determined by the final cation states, as: $KE = h\nu - (IP + E^i)$ where $E^i$ is the final vibronic energy of the cation. This kinetic energy KE of fast photoelectrons can then be transferred to any collision partner available in the local ISM. This whole process (Fast photoelectron production + Collisional energy transfer) is responsible for the so-called photoelectric heating of the ISM.

Thanks to the availability of the DELICIOUS3 set-up on the DESIRS VUV beamline at the SOLEIL synchrotron facility, we have conducted a systematic study to characterize in details the photoionization overall behavior of a series of nine PAHs, covering a broad range for the number of C-atoms (Nc =13 to 20) and differing in their structures (compact or not, presence of pentagons, methyl substituents, non-planarity). For a majority of them we have also obtained information on the dissociative ionization channels (from one to three H-losses).

It has been confirmed that the total VUV ionization yield (TIY) get to a maximum in agreement with the simple VUV absorption peak, which remains close to 18-20 eV for the parent PAHs, as well as for the dehydrogenated species. The slow photoelectron spectra (SPES) of the whole series of PAHs have allowed to distinguish in each case a structure of several bands, revealing the vibronic structures of the relevant cation excited states. Appearance energy potentials for de-hydrogenation (H-loss), as well as the vibronic structures of the corresponding product species, have been properly characterized. Some major results of this extensive study will be presented and discussed.

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# Ion reactivity with CRESU: insights into the chemistry of the interstellar medium

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Gas-phase ion-molecule reactions may play some role in the synthesis of large interstellar molecules. However, the nature of the products and the kinetics of ion-molecule reactions relevant for cold environments are not well known, in particular at low temperature. We have recently developed a unique approach to investigate the reactivity of ions. Our method relies on the implementation of a mass-selective source of ions on the uniform supersonic flow chamber (better known as the CRESU – Cinétique de Réaction en Ecoulements Supersoniques Uniformes) [1]. Our efforts first focused on the reactivity of $CH_2CN^+$ with four hydrocarbons: methane ($CH_4$), acetylene ($HC{\equiv}CH$), ethylene ($H_2C{=}CH_2$), and ethane ($H_3C{-}CH_3$) over the 36—300 K range. Branching ratios into the various exit channels were measured. We also explored the reaction of the molecular ion $N_2^+$ with propyne ($HC{\equiv}C{-}CH_3$). Our results will be discussed and preliminary conclusions drawn. Beyond the interstellar medium, our work may also have some implications for the chemistry of Titan's atmosphere.

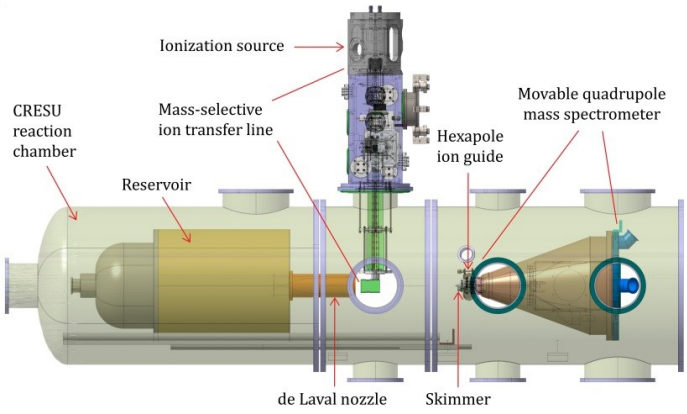


Figure 1: The CRESU reaction chamber incorporating the new mass-selective ion transfer line.

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# The protostellar collapse of a gas and dust cloud

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Dust grains are the building blocks of protoplanetary disks and planets. Dust regulates the thermal evolution of the disk through its opacity. In addition, it plays a major rôle in the coupling between the gas and the magnetic field, hence in the disk and jet formation. In observations, the polarized light emitted by the grains can be used to measure the magnetic fields orientation or to estimate the maximum grain size. Nevertheless the dust evolution remains poorly constrained during the early phases of star formation. The dependence of the drag force on the grain and gas properties can lead to a dynamical sorting, in particular for the large dust grains. Assumed to be uniform at low densities, the dust-to-gas can increase up to large values during the protostellar collapse that leads to the protostar and disk formation (Bate and Loren Aguilar 2017, Lebreuilly et al. 2019). I will present our dust dynamics algorithm (Lebreuilly et al, 2019) in the adaptive-mesh-refinement code RAMSES (Teyssier 2002) and first collapse and turbulent cloud simulations of gas and dust mixtures with a simultaneous treatment of multiple grains species of different sizes (Lebreuilly et al, in prep; Commerçon et al, in prep).

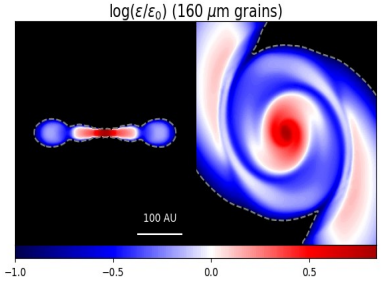


Figure 1 : Logarithm of the dust-to-gas ratio over the initial dust-to-gas ratio for a solar mass protostellar collapse 2 kyr after the first core formation.

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# Modeling the origin and chemistry of protostellar outflows: New insights from the IRAM-CALYPSO survey and ALMA

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Slow molecular outflows and high-velocity collimated jets are the earliest and most spectacular manifestations of the birth of a new star. They may actually play a fundamental role in star and planet formation : By removing angular momentum, they could facilitate accretion of keplerian material onto the growing star, and thus contribute to solve the angular momentum problem of star formation (Franck et al. 2014). Magnetized disk winds could also modify the disk structure, creating disk gaps and halting planet migration (eg. Suriano et al. 2019, Ogihara et al. 2018). Determining the exact origin of protostellar outflows is thus an essential step to build a complete picture of star and planet formation. The flow chemistry is an important tool to reach this goal, as it offers an indirect clue to the jet launch zone and dust content.

In the present contribution, we will review the results on jets and outflows from the IRAM-PdBI CALYPSO survey (see companion abstract by A. Maury) where a uniquely *large sample* of 24 outflows from the youngest protostars (Class 0/1) were mapped in CO, SiO, and SO. This survey gives for the first time a statistical view of the flow occurrence, chemical stratification, collimation, kinematics, and their correlation with the source properties (Podio et al. in prep ; Lefèvre et al. 2017). We will then present further constraints on the flow origin from high-resolution ALMA data in $^{29}$SiO and SO (Cabrit, in prep., Tabone et al. 2020b), and new chemical models of molecule formation in dust-poor disk winds (Tabone et al. 2020a), showing that SiO jets could trace disk winds launched within the dust sublimation radius.

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# Recent Advances in the Complex Chemistry of the ISM

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Complex Organic Molecules in the interstellar medium were defined by Herbst and Van Dishoeck (2009) as any organic molecules with 6 atoms or more. It is now well established that molecular complexity in that sense is already present at the very early stages of the star formation process.

In the past years, new molecular species have been discovered, some of which of prebiotic interest. Strong efforts are being made in close collaboration with theoretical and experimental chemists to constrain the possible formation and destruction pathways of these species, depending on the environmental conditions. Beyond (apart from) the detection of increasingly larger molecules, new results have been obtained which unveil a complex chemistry at work in the interstellar medium.
In this presentation, I will review the recent observational progress and the challenges in the exploration of this complex chemistry in the interstellar medium.

# Theoretical study of adsorption energies of small molecules on interstellar ice surfaces

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The adsorption energies of a series of atoms and small molecules (H, C, N, O, NH, OH, $H_2O$, $CH_3$, $NH_3$) on a model cluster of hexagonal crystalline ice have been calculated using a QMHigh/QMLow ONIOM method. Eight different sites with different dangling bonds were probed. The cluster size consists in 156 and 162 water molecules, with the QMHigh region containing 20 and 24 water molecules, respectively. Several basis sets (6-31G** and def2-TZVP), density functionals (wb97X-D and M06-2X) and semi-empirical methods (PM6 and PM7) have been employed. In some cases, the results will be compared to the ONIOM QM/MM results of Sammeera et al. [1,2].

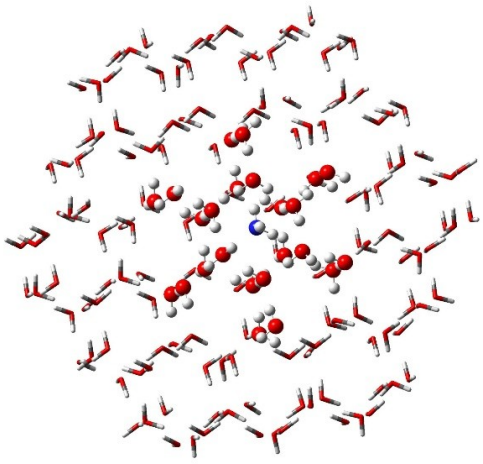

Figure 1 : $NH_3$ adsorption optimized geometry on ice surface

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# Chemical analysis of the Pirenópolis meteorite using non-destructive techniques

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This work is part of a project that intends to propose a protocol of analysis and characterization of the meteorites, so they can be fully characterized by most modern techniques accessible to researchers of the group. The specific objective of this work is to characterize the Pirenópolis, a poorly studied meteorite, by elemental analysis using PIXE (Particle Induced X-ray Emisson) and SEM (Scanning Electron Microscopy) techniques. Both techniques are very functional due to its non-destructive nature and multi- elemental analysis simultaneously, allowing the reuse of the meteorite for other purposes. The experiments were performed at Centro Atómico de Bariloche, in Bariloche, Argentina.

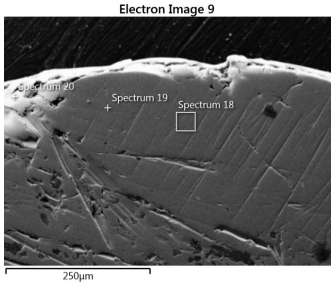


Figure 1 : Caption

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# Linking Galactic and Extragalactic Star Formation through Water Emission

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Observations of Galactic protostellar sources reveal that water vapor is almost uniquely associated with molecular outflows from the accreting stars. However, when we go to the extragalactic (high-z) regime, water emission is often associated with the giant molecular clouds in which the stars form, and not outflows as observed in the Galaxy. Thus, the question is, is water tracing a different component in extragalactic sources, or is it tracing the outflows as in Galactic sources?

To address that question, we perform a detailed statistical comparison of observed water transitions toward both regimes to provide a significant characterization of water emission. As part of this process, we are developing the Water Emission Database (WED) containing all available information on observed water emission toward Galactic and high-z sources. In this poster, I will present some preliminary results from this project.

# PAHs on/in water ice: structures, energetics and spectra from FTIR experiments and a multi-method theoretical study

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Polycyclic Aromatic Hydrocarbons (PAHs) have been proposed to be the carriers of the Aromatic Interstellar Bands (AIBs), a set of infrared (IR) emission bands observed in the [3 - 15 μm] range in many regions of the interstellar medium (ISM). In dense environments, PAHs are likely to condense onto or integrate into water ice mantles covering dust grains and to contribute to the complex grain chemistry [1]. Understanding the role of ice in the processes involving adsorbed PAHs is therefore a key issue in astrochemistry.

Our joint theoretical (classical molecular dynamics/force field simulations and SCC-DFTB calculations) and experimental (matrix isolation/solid phase FTIR spectroscopy) study has given rise to several conclusions, namely: the role of water clusters [2] and of the ice structure [3] on the photo-reactions of PAHs with water ice. We will present evidence of how the surface of amorphous solid water (ASW) is perturbed by the adsorption of PAHs [4] and a complete description of PAH-ice interaction in the ground electronic state at low temperature, providing the binding energies and barrier heights necessary to the on-going improvement of astrochemical models [5a]. The influence of ice on the ionization potential (VIP) of PAHs [5b] will be discussed, together with its astrophysical implications.

This work has been supported by ANR, PN PCMI, and GDR EMIE.

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# Density Functional Theory for Radio Spectrum Simulations of Interstellar Organic Molecules

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In the field of observational astrochemistry, rotational spectroscopy is majorly employed to unveil the chemical composition and evolution of astrophysical environments. In special, the Interstellar Medium (ISM) is known for its chemical lavishness, with radiofrequency line detections of more than 200 species including small hydrocarbons, molecular radicals and a plethora of Complex Organic Molecules (COMs) to date. In this context, quantum chemistry is a powerful tool to the investigation of the molecular inventory of astrophysical environments.

In this work, Density Functional Theory (DFT) calculations of spectroscopic parameters of astrochemically relevant species followed by rotational spectra simulations were performed, aiming to further contribute to the assignment and interpretation of radio spectra from the ISM. Case studies encompass both symmetric, quasi-symmetric and asymmetric tops, such as $H_2CO$, HCOOH, $H_2CS$ and $CH_3CN$. Spectroscopic parameters' predictions were comparable to state-of-the-art methods[1], with errors of less than 1% for zeroth order and ~5% for first order constants, thus yielding accurate spectral simulations with much less computational effort (i. e. Figure 1). Additionally, the rotational spectra of acetonitrile ice radiolysis products were predicted with an estimated uncertainty of around 100 MHz.

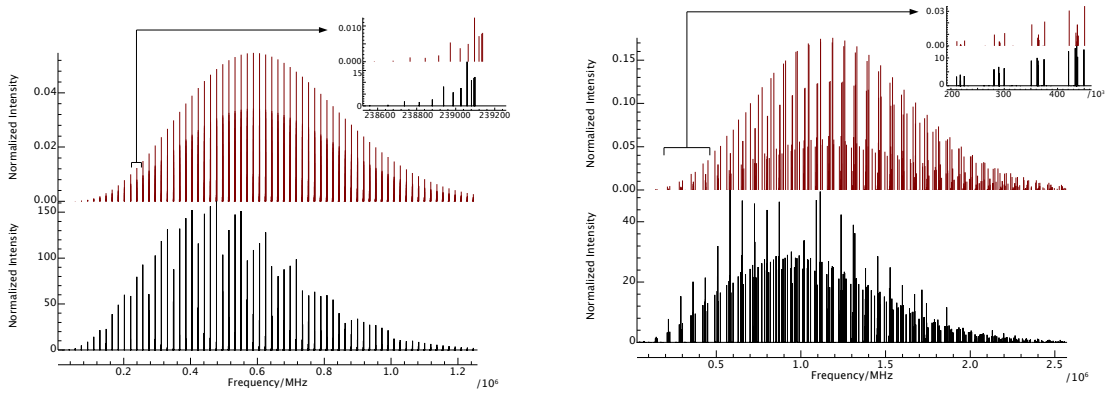


Figure 1: Experimental (red) and simulated (black) microwave spectra of $CH_3CN$ (left) and $H_2CO$ (right).

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# Variability of the Proton-to-Electron Mass Ratio from Splittings in the Molecular Spectra

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The cosmological variability of the fundamental constants in function of the look-back time, the local gravitational field or the local density of matter was addressed in modern theories [1]. The molecular spectra in the microwave domain provided a testground for astrophysical searches for a variation of the proton-to-electron mass ratio constant $\mu$. Narrow molecular lines with enhanced sensitivity coefficients to a variation of $\mu$ allowed to constrain a variation of $\mu$ at the $10^{-7}$ level [2].

This contribution proposes an approach to constrain $\mu$ from frequency splittings between the microwave and millimeter-wave transitions of CO [3], LiH [4] and $NH_3$ [5] detected in the spectra of the B0218+357 quasar at z=0.68 redshift. The rotational energy levels of CO and LiH are expressed in the form of the semiempirical expansion of Dunham. That allows to calculate the sensitivity coefficients to a variation of $\mu$ and their uncertainties for splittings between the rotational transitions [6]. The linear adjustment of the $NH_3$ inversion transitions (J,K)=(1,1), (2,2), and (3,3), and of the frequency intervals between the isotopic CO J=1->2 rotational transitions to the LiH J=0->1 transition allows to constrain $\Delta\mu/\mu=(5.1\pm3.7)\times10^{-6}$, as shown in Fig. 1.

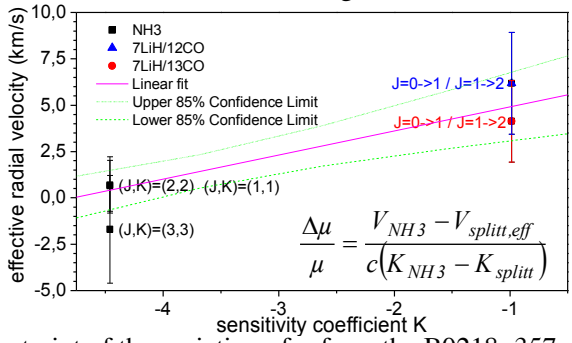


Figure 1 : Constraint of the variation of $\mu$ from the B0218+357 quasar spectra

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# Rotational quenching of an interstellar gas thermometer: $CH_3CN$-He collisions.

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Among all the molecular species found in the interstellar medium, molecules with three-fold symmetry play a special role, as their rotational spectroscopy allows them to act as practical gas thermometer. Methyl-cyanide ($CH_3CN$) is the second more abundant of those (after ammonia). We compute in this paper the collisional dynamics of methyl-cyanide in collision with helium, for both the A- and the E- symmetry of $CH_3CN$. The Potential Energy surface is determined using the CCSD(T)-$F_{12b}$ [1] formalism and fit onto relevant functionals. We compute the rotationally inelastic cross-sections for all levels up to 510 $cm^{-1}$ of collisional energy, thanks to low energy exact coupled channels (CC) methods [2] and higher energies approximate Coupled States (CS) methods [3]. For temperatures from 7 K up to 300 K rates of quenching are computed and most are found to vastly differ from earlier published ones (up to a factor of a thousand), calling for a possible reexamination of the temperatures found in low density gasses.

Figure 1 : Rates temperature dependence of *A*-$CH_3CN$ and *E*-$CH_3CN$ in collision with He for transitions corresponding to the 220 GHz observation band.

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# Complex Organic Molecules (COMs) in protoplanetary disks : X-ray photodesorption from methanol containing ices

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Small organic molecules are now commonly detected in the coldest regions of the interstellar medium (ISM, star and planet formation regions) by the last generation of space and ground-based telescopes (ALMA, NOEMA). These Complex Organic Molecules (COMs, such as methanol or formic acid), tend to form or accrete on the surface of dust grains. Thus, they are expected to be mainly present in the condensed phase into the interstellar ices, diluted in their main constituants such as $H_2O$ and CO. As COMs cannot thermally desorb from ices in these regions where they are detected, it is expected that photons coming from various sources in the ISM could trigger their ejection into the gas phase. This process, known as photodesorption, can participate to the overall gas-to-ice balance of these cold regions, and needs to be qualitatively understood and quantitatively constrained.

So far, very few experimental data exist on the photodesorption of COMs-containing ices (methanol [1], [4], formaldehyde [2]), and they concern only the photons in the VUV range (<13.6 eV). However, in some regions like protoplanetary disks, soft X-rays (500-2000 eV) can also participate to the desorption. X-ray photodesorption has already prooven to be efficient for "simple" species like water [3], [5] but its role in the origin of gaseous COMs is still uncertain. Thus, we have recently studied the X-ray photodesorption of methanol in pure and $H_2O$/CO rich ices using the SEXTANTS beamline at the SOLEIL synchotron in France.

We will summarize the main findings of our studies, i.e. the critical influence of several physical parameters such as ice composition, and the identification of competing processes of desorption (X-ray induced electron-stimulated desorption, true photon-stimulated desorption ...) and we will discuss the astrophysical implications of these findings.

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# Polarization mapping of B335 and L483: magnetic fields and dust evolution from cloud to core scales

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Interstellar magnetic fields are believed to play an important role in regulating the cloud-core gravitational collapse that leads to star formation. However, the differences in magnetic field structure and grain properties from cloud-core scale down to the scale of the protostellar disk are poorly understood. Using new optical and near-infrared polarization data toward two well-known Class 0/I sources (B335 and L483), we investigate how the cloud-scale magnetic field morphology is affected by the bipolar outflows, and how it connects with the inner portions near the forming protoplanetary disk. For B335, this is made possible by comparing with ALMA polarization data and MHD simulations.

The magnetic field direction was compared to the bipolar outflow orientation of B335 (e.g., see Figure 1) and L483. For B335, we employ polarization spectrum Serkowski curve fits to estimate the $\lambda_{MAX}$ parameter, which represents the wavelength at which the spectrum reaches its peak polarization degree value. For both sources, the bipolar outflow orientation is strongly correlated with the magnetic field direction up to the ~0.15 pc scale, which covers the full length of the CO emission that traces de outflow. B335 shows a smooth increase in $\lambda_{MAX}$ from the cloud outskirts into the inner core portions. After discarding possible grain alignment effects, this result is interpreted as due to grain growth correlated to the increased density near the core center. This provides a connection with a recently published indirect evidence of large grains near the B335 protostellar disk, as revealed from analysis of the ALMA data.

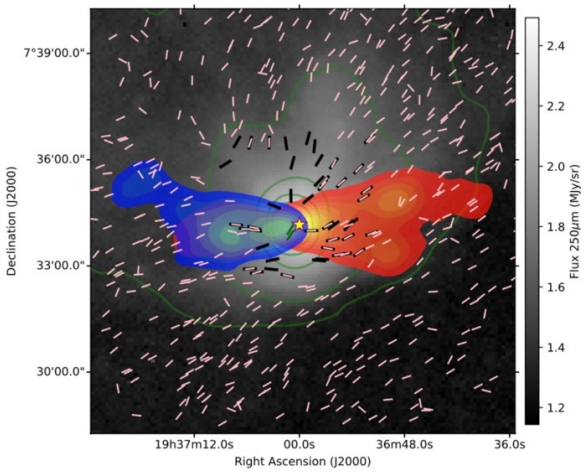


Figure 1: *Herschel* dust emission map of B335 with polarization vectors overlaid. Different vector colors represent different observed wavelengths. The bipolar outflow CO emission is represented by the blue/red lobes.

The bipolar outflows in B335 and L483 likely dominate the energetics over the magnetic field, up to the entire length of the outflow itself. The presence of larger grains near the B335 protostellar disk, as evidenced from ALMA data, is likely a result from a smooth grain growth process that begins in the outskirts of the star forming core.

# Desorption of ammonium salts from cold surfaces

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The chemical evolution of the gas-phase during the protostellar stage is largely governed by the desorption of species present in the dust grains. In environments where the dust grains are slowly heated, such as in regions around low-mass protostars, the desorption of molecules can occur in more than one temperature range [1, 2]. How, where and when these species are released to the gas-phase depends on the chemical nature of the molecule involved and its chemical environment. Ammonia desorption when present in an icy water matrix should occur at the same time as water desorption [1, 2]. However, ammonia in its protonated form, $NH_4^+$, presents a more refractory character [4] and could remain on the surface of the dust grains until higher temperatures. The temperature dependence on the location of these different N reservoirs, in relation to water and methanol snow lines, is a fundamental step to understand planetary formation [4]. For this purpose, data on the kinetic parameters of desorption of these different nitrogen carriers are essential to optimize gas-grain astrochemical models.

In this work, we perform experiments to investigate the desorption of ices made of ammonium salts in a set-up that mimic interstellar medium conditions. $NH_3$ and an organic acid (formic or acetic acid) were co-deposited on a on inert substrate (gold) and on amorphous water ice at low temperatures (10 and 120 K) under ultrahigh vacuum conditions. IR measurements show the formation of ammonium salts upon deposition. Using temperature programmed desorption experiments we quantify the different desorption parameters and determine the binding energies of the salts. An experimental evidence is also provided to show that ammonium salts are released to the gas-phase as neutral species, $NH_3$ and the organic acid, at temperatures higher than the temperature of thermal desorption of water ice. Finally, we discuss the implications of the desorption of ammonium salts in the composition of comets and to model planet formation.

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# Inelastic rate coefficients for collisions of $N_2H^+$ with $H_2$

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$N_2H^+$ observations are of particular interest to probe the physical conditions of cold molecular clouds. Accurate modelling of the observed spectra requires the knowledge of the excitation conditions of $N_2H^+$ in the ISM. Thus, we have calculated rate coefficients for the excitation of $N_2H^+$ by $H_2$, the most abundant collisional partner in cold molecular clouds. The calculations are based on a new potential energy surface (PES) obtained from highly correlated ab initio calculations. This 4D-PES exhibits a very deep well of ~2530 $cm^{-1}$ making fully converged scattering calculations very difficult to carry out. To overcome this difficulty, two approximate approaches, the Adiabatic Hindered Rotor approach (AHR) and the Statistical Adiabatic Channel Model (SACM), were tested and compared to results obtained from full 4D Close-Coupling (CC) calculations. The AHR treatment, which reduces the scattering calculations to a 2D problem was found to give the best results at all temperatures and even for transitions involving high $N_2H^+$ rotational levels. State-to-state rate coefficients between the 26 first $N_2H^+$ rotational levels were then calculated for temperatures ranging from 5 K up to 500 K.

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# Hydrogenation of formic acid on cold dust grain analogue surfaces

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Formic acid (FA) is the simplest organic carboxylic acid in chemical synthesis and the significant species in interstellar chemistry. It is a complex organic molecule containing two oxygen atoms and tow chemical conformations. It was observed in cold dense molecular clouds [1], detected together with methanol ($CH_3OH$) and formaldehyde ($H_2CO$) in potoplanetary disks in trans conformer, and even in comets of planetary system by IRAM 30 m telescope [2]. Our LERMA-Cergy laboratory hydrogenation experiments of HCOOH molecules with H atoms were performed with two cryogenic ultra-high vacuum devices on amorphous solid water (ASW) ices, graphite (HOPG) and gold surfaces at low surface temperature 10 K, low surface coverage of one monolayer to three layers, and low H-atom flux [3]. The experiments have shown a consumption of 30 % of formic acid molecules and the formation of some products, sucha as carbon dioxyde and water molecules, which were identified by absorption reflexion infrared spectroscopy (RAIRS) and temperature programmed desorption (TPD) mass spectrometry. A chemical surface reaction route for the hydrogenation reaction is proposed involving both the monomers and the dimers of HCOOH which were evidenced experimentally by TP-DED mass spectroscopic method. The consumption yields of HCOOH by H is discussed, and it depends probably on many factors, such as the effect of the substrate, the diffusion of atoms and radicals on the surface, the chemical desorption, the chemical conformation of molecules, the orientation of molecules in a specicfic direction favoring or enabling the H/OH abstraction reactions. We present the experimental results and the different possible chemical routes for the product formation. The hydrogenation reactions of FA on cold grain surfaces may help astrophysicists and astrochemists to further understand the chemistry in gas-grain interfaces of protoplanetary disk regions, where gaseous molecules CO, $CH_3OH$ and HCOOH are expected to be abundant according to the recent atrochemical models of Ruaud & Gorti [4]. These astrophysical environments are believed to be birthplaces of planetary systems and comets.

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# Large-scale Turbulent Driving Regulates Star Formation in High-redshift Gas-rich Galaxies

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The question of what regulates star formation is a longstanding issue. To investigate this issue, we run simulations of a kiloparsec cube section of a galaxy with three kinds of stellar feedback: the formation of H II regions, the explosion of supernovae, and ultraviolet heating. We show that stellar feedback is sufficient to reduce the averaged star formation rate (SFR) to the level of the Schmidt-Kennicutt law in Milky Way-like galaxies but not in high-redshift gas-rich galaxies, suggesting that another type of support should be added. We investigate whether an external driving of the turbulence such as the one created by the large galactic scales could diminish the SFR at the observed level. Assuming that the Toomre parameter is close to 1 as suggested by the observations, we infer a typical turbulent forcing that we argue should be applied parallel to the plane of the galactic disk. When this forcing is applied in our simulations, the SFR within our simulations closely follows the Schmidt-Kennicutt relation. We found that the velocity dispersion is strongly anisotropic with the velocity dispersion alongside the galactic plane being up to 10 times larger than the perpendicular velocity.

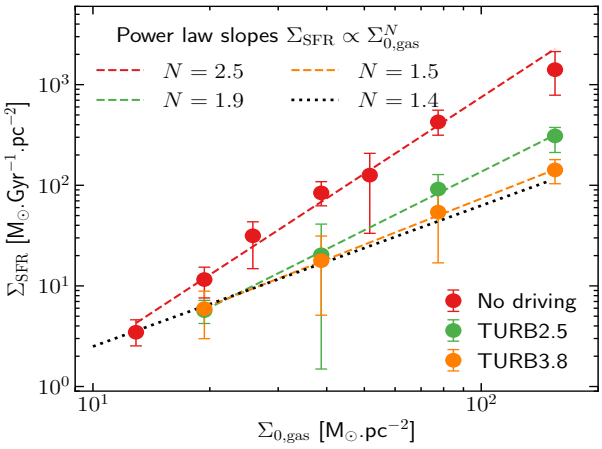


Figure 1 : Averaged surfacic SFR as a function of the initial column density.

# Hunting the relatives of benzonitrile: Rotational spectroscopy of dicyanobenzenes

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The presence of large and aromatic C-bearing molecules in the interstellar medium (ISM) has been the subject of numerous studies [1]. The recent detection of benzonitrile ($C_6H_5$-CN) [2] by radio-astronomy has confirmed the presence of this family of species in the ISM and brings renewed interest in related molecules that could participate in similar reaction networks. New unambiguous interstellar detection of such species, however, requires thorough laboratory spectroscopic investigations.

We have recorded the pure rotational spectra of *ortho*- and *meta*-dicyanobenzene ($C_6H_5$-$(CN)_2$), from the centimeter to the millimeter-wave domain. The centimeter-wave region was investigated using a supersonic jet Fourier-transform microwave (FTMW) spectrometer. The room temperature, gas phase absorption spectra of both species in the millimeter-wave domain have been recorded using millimeter-wave spectrometer based on a multiplication frequency chain. Quantum chemical calculations with the DFT methods, B97-1 and MP2, both at cc-pVTZ level in the harmonic approximation have been performed to support the analysis enabling the assignment.

Using a combinaison of Pgopher [3], LWW [4] and SPFIT/ SPCAT [5] softwares, accurate spectroscopic parameters have been derived from the analysis of the experimental spectra, allowing for reliable predictions at temperatures of interest for astronomical searches.

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# Rotational (de-) excitation of ortho-$CH_3Cl$ byHe:three dimensional potential energy surface and collision rate coefficients

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Chloromethane ($CH_3Cl$) is the first organohalogen molecule to be detected in the interstellar medium[1]. Therefore it is a key to understand the chemistry of the interstellar clouds.

We present the inelastic scattering of both ortho-$CH^{35}Cl$ and ortho-$CH^{37}Cl$ isotopes by helium atom. A new three dimensional potential energy surface (3D-PES) between $CH_3Cl$ and He was mapped using CCSD(T)-F12 method[2] and AVTZ basis set[3] implemented in the MOLPRO package. This PES was incorporated later into dynamical computation code MOLSCAT. The treatment of the nuclear motions of both isotopes colliding with He was supported by calculations of state-to-state cross-sections for transitions among the first 39 rotational levels of ortho-$CH_3Cl$ (up to $J_{K\varepsilon}=13_{3+}$) using the quantum close-coupling methodology for total energies up to300 $cm^{-1}$and the coupled state approach for higher energies up to 720$cm^{-1}$.Rate coefficients for temperatures ranging from 5 to 50K are calculated by averaging the cross-sections over a Maxwell–Boltzmann distribution.We expect that our results will be helpful for understanding the chemistry of such species in the interstellar medium and interpreting data that powerful instruments like ALMA or Herschel will provide.

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# Electron-induced kinetics of $HD^+$ in the Early Universe

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$HD^+$ is considered a key species in the evolution of the Early Universe [1]. It can either ro-vibrationally excite/de-excite (Ro-Vibrational Transitions, RVT), or recombine (Dissociation Recombinaison, DR). This latter process received particular attention in the storage-ring type experiments, resulting in very accurate state-to-state rate-coefficients. Using Multichannel Quantum Defect Theory (MQDT) [2, 3], we have recently produced a complete set of cross sections and Maxwell rate coefficients for the lowest 30 ro-vibrational states of this ion, as shown in the figure below.

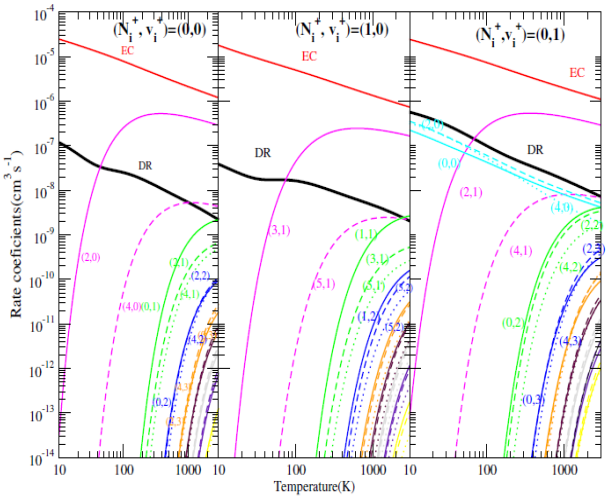


Figure 1. Maxwell rate coefficients for DR, elastic collisions (EC) and ro-vibrational transitions (RVT) of $HD^+$. Left-panel: Target in its ground state ($Ni^+$,$vi^+$)=(0,0). Middle-panel: Rotationally excited target ($Ni^+$,$vi^+$)=(1,0). Right-panel : Vibrationally excited target ($Ni^+$,$vi^+$)=(0,1). For RVT, the final quantum numbers ($Nf^+$,$vf^+$) of the ion are indicated.

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# The headlight cloud in NGC 628: An extreme giant molecular cloud in a typical galaxy disk.

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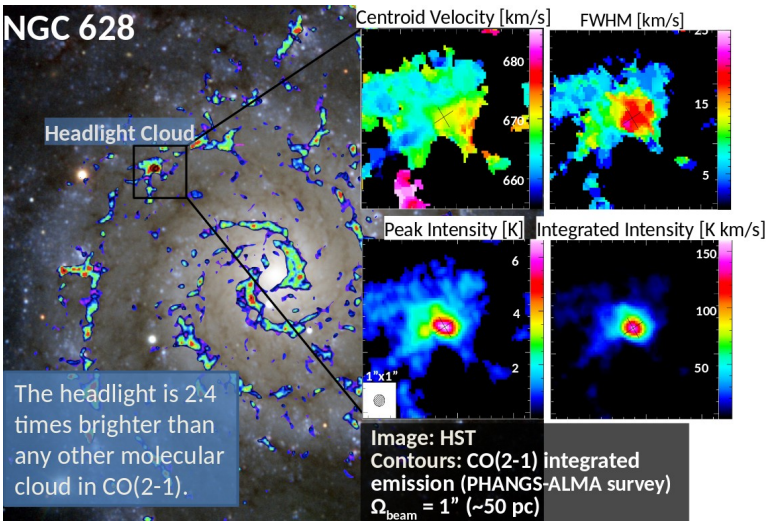
Cloud-scale surveys of molecular gas trace the link between cloud properties and star formation (SF) across galactic environments. Cloud populations in disks are considered to represent the normal SF process, while centers tend to harbor denser gas with more extreme SF. At high resolution, however, molecular clouds with exceptional gas properties and SF activity may also be observed in normal disks. I will present one of such clouds in NGC 628.

High-resolution ALMA CO observations (see fig.) revealed an unusually massive ($2x10^7 M_\odot$) molecular cloud, which has embedded a young (2-4 Myr) and massive ($3x10^5$ $M_\odot$) stellar population. It has a low virial parameter, suggesting that its CO emission is overluminous due to the feedback from the vigorous SF happening within the cloud, captured just prior to its destruction. This is possible given the longer survival times expected for the most massive objects. Its extreme mass may be related to its location at the intersection of a spiral arm and a co-rotation radius, a special location against the disruptive effect of galactic shear and a sustained inflow of gas favorable to enhanced mass growth.

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# The $X_{CO}$ conversion factor in galactic disk simulations

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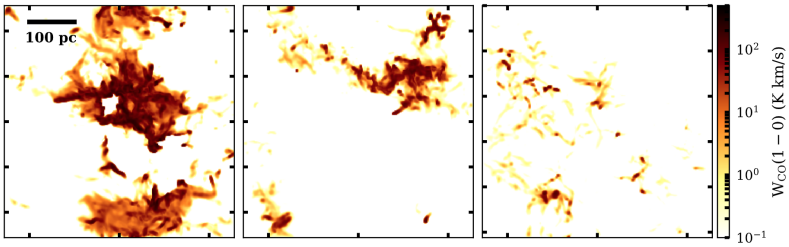


Figure 1 : Synthetic CO (J=1-0) line emission maps from simulations. From left to right, the panels show the simulations at distances 2, 4, and 8 kpc from the Milky Way galactic center.

CO emission is a widely used observational tracer of molecular gas, rendering essential the $X_{CO}$ factor, which is applied to convert CO luminosity to $H_2$ mass. We use the TIGRESS (Three-phase Interstellar Medium in Galaxies Resolving Evolution with Star Formation and Supernova Feedback) simulations of galactic disks to study $X_{CO}$ in a wide range of physical environments. Molecular clouds form in the simulations in the three-phase ISM with self-consistent star formation feedback. Figure 1 shows the synthetic CO maps generated from the simulations using chemistry and radiation post-processing. We successfully reproduce the observed CO line widths and excitation temperatures in the PHANGS survey (Sun et al. 2018) and the line ratios in the EMPIRE survey (Cormier et al. 2018). We find that as the density increases, $X_{CO}$ first decreases due to the increasing excitation temperature, and then decreases when the emission is fully optically thick. We identify direct observable quantities which can be used to calibrate $X_{CO}$. Figure 2 shows that using a constant $X_{CO}$ introduces large systematic biases, which can be corrected using CO line properties or line ratio. We also investigate the large scale variations of $X_{CO}$ as functions of metallicity, cosmic ray ionization rate, and the FUV radiation. We provide the CO-dark $H_2$ fraction as a function of observational sensitivities and beam-sizes.

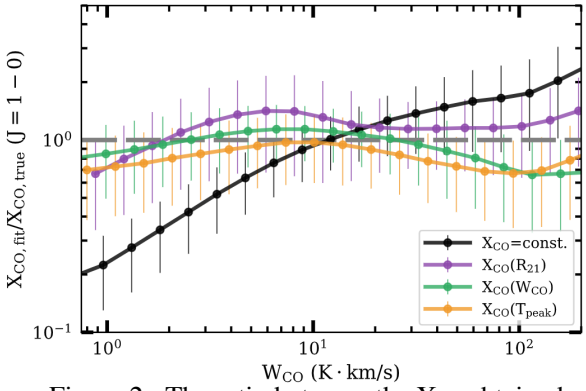


Figure 2 : The ratio between the $X_{CO}$ obtained from various fitting formulas and the true $X_{CO}$. The black line shows the constant $X_{CO}$. The other lines show $X_{CO}$ corrected by observables, such as the CO (J=2-1)/(J=1-0) line ratio ($R_{21}$), brightness ($W_{CO}$), peak excitation temperature ($T_{peak}$).

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# Dynamical Effects of the Radiative Stellar Feedback

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The photodissociation region (PDR) is the layer of interaction between molecular cloud and stellar radiation ionizing and dissociating the gas. The photodissociation front separating the atomic and molecular regions is critical in the determination of the $H_2$ mass fraction on which rely the Kennicutt-Schmidt relations. The analytical theory of Sternberg *et al*. 2014[1], a static and stationary description, has become widely used to estimate atomic fractions in galactic and extragalactic giant molecular clouds. But recent observations from ALMA [2,3] and from Herschel [4,5] providing a vast number of CO rotational lines showed important dynamical effects. The observations were explained by a time-dependent hydrodynamical PDR code[6] highlighting a mechanism called the photo-evaporation. It consists in the evaporation of photo-ionized gas through the ionization front that creates a compression layer behind this front, propagating inside the cloud and responsible for the excitation of the molecules. In the simulated models, the dynamics changed the position and sharpness of the photodissociation front.

That is why we extended previous work (*e.g*. Sternberg *et al*. 2014[1]) by building a semi-analytical model of H-to-$H_2$ transition that includes the impact of the dynamics. In the ionization front frame, the evaporation acts like an advection term. We showed that in the presence of this advection, the photodissociation front is shifted toward the ionization front, and is sharper than predicted with a static approach. We also found the existence of physical conditions in which the advection is so strong that the ionization and dissociation fronts are merged, and present an updated criterion [7,8] for this front merging. With molecular hydrogen closer to the border we can expect it to be warmer and with more excited lines that could be more easily detected by the James Webb Space Telescope (JWST) that will bring well resolved observations of such regions.

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# $C^{18}O$, $^{13}CO$, and $^{12}CO$ abundances and excitation temperatures in the Orion B molecular cloud: An analysis of the precision achievable when modeling spectral line within the Local Thermodynamic Equilibrium approximation

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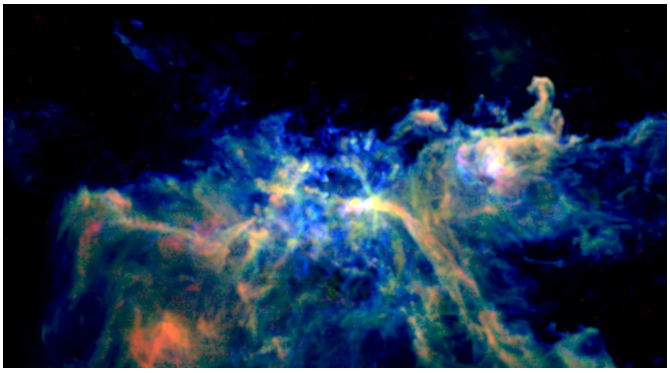

*Illustration 1: Composite image of the emission of 12CO(1-0) in blue, 13CO(1-0) in green, and C18O(1-0) in red.*

CO isotopologue transitions are routinely observed in molecular clouds to probe the column density of the gas, the elemental ratios of carbon and oxygen, and to trace the kinematics of the environment. We aim at estimating the abundances, excitation temperatures, velocity field and velocity dispersions of the three main CO isotopologues towards a subset of the Orion B molecular cloud. We use the Cramer Rao Bound (CRB) technique to analyze and estimate the precision of the physical parameters in the framework of local-thermodynamic-equilibrium excitation and radiative transfer with an additive white Gaussian noise. We propose a maximum likelihood estimator to infer the physical conditions from the 1-0 and 2-1 transitions of CO isotopologues. Simulations show that this estimator is unbiased and efficient for a common range of excitation temperatures and column densities (Tex > 6 K, N > 1e14 - 1e15 cm-2). Contrary to the general assumptions, the different CO isotopologues have distinct excitation temperatures, and the line intensity ratios between different isotopologues do not accurately reflect the column density ratios. We find mean fractional abundances that are consistent with previous determinations towards other molecular clouds. However, significant local deviations are inferred, not only in regions exposed to UV radiation field but also in shielded regions. These deviations result from the competition between selective photodissociation, chemical fractionation, and depletion on grain surfaces. We observe that the velocity dispersion of the C18O emission is 10% smaller than that of 13CO. The substantial gain resulting from the simultaneous analysis of two different rotational transitions of the same species is rigorously quantified. The CRB technique is a promising avenue for analyzing the estimation of physical parameters from the fit of spectral lines.

**References** [1] Roueff et al, accepted to A&A, https://arxiv.org/abs/2005.08317

# Quantitative inference of the $H_2$ column densities from 3 mm molecular emission: A case study towards Orion B

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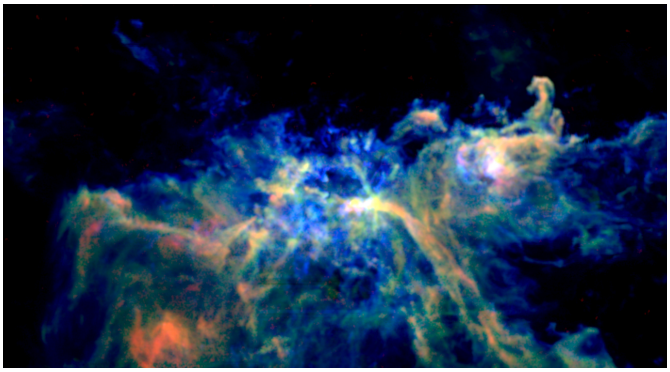

*Illustration 1: Composite image of the emission of 12CO(1-0) in blue, 13CO(1-0) in green, and C18O(1-0) in red.*

Molecular hydrogen being unobservable in cold molecular clouds, the column density measurements of molecular gas currently rely either on dust emission observation in the far-IR, which requires space telescopes, or on star counting, which is limited in angular resolution by the stellar density. (Sub-)millimeter observations of numerous trace molecules are effective from ground based telescopes, but the relationships between the emission of one molecular line and the $H_2$ column density is non-linear and sensitive to excitation conditions, optical depths, abundance variations due to the underlying physico-chemistry. We aim to use multi-molecule line emission to infer the $H_2$ molecular column density from radio observations. We propose a data-driven approach to determine the $H_2$ gas column densities from radio molecular line observations. We use supervised machine learning methods (Random Forests) on wide-field hyperspectral IRAM-30m observations of the Orion B molecular cloud to train a predictor of the $H_2$ column density, using a limited set of molecular lines between 72 and 116 GHz as input, and the Herschel-based dust-derived column densities as ``ground truth'' output. For conditions similar to the Orion B molecular cloud, we obtain predictions of the $H_2$ column density within a typical factor of 1.2 from the Herschel-based column density estimates. A global analysis of the contributions of the different lines to the predictions show that the most important lines are $^{13}$CO(1-0), $^{12}$CO(1-0), C$^{18}$O(1-0), and $HCO^+$(1-0). A detailed analysis distinguishing between diffuse, translucent, filamentary, and dense core conditions show that the importance of these four lines depends on the regime, and that it is recommended to add the $N_2H^+$(1-0) and $CH_3OH$ ($2_0$-$1_0$) lines for the prediction of the H2 column density in dense core conditions. This opens a promising avenue to directly infer important physical parameters from the molecular line emission in the millimeter domain. The next step will be to try to infer several parameters simultaneously (e.g., the column density and far-UV illumination field) to further test the method.

**References** [1] Gratier et al, submitted to A&A

# Explicitly correlated potential energy surface of the CO2-CO van der Waals and applications

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The four-dimensional-potential energy surface (4D-PES) of the CO2-CO van der Waals complex is generated using the explicitly correlated coupled cluster with single, double, and perturbative triple excitation (CCSD(T)-F12) method[1,2]in conjunction with the augmented correlation-consistent triple zeta (aug-cc-pVTZ) basis set. This 4D-PES is developed over the set of inter-molecular coordinates and where the CO2 and CO monomers are treated as rigid rotors. Afterwards, analytic fits of this 4D-PES are done. In addition to the already known C-bound and O-bound stable structures of CO2-CO, we characterise a new isomer: it has a T-shaped structure where the O atom of the CO2 moiety points into the centre of mass of CO. We also find the saddle points connecting these minimal structures. This new isomer may play role during the intramolecular isomerization processes at low energies. Then, the 4D-PES expansion is incorporated into bound vibrational state computations of C-bound and O-bound complexes. We also computed the temperature dependence of the second virial coefficient for CO2-CO. A good agreement with experiment[1,2]is found.

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# Rotational transitions and dissociative recombination of $D_2^+$ induced by collisions with slow electrons

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Using the Multichannel Quantum Defect Theory (MQDT)[1], a new series of computations has been performed to obtain cross sections and rate coefficients for rotational transitions of $D_2^+$ induced by collisions with very low-energy electrons. Following our previous work [2, 3] and using the same molecular structure data sets, the excitation $N_i^+ \rightarrow N_i^+ + 2$ for $N_i^+ from 0$ to 10, and the de-excitation $N_i^+ \rightarrow N_i^+ - 2$, for $N_i^+ from 1$ to 10, in the energy range 0.01 meV - 0.3 eV have been explored. The calculated cross sections have been convolved in order to obtain Maxwell rate coefficients for electronic temperatures up to a few hundred of Kelvin - Figure 1. Rate coefficients for dissociative recombination have been also calculated for the same initial rotational levels.

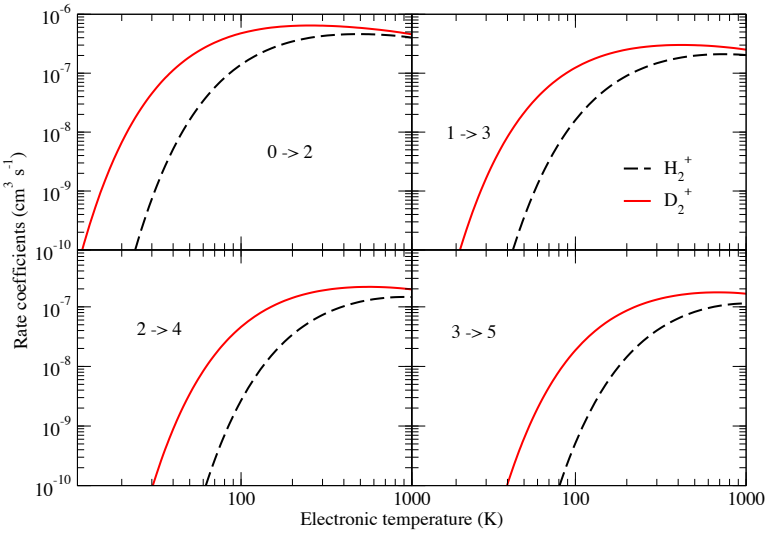


Figure 1: Isotopic effects in rotational excitation: rate coefficients for $N_i^+ \rightarrow N_i^+ + 2$ transitions, $N_i^+ = 0, 1, 2, 3$, for vibrationally relaxed $X^2\Sigma_g^+$ $H_2^+$ and $D_2^+$ systems.

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## Reactive collisions of electrons with $ArH^+$

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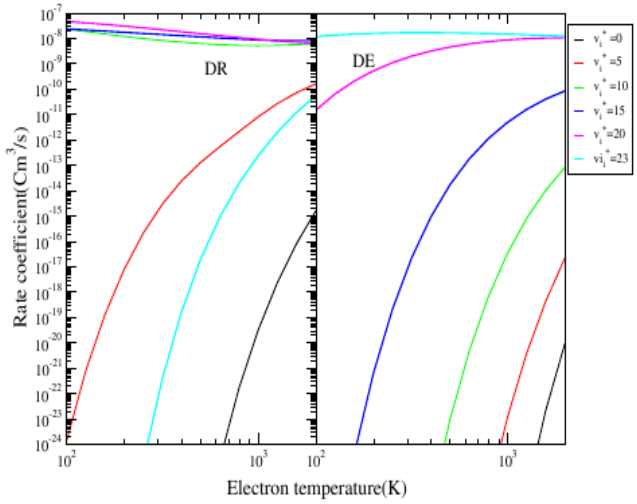
Electronic collisions are major processes in cold ionized media such as interstellar molecular clouds and polar auroras. $ArH^+$ molecular is considered a good tracer of hydrogen gas in the interstellar medium (ISM)[1]. The knowledge of accurate values of its dissociative recombination rate coefficient of this molecular ion is important for the ISM modelers. To better describe the kinetics of this media, increasingly sophisticated experiments are being carried out, complemented by theoretical calculations of increasing precision. With the latter we can overcome experimental limitations, such as difficult access to excited levels of targets and state-to-state descriptions.

Using Multi-channel Quantum defect Theory (MQDT) [2-8], we calculated the cross sections and the rate coefficients for dissociative recombination (DR) (1.1) and for its competitive processes, inelastic collisions ($vf^+ > vi^+$) or vibrational excitation (VE), super-elastic collisions ($vf^+ < vi^+$) or vibrational de-excitation (VdE), and dissociative excitation (DE):

$$ArH^+(vi^+) + e^- \longrightarrow Ar + H \ \text{(DR)}, \quad ArH^+(vf^+) + e^- \ \text{(VE, VdE)}, \quad Ar + H^+ + e^- \ \text{(DE)}$$

where $vi^+$ and $vf^+$ are respectively the initial and the final vibrational levels.




*Rate coefficient of Dissociative Recombination (DR) and Dissociative excitation (DE).*

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# La vie a-t-elle pu apparaître ailleurs que sur la Terre ?

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La recherche d'une autre forme de vie que la nôtre ailleurs dans l'univers repose sur notre compréhension de l'origine de la vie terrestre, seul exemple connu à ce jour. Les études concernant l'évolution de la chimie vers la biologie dans l'environnement primitif terrestre, l'universalité de la chimie organique et le rôle éventuel d'un apport sur Terre de molécules extraterrestres, nous permettent d'approcher rationnellement la possibilité de l'apparition de la vie ailleurs que sur notre planète, dans le système solaire ou autour d'autres étoiles. Où en sommes-nous à l'heure actuelle de ces recherches, et quelles en sont les perspectives à plus ou moins long terme ?

# Scientific capabilities of the Canada-France-Hawaii Telescope

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The Canada-France-Hawaï Telescope is a 4m optical observatory located at at the summit of Maunakea, Hawaii. It hosts 3 wide field imagers and two high resolution spectropolarimeters operated in Queue Scheduled Observing mode. I will present the science capabilities of the instrument suite, focusing on the physics and chemistery of the ISM. One of our instruments, SITELLE, has capabilities that are unique for this type of studies. I will also give an update on the status of the Maunakea Spectroscopic Explorer and its expected scientific capabilities.

# Molecules and Dust in High-Redshift Galaxies

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With the advent of increased capabilities in sub/millimeter facilities over the past decade, particularly with ALMA and NOEMA, observations of the cool interstellar medium in galaxies throughout cosmic time have made remarkable progress. Molecular and atomic gas, together with the underlying dust continuum, have been observed in hundreds of high-redshift galaxies up to z~9, from extreme starbursts to main sequence galaxies. These observations have enabled, e.g., detailed dynamical studies at sub-kpc scales and multispecies studies, probing the physical and chemical conditions in early galaxies and their evolution with cosmic time up to the era of re-ionization.

In this review, I will summarize recent studies illustrating the rapid progress in observations of molecular species other than CO (e.g., $H_2O$, molecular ions and isotopes) and of atomic fine-structure lines (carbon, oxygen and nitrogen). The emphasis will be put on what we have learned from these various species, addressing issues such as galaxy dynamics, the underlying chemistry and feedback. In addition, I will present the current status on the dust properties and their evolution with redshift.

Finally, after identifying some fundamental questions brought up by the currently available data, I will outline future prospects that will be made possible with upgrades of the current facilities and the forthcoming launch of the JWST.

# From spectroscopic studies to astrophysical detections: recent results and prospective

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Laboratory analysis of spectra of potential interstellar molecules from the radio-frequency to the THz range is a primary tool for their subsequent identification by radioastronomical techniques. The spectral analysis allows us to derive molecular parameters that are able to model the frequency and intensity patterns of the transitions, as well as to predict with a high degree of precision the frequencies of transitions not measured in the laboratory. In Lille Spectroscopy Group, different spectrometers using both absorption and emission techniques cover the frequency range from 2 GHz up to 1.52 THz and are capable of measuring the rotational spectra with high spectral resolution, accuracy, and sensitivity. Recent spectroscopic studies of our group resulted in the interstellar detection of methoxymethanol [1] and hydroxyacetonitrile [2], and in the tentative detection of N-methylformamide [3], but also in many non-detections. The latter receives much less attention from the astrophysical and astrochemical community whereas it may also contribute into the development of interstellar and circumstellar chemistry models. Rotational spectroscopy is extremely sensitive to molecular geometry and/or mass variation. Therefore, it allows independent and simultaneous analysis of tautomers, isomers, conformers, or isotopomers, and it is suitable for laboratory analysis of the gas phase samples. Recent advances in chirped pulse (CP) millimeter-wave spectroscopy allowed fast spectral recording within broad frequency range. For example, we show that in about 0.2 s we may record relatively broadband portion of spectrum in which a species with partial pressure as low as 10 nbar or $5 \cdot 10^{-13}$ $cm^{-2}$ in column density may be detected [4]. The microsecond time scale of typical CP experiment is an asset for rapid spectral acquisition of transient species like radicals and ions. In coupling with high specificity, it makes the rotational spectroscopy a promising tool for studying chemical reactions kinetics. Current state-of-the-art of the terahertz rotational spectroscopy will be presented, and future prospects will be discussed.

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# A (Re)view of the Interstellar Media of the Local Universe

Suzanne Madden

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The cycling of matter between gas, dust and stars in galaxies influences how the different phases structure themselves and, in general, forms the basis for the evolution of galaxies. I will review some advances we have made in these areas, given the numerous surveys carried out on galaxy scales in the local universe (e.g. Spitzer, Herschel, SOFIA, IRAM and other ground-based telescopes) as well as what we are learning on resolved scales of atomic/molecular clouds and HII regions with, e.g. ALMA, NOEMA, VLT/MUSE and HST. Characterisation of the variations of dust and gas properties with local and galactic environment and the interplay of the ISM with star formation is emerging from local galaxy surveys. The laboratories of the local universe offer a wide range of parameter space giving us a broad picture of the physics and chemistry of star formation activity, heating and cooling processes, atomic-molecular phase transition and the presence of a molecular phase not traced by CO as well as the dust and molecular complexity within galaxies. With such detailed studies we can better make the link with the physics and chemistry of the gas and dust in high-z systems to understand the evolution of cosmic dust and how molecular gas is transformed into stars in extremely metal-poor systems, for example.

Taking into account where we have come to as of today, I will attempt to lay out some major questions we will have and where we may go in the next 5 years with the many exciting, new telescopes and instruments we look forward to.

# Dust and gas as tracers of star formation

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While $H_2$ is the most abundant molecule in the Interstellar Medium (ISM), the study of the star formation process is carried out using more favorable dust observations at FIR wavelengths or millimeter line transitions of less abundant molecules such as CO or HCN. The detailed characterization of these observational tracers provide crucial information about the physical and chemical properties of molecular clouds, the evolution of the ISM, and ultimately the origin of stars across Cosmic Times. During my talk I will discuss how the use of a new generation of galactic studies carried out by space and ground telescopes such as Herschel, IRAM30m, and ALMA (e.g. [1], [2]), are revolutionizing our contemporary description of the star formation process. Moreover, I will summarize how some of our recent studies on classical star formation tracers such as HCN are posing important challenges for the interpretation of both local and extragalactic observations.

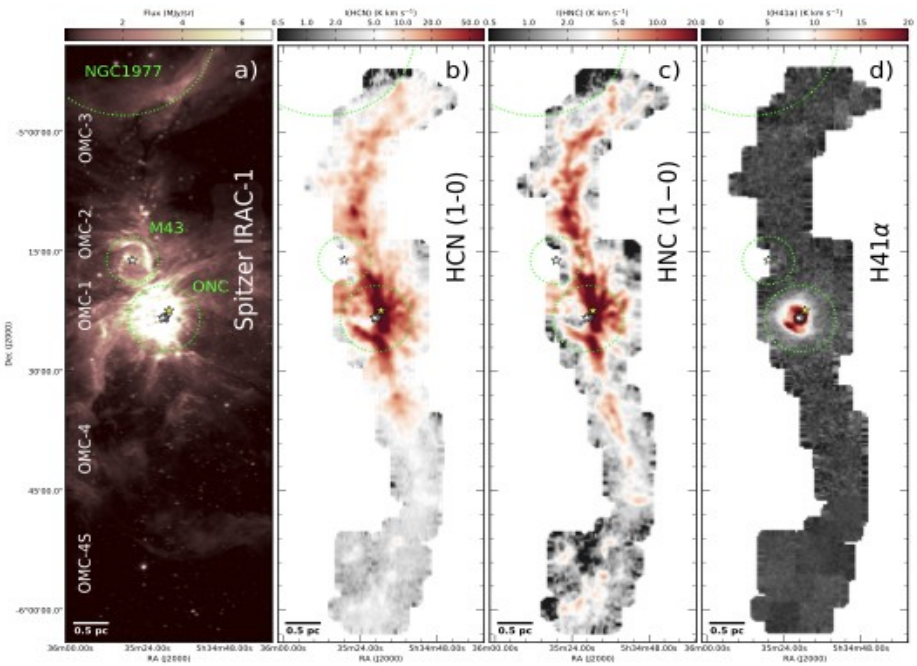


Figure 1 : HCN observations in the Orion A cloud [2]

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# An update on (some of the) Nanocosmos results

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Evolved stars are major dust factories. Stardust is composed of tiny grains that are injected into the interstellar medium where they can evolve through interactions with gas, photons and energetic ions. The resulting cosmic dust plays a key role in regions of star and planet formation but models suffer from our poor knowledge of these grains. In this context, the main goal of the Nanocosmos synergy project [1], funded by the European Research Council, is to tackle the formation of stardust by combining experiments using sophisticated laboratory setups with astrophysical observations and chemical modelling.

The Stardust machine [2], the key setup of Nanocosmos, can produce stardust analogues in controlled conditions. Their molecular content can be probed by AROMA [3], another experimental setup, which is highly sensitive to (hydrogenated) carbon clusters, polycyclic aromatic hydrocarbons (PAHs) and fullerenes. These studies bring new insights into the chemical pathways involved in carbon dust formation. Specific results will be shown in the case of $C/C_2+H_2$ [4] and $C/C_2+C_2H_2$ [5] chemistries, providing constraints on the formation of PAHs and fullerenes in evolved star environments.

The PIRENEA 2 setup is a future step in laboratory experiments that aims to produce stardust grain analogues and study their evolution in interstellar-like conditions. The setup is equipped with both a molecular aggregation source [6] and a laser vaporisation source. I will describe how PIRENEA 2 can specifically mimic the interactions of nano-sized cosmic dust analogues with gas and UV photons.

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