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# Accelerated Macroscopic Monte Carlo method for gas-grain chemical simulations

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Current macroscopic Monte Carlo (MC) method cannot be used to simulate a gas-grain reaction network that includes the accretion of gas phase molecular hydrogen onto grain surfaces. Moreover, the computational cost for MC method to simulate the chemical evolution of protoplanetary disks is also too high. An efficient macroscopic MC method that can solve the problem is presented in this talk. Our new method is based on quasi-steady-state assumption. Numerical comparisons by the exact macroscopic MC method and our approximations will be discussed. We expect our new method can be used to simulate disk chemistry.

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\*Speaker

# Chemical modelling of formamide and methyl isocyanate in star-forming regions

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Comets are thought to contain relatively pristine material from the origin of the solar system, having condensed directly out of the pre-solar nebula (e.g., Mumma & Charnley 2011). It is postulated that comets may have even delivered some of the water and organic matter found on the Earth via impacts (e.g., Hartogh et al. 2011). Over 22 molecules have been identified in comets via radio observations (Crovisier et al. 2004), including organic species such as formamide (NH<sub>2</sub>CHO, Biver et al. 2014). Formamide and methyl isocyanate are particularly interesting for their potential role in prebiotic chemistry (Saladino et al. 2012).

Formamide has been detected in a large variety of star-forming environments, as well as in Solar System comets, thus supporting the hypothesis that molecules with a strong prebiotic potential could have been delivered to Earth by comets after being synthesized in prestellar environments (e.g. Caselli & Ceccarelli, 2013).

Recently, the Rosetta spacecraft's Philae lander may have detected methyl isocyanate (CH<sub>3</sub>NCO) in the comet 67P/Churyumov–Gerasimenko (Goesmann et al. 2015). Methyl isocyanate has been detected for the first time recently towards SgrB2(N) (Halfen et al. 2015) and most recently towards Orion KL (Cernicharo et al. 2015). Finally, using all the available ALMA data, CH<sub>3</sub>NCO has been detected for the first time towards a low-mass proto-star, IRAS16293-2422 (Martín-Doménech et al. 2017; Ligterink et al. 2017).

The chemistry of formamide and methyl isocyanate in the ISM, and of its precursors, is highly uncertain. This chemistry has theoretically been explored only for massive hot cores at high temperatures (Garrod et al. 2013) but only a few modellings has been done for the chemistry of these molecules under the physical conditions found in pre-stellar cores or low-mass proto-stars. There is increased evidence that chemical processes unaccounted for in past theoretical modelling (e.g. UV photo-desorption, cosmic-ray-induced diffusion, and/or chemical reactive desorption) are required to explain the formation, and detection, of complex organics in those regions.

In this talk, I will present a detailed modelling of the chemistry of formamide and methyl isocyanate in star-forming regions such as pre-stellar cores (L1544) and hot corinos (IRAS16293-2422). This chemical modelling aims at fully characterising the main formation/destruction routes of these two species, establishing their expected abundances, and compare them to available observations. This study identifies their precursors and other related species, providing good molecular targets to test our models against observations.

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\*Speaker

# X-ray photodesorption of water ice

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The icy mantle of interstellar dust grains is exposed to a variety of processes, including cosmic ray bombardment, collisions and irradiation, which can eject molecules back into the gas phase and have chemical and structural effects on the ice. Providing experimental constraints on these processes is important for astrophysical modeling. UV photodesorption, for example, has been well studied in the last few years, since UV irradiation is thought to be significant in several interstellar environments [1]. In protoplanetary disks, however, the young star is a source of intense X-ray radiation. X-rays are more penetrating than UV radiations, and therefore the X-ray field is much higher than the UV field in large portions of the disk [2]. The photodesorption induced by this X-ray field may have consequences on the gas-phase abundances of some species, and may also play a role in the position of the " snow line " of some molecules, i.e. the distance from the star at which a given molecule freezes onto the grains, the most important of which is the water snow line. Only a few experimental studies exist on quantified X-ray photodesorption for astrophysically relevant systems so far, e.g. for methanol [3].

Here we report an experimental study of the X-ray photodesorption of water ice around the O 1s edge (500 – 600 eV). Using our upgraded SPICES 2 set-up at the SEXTANTS beamline of the SOLEIL synchrotron, we measured and quantified photodesorption of neutral species, as well as positive and negative ions. Besides the intact H<sub>2</sub>O molecule, a variety of neutral and ionic fragments and products are observed. Photodesorption spectra of the species give us some insights regarding the physical mechanisms behind dissociation and desorption.

## References:

See e.g. Óberg et al., *A&A* 496, 281 (2009a) ; Fayolle et al., *ApJ* 739, L36 (2011) ; Muñoz-Caro et al., *A&A* 589, A19 (2016)

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\*Speaker



# Carbon Chemistry in AGB stars. The first results of the Nanocosmos Project

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We present in this talk the first results of the Stardust machine concerning Carbon-chemistry. In evolved stars chemical models have problems to produce abundant C<sub>n</sub> species for n > 3 due to the presence of many competitive reactions, mainly those producing C<sub>2</sub>H<sub>2</sub>, CH<sub>4</sub> and C<sub>2</sub>H<sub>4</sub>. In our experiments we have observed that the yield of nanoparticles from a cloud of atomic carbon is very low compared to other materials. Our interpretation is based on the difficulty to produce large clusters from small ones due to many forbidden reactions involving small clusters. We have modelled the formation of C<sub>2</sub>, C<sub>3</sub>, and larger carbon clusters, together with silicon-carbon clusters, in the atmosphere of carbon-rich evolved stars and contrasted these models with observations from ALMA, the 30m IRAM telescope. The first results from the stardust machine will be also shown.

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\*Speaker

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# Determining the effect of a non-uniform AGB outflow on its chemistry

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The chemistry in the outflow of an AGB star is dominated by its C/O abundance ratio. For C-rich stars, no O-rich species are expected in the inner wind since oxygen is locked up in CO, and vice versa for O-rich stars. However, several of these unexpected molecules have been detected. Non-equilibrium chemistry in the inner wind, caused by shocks due to the pulsating AGB star, can in most cases explain their existence and abundance. An alternative mechanism is the penetration of harsh UV photons in a non-uniform outflow. In a non-uniform or "clumpy" outflow, which can be caused by e.g. binary interaction, interstellar UV photons can reach the formerly shielded inner wind and break up CO. Using the porosity description, we take a clumpy density distribution into account by modifying the optical depth of the outflow. The porosity description provides us with a solid mathematical framework. We explore the parameter space characterising clumpiness in our chemical model and describe its effect on the chemistry throughout the outflow. We find that our results can explain the existence of certain species in the inner wind and add to the results of the non-equilibrium models.

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\*Speaker

# PAH destruction by heavy cosmic rays – carbon chains production rates

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The ISM contains both CR and PAH. The frontal impact of a single heavy CR with one PAH, strips out many electrons. The highly charged species then relax by multifragmentation, potentially feeding the interstellar medium with hydrocarbon chains. I will present results of calculations for this process. The IAE model was used for collisional purposes while a new microcanonical model was used for fragmentation. Both models agree with experiments. The production rate of low hydrogenated hydrocarbon chains ( $N_c = 5-15$ ) is found to be within 0.1 to 1 zeta depending on the size and morphology of the PAH, and on the adopted content of heavy particles in the impinging CR flux.

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\*Speaker

# Adsorption of PAHs on interstellar ice viewed from molecular dynamics

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Polycyclic Aromatic Hydrocarbons (PAHs) have had an astrophysical interest since they were proposed, in the mid-eighties, to be the carriers the Aromatic Interstellar Bands (AIBs), a set of infrared (IR) emission bands observed in the [3 - 15  $\mu\text{m}$ ] range in many regions of the interstellar medium (ISM). PAHs would also be potential candidates to carry the Diffuse Interstellar Bands (DIBs), which are weak absorption bands measured between 0.38 and 1.3  $\mu\text{m}$  on the extinction curve of our galaxy. Besides, PAHs are likely to play a role in the chemistry of the ISM as, for instance, they would form stable complexes with iron, thus contributing to the iron depletion from the gas phase of the ISM. In molecular clouds, some gases are condensed on dust particles and form ice mantles essentially made of water. PAHs may also condense on/in these ices and contribute to the complex grain chemistry [1]. This heterogeneous chemistry plays a fundamental role in presence of the adsorbed water, which catalyzes photochemical processes. Although ice has been extensively investigated by IR spectroscopy [2], few studies of ices containing PAHs have been reported. To shed light on the unexpected role played by PAHs in cosmic ice chemistry, IR spectroscopy experiments on the cryogenic codeposition [3] of PAH and water are achieved at the Institut des Sciences Moléculaires (ISM, Bordeaux).

In connection with these experiments, we model PAHs interacting with various icy environments using a multi-method approach. The aim is to identify configurations that could best describe the experiments and provide quantitative indications on the effect of the environment on the IR spectra. Our strategy consists in (i) determining the most relevant PAH-ice configurations with a MD/FF (Molecular Dynamics/Force Field) approach [4] and (ii) extracting from such structures starting point finite-size configurations for further Density Functional based Tight Binding (DFTB) calculations, the latter approach describing the electrons explicitly. Results on the effects of the icy environment on the ionization potentials of PAHs and on PAHs' IR spectra - and reciprocally on the effect of PAH adsorption on the IR spectrum of ice- obtained with such a DFTB-based approach will be presented.

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Z. Guennoun, C. Aupetit, and J. Mascetti *J. Phys. Chem. A*, 115(10):1844–1852, (2011).

E. Michoulier et al. submitted

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# PDR-Modelling with the KOSMA-tau PDR code - Recent developments and applications

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The study of star formation and of the interstellar medium gained large momentum during the last years, thanks to the immense amount of radio, infrared and far-infrared data observed with the latest instruments on Spitzer, Herschel, ALMA and SOFIA. The interaction of massive star formation and its ambient medium, e.g. the heating of the dust and gas by strong UV radiation, gives rise to Photodissociation Regions (PDRs), an interface region between the ionized gas in HII regions and the cold molecular gas. PDR-models solve the complex problems of astrochemistry, thermodynamics and radiative transfer and provide observable properties that can be compared with observations.

The Cologne PDR-code KOSMA-tau models spherical PDRs including the local gas-phase and surface chemistry, the line and continuum radiative transfer including a variety of possible dust compositions, and the local heating and cooling balance to approximate the chemical and physical structure of the observed PDRs. The spherical clouds can be combined to form a clumpy ensemble of PDRs: The recent development of KOSMA-tau-3D allows to model arbitrary 3-dimensional PDR structures ranging from local star forming regions”, e.g. Orion (Andree-Labsch et al. 2017), to whole galaxies, e.g. the Milky Way (Cubick et al. 2007, Bruckmann et al.).

In this talk I will give an overview of the recent code developments, e.g. the full surface chemistry update and the self-consistent continuum radiative transfer and dust modelling including low-metallicity environments such as the Small and Large Magellanic Clouds. I will also present a number of recent applications of the KOSMA-tau results to new data.

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\*Speaker

# A new study of the chemical structure of the Horsehead nebula: the influence of grain-surface chemistry

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A wide variety of molecules have now been detected in the Horsehead nebula photodissociation region (PDR) suggesting that: (i) gas-phase and grain chemistries should both contribute to the formation of organic molecules, and (ii) far-ultraviolet (FUV) photodesorption may explain the release into the gas phase of grain-surface species. In order to tackle these specific problems and more generally in order to better constrain the chemical structure of these types of environments we present a study of the Horsehead nebula gas-grain chemistry. To do so we used the 1D astrochemical gas-grain code Nautilus with an appropriate physical structure computed with the Meudon PDR Code and compared our modeled outcomes with published observations and with previously modeled results when available. The use of a large set of chemical reactions coupled with the time-dependent code Nautilus allows us to reproduce most of the observations well, including those of the first detections in a PDR of the organic molecules HCOOH, CH<sub>2</sub>CO, CH<sub>3</sub>CHO and CH<sub>3</sub>CCH, which were thought to be mostly associated with hot cores. We also provide some abundance predictions for other molecules of interest. Understanding the chemistry behind the detection of these organic molecules is crucial to better constrain the environments these molecules can probe.

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\*Speaker

# Time-dependent chemical modeling of H<sub>2</sub> and C<sup>+</sup>/C/CO transitions in Orion Bar

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High-resolution ALMA millimeter-band images show no significant offset between the peak of H<sub>2</sub> emission in the photon-dominated region and CO(3-2) and HCO<sup>+</sup>(4-3) emission toward the molecular region in Orion Bar (Goicoechea et al., Nature, 2016). We verify whether time-dependent astrochemical calculations could reproduce nearly coincident positions of the H<sub>2</sub> and CO dissociation fronts. We use chemo-dynamical model MARION (Kirsanova et al., ARep, 2009; Akimkin et al., MNRAS, 2015, 2017) to predict positions of the H<sub>2</sub> and CO dissociation fronts relative to the ionization front on the interface between the Orion Bar and the Orion Nebula. We present results of three calculations with different dust models: MRN, Weingartner & Draine for R<sub>v</sub>=3.1, and Weingartner & Draine for R<sub>v</sub>=5.5 to study the effect of self and mutual shielding on the H<sub>2</sub> and CO dissociation front positions. We find that in all the three models gas expansion velocity is nearly the same. The absence of the significant (more than 5 arcsec) offset between the H<sub>2</sub> and CO dissociation fronts is obvious after 2000-3000 years of the gas expansion and shock propagation into the molecular gas. At the same time the offset of about 5 arcsec between CO(3-2) and HCO<sup>+</sup>(4-3) peak emission is visible in Orion. We see this small offset in our results utilizing RADEX modeling in the very beginning of the shock propagation prior to the time when the fronts of H<sub>2</sub> and CO dissociation coincide. Our models predict that HCO<sup>+</sup> is converted to CO in the shocked layer but at later computational times the shocked layer is too thin to be resolved by ALMA.

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# Radiation-induced formation of formic acid in the H<sub>2</sub>O–CO system: a matrix-isolation study

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Formation of complex organic molecules under astrophysically relevant conditions is a basically important problem widely addressed in the laboratory simulations. Water and carbon monoxide are among the most abundant molecules in the astrophysical ices, thus the radiation-induced chemistry in the H<sub>2</sub>O–CO system is of significant interest for astrochemistry. It has been shown previously [1] that irradiation of the frozen H<sub>2</sub>O/CO mixtures may lead to the formation of formic acid (HCOOH). In the present work, we investigated the radiation-chemical evolution of the H<sub>2</sub>O–CO molecular system using the matrix-isolation technique, which provides versatile information on both formation and low-temperature reactions of the radiation-induced intermediates.

H<sub>2</sub>O/CO/Ng mixtures (Ng = Ar, Kr, or Xe; typical concentration is 1/1/1000) were deposited onto a cold (15–25 K) KBr substrate mounted in a closed-cycle helium cryostat. Prepared matrices, containing significant amounts of the H<sub>2</sub>O–CO 1:1 intermolecular complexes, were cooled down to 5 K, irradiated with X-rays (energy ca. 20 keV), and then annealed stepwise at various temperatures (up to 45 K). FTIR spectroscopy was used to monitor the formation and decay of different species.

Radiolysis of the H<sub>2</sub>O–CO complexes leads to the loss of H-atoms yielding the OH–CO complexes and some amount of *trans*-HOCO radicals (the less stable *cis*-HOCO conformer is not observed in the noble-gas matrices) [2]. The radiation-induced H-atoms are stabilized at 5 K and could be mobilized by subsequent matrix annealing to react with other matrix-isolated species (for example, H + CO → HCO). Another thermally-induced reaction observed in the studied system is transformation of the OH–CO complexes to the *trans*-HOCO radicals. In Ar and Kr matrices, both the OH–CO → *trans*-HOCO reaction and reactions of H-atoms occur within the same temperature range (25–35 K). In the case of Xe matrices, annealing at 35 K results in complete transformation of OH–CO to *trans*-HOCO, whereas H-atoms mobility is activated at higher temperatures. Formation of HCOOH (detected by the characteristic IR absorptions) was observed in Xe matrices upon annealing at 40–45 K, which evidences the H + *trans*-HOCO → HCOOH reaction. We suggest that this reaction pathway could be more favorable than the H + OH–CO → OH–HCO → HCOOH reaction since formation of HCOOH is not observed in Ar and Kr matrices (where the latter process may happen because H-atoms are reacting at the temperatures low enough, when the OH–CO complex can survive).

To sum up, this work provides some insight into the possible mechanisms responsible for the formation of formic acid in the astrophysical ices. We also believe, that similar experimental approach could be applied in model astrochemical studies related to other prebiotic molecules. The work was supported by the Russian Science Foundation (grant 14-13-01266).

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# Chemical differentiation in the inner envelope of a young high-mass protostar

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The origin of the highest mass stars is still an enigma in modern astrophysics. Only massive clumps, at the onset of star formation, can reveal the initial conditions and shed light on the necessary physical processes leading to their formation. From the 870 micron ATLASGAL survey of the inner Galaxy, we identified the complete sample of infrared quiet massive clumps located closer than 5 kpc. We targeted this sample in the frame of the SPARKS project with ALMA, reaching the physical scales of individual collapsing envelopes. Our sample uncovers a significant sample of the so far known highest mass Class 0 like protostars. Here I will discuss the first insights of the chemical diversity of the immediate vicinity of a young high-mass protostar in its main accretion phase.

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\*Speaker

# New calculations of radiative charge transfer and of radiative association rate coefficients

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Recent calculations of radiative charge transfer and radiative association rate coefficients are presented. In the case of C and He+, both in their ground states, radiative charge transfer is found to be large compared to direct charge transfer at thermal and lower energies [1]. In the case of C and H+ interacting via triplet molecular potentials, the rate coefficients for radiative association are found to be about 100 times larger than the (well-studied) values for radiative association via singlet molecular potentials [2]. New calculations of the radiative association rate coefficients for Si and O are discussed [3].

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# Gas Phase Kinetics of OH Radical With COMs at Temperatures of the Interstellar Medium ( $T = 22\text{-}107\text{ K}$ )

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A great variety of complex organic molecules (COMs) have been detected by astronomical observations in the interstellar medium (ISM) in the last 50 years. Formaldehyde ( $\text{H}_2\text{CO}$ ) and ethanol ( $\text{CH}_3\text{CH}_2\text{OH}$ ) are two of these COMs of importance in prebiotic chemistry in space. In order to model their observed abundances, chemical models need the rate coefficients ( $k$ ) of the processes in which the COM is involved at the temperatures of ISM ( $\sim 10\text{-}100\text{ K}$ ). For many gas-phase reactions with OH radicals, ubiquitous in the ISM,  $k$  is unknown at these ultra-low temperatures, mainly because of the experimental difficulty of reproducing those extreme temperature conditions without condensation of the species. The pulsed and continuous CRESU technique is a powerful tool that allows measuring rate coefficients of IS reactions [1,2]. In our group, some OH-molecule reactions have been recently investigated for methyl formate [3] and methanol [4] between 22 and 61 K using this technique coupled to pulsed laser photolysis and laser induced fluorescence. Currently, this temperature range has been extended up to 107 K and the OH+ $\text{H}_2\text{CO}$  reaction has been investigated for the first time between 22 and 107 K (submitted to PNAS) as well as the OH +  $\text{CH}_3\text{CH}_2\text{OH}$  for which, up to now, there is only a previous study at ISM temperatures between 54 and 148 K [5]. In both cases, we found a significant increase of the rate coefficient below 200 K making these processes potentially interesting for the chemistry in the ISM.

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# Photochemistry vs. Radiation Chemistry of Cosmic Ice Analogs

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While gas-phase reactions and surface reactions on bare carbonaceous or siliceous dust grains contribute to cosmic chemistry, energetic processing via photochemistry and radiation chemistry of cosmic ices is thought to be the dominant mechanism for the cosmic synthesis of prebiotic molecules. Radiation chemistry is defined as the "study of the chemical changes produced by the absorption of radiation of sufficiently high energy to produce ionization." Ionizing radiation in cosmic chemistry includes high-energy particles (e.g., cosmic rays consisting mostly of protons) and high-energy photons (e.g., extreme-UV (12.4 –124 eV), X-rays, and g- rays). In contrast, photochemistry is defined as photon-induced electronic excitation not involving ionization. In addition to photochemistry, vacuum-UV (6.2 –12.4 eV) light may initiate radiation chemistry because the threshold for producing low-energy electrons in condensed matter is lower than the gas phase ionization energy for a given molecule. For example, photoelectric emission threshold of amorphous ice (the main constituent of cosmic ices) is  $\sim 10.2$  eV, which is smaller than the gas phase ionization energy of 12.6 eV for water. Because most previous astrochemical studies have used light sources that produce  $> 10$  eV photons, discerning the role of photochemistry vs. radiation chemistry in astrochemistry is challenging. By using a source whose photon energy does not exceed 8 eV, we have studied ammonia cosmic ice reactions attributable solely to photochemistry. We will compare and contrast these results to those obtained in the same ultrahigh vacuum chamber with 1 keV electrons which initiate radiation chemistry in condensed ammonia.

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# Atom-diatom reactions and molecular clusters in the interstellar medium

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In recent investigations we have investigated reactions of astrophysical interest performing quantum mechanical, quasiclassical trajectory and statistical calculations to obtain cross sections and rate constants. Examples of such processes are reactive collisions between either  $\text{NeH}^+ +$  or  $\text{HeH}^+ +$  with Ne/He [1-4] or the  $\text{H}^+ + \text{H}_2$  [5]. For this latter reaction, rate constants [6] have been employed to design chemical clocks to trace the age of dark clouds of proto-star material in the interstellar medium [7,8]. Rate constants for higher temperatures have been recently reported [9].

On the other hand we have focussed our studies on polycyclic aromatic hydrocarbons (PAH) doped with rare gas and molecular hydrogen [10,11]. These PAHs have been suggested in the past as possible sources of unidentified absorption lines from diffuse interstellar bands. Energy and structure of some of those clusters with an increasing number of impurity atoms were calculated.

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\*Speaker

# Complete Hydrogenation of a PAH cation

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The H<sub>2</sub> molecule is the most important in the Universe. The polycyclic aromatic hydrocarbons (PAH) are well known to be catalyst of the H<sub>2</sub> formation [1]. In this work [2], experimental and theoretical studies have been performed on the hydrogenation of a coronene cations as prototypical PAH molecules. The main results show the existence of magic numbers in the sequential hydrogenation process. The quantum chemistry calculations show that hydrogenation follows a site-specific sequence leading to the appearance of cations having 5, 11, or 17 hydrogen atoms attached, in agreement with the magic numbers found in the experiments. Furthermore, these calculations also allow to propose a complete hydrogenation sequence

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\*Speaker



# Hydrogenation of a PAH deposited on a graphene surface

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The H<sub>2</sub> molecule is the most important in the Universe. The polycyclic aromatic hydrocarbons (PAH) are well known to be catalyst of the H<sub>2</sub> formation [1]. Neutral PAHs are known to exist as the gas phase species [2] or condensed on interstellar dust grains [3]. The study of the hydrogenation of the PAH adsorbed on a graphite surface is essential to understand the H<sub>2</sub> formation. In this work [4], theoretical study has been performed on the first steps hydrogenation of the PAH deposited on a graphene surface using Density Functional Theory including a van Der Waals functional. The role of the surface is determined by comparing hydrogenation reactions in the gas phase and on the surface. The main results are of these work are that the radical product of the H with a closed-shell system is more stable on the surface whereas the closed-shell product of the H with a radical species is more stable in the gas phase.

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\*Speaker

# On the formation of glycine via ion-molecule reaction: theory and experiments

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Different organic molecules have been observed in the space and recently glycine was found in the comet 67P/Churyumov-Gerasimenko.[1] While these molecules have been observed, the mechanisms by which they are formed under astrophysical conditions are not clear. One main problem is that these molecules are very cold such that they do not always have enough activation energy to react under thermodynamic conditions. Ion molecule-reaction is a possibility, which merits to be investigated since the barriers are generally low and the ions can be accelerated under astrophysical conditions and they can use this energy to react.

Here we have studied the formation of glycine, inspired by the earlier works of Bohme,[2] in which the reactants were  $\text{NH}_3\text{OH}^+/\text{NH}_2\text{OH}_2^+$  and  $\text{CH}_3\text{COOH}$ . At this end we have coupled chemical dynamics simulations, in which the ion-molecule collision can be tuned, with novel gas phase experiments, where the reactants and products can be studied via infra-red multi photon dissociation (IRMPD) spectroscopy, thus giving information on their structure.

Collisional simulations dynamics have shown that it is possible to form ions with the same mass-to-charge ratio (which is the observable in mass spectrometry experiments) of protonated glycine ( $m/z$  76) but with different structures. Reaction cross sections are obtained as a function of collision energies and the isomer distribution is also function of the collisional conditions. Independently on the structure of protonated hydroxylamine ( $\text{NH}_3\text{OH}^+$  or  $\text{NH}_2\text{OH}_2^+$ ) we formed molecules with  $m/z$  76, while the isomer distribution is dependent on the reactant employed. Finally, the internal temperature of the ions (300K or 15K) has only a minor effect on products, the most important parameter being the collisional energy.

We have thus studied the same reaction in an ion trap, in which protonated hydroxylamine is formed by electrospray and stable products can be investigated by IRMPD. We have first characterized the structure of protonated hydroxylamine, being likely in the more stable form ( $\text{NH}_3\text{OH}^+$ ). By adding neutral  $\text{CH}_3\text{COOH}$  in the gas phase we obtained as product a stable complex made by the ion and the neutral ( $m/z$  94), which was characterized as well via IRMPD. Band and structure assignment were assisted by quantum chemistry calculations. Very interestingly from the examination of  $m/z$  94 photoproducts we observed that, in particular at

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\*Speaker

some given wavelengths, the  $m/z$  76 (likely corresponding to protonated glycine) is produced. Our future works will go in the direction of a better understanding of this reaction, which can propose as synthetic route in space the coupling of ion-molecule and infra-red induced reactions.

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# Photochemistry of PAH in water ice and of PAH:water complexes. Reaction mechanism and astrophysical implications

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Polycyclic aromatic hydrocarbons (PAHs) are believed to contribute to both the Diffuse Interstellar Bands (DIBs) and the Unidentified/Aromatic Infrared Bands (UIR/AIBs) widely observed along interstellar lines of sight. In star forming regions, PAHs in the solid and gas phases play key roles in the chemical evolution. Several groups have shown that PAHs in water ices react, upon UV irradiation, to produce oxygenated species [1,2,3].

We present the results of a recent experimental and theoretical study of the PAH:water system. FTIR spectroscopy has been used to investigate the photo- reactivity of coronene and pyrene with water molecules at low temperatures in both argon matrices and in solid water ices. Ab-initio (DFT, DFTB) calculations of water:PAH clusters have been used to study intermolecular interactions and the effect of the argon matrix on such aggregates [4].

We show that PAH:water systems are highly photoreactive, producing oxygenated products after short UV irradiation times. We also show that the presence of a water ice is not necessary to catalyse the PAH:water reaction, but rather that small water clusters ( $n < 6$ ) can react with PAH molecules to form alcohols and quinones. Calculations performed on PAH:water systems involving water clusters and water ices support the conclusion that the orientation of the PAH compared to the water molecules is a key factor controlling the photo reactivity pathway [4] [5]. Both the matrix and water ice environments favour water reaction with the edges of PAH molecules.

These results suggest that oxygenated PAHs could be formed in dense clouds with low water abundance, where there is low energy UV field and where water does not condense onto grain surfaces in the form of an icy layer.

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# Data of fragmentation for neutral, cationic and anionic C<sub>n</sub>N molecules (n=1-3)

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Data of fragmentation for neutral, cationic and anionic C<sub>n</sub>N molecules (n=1-3)  
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Carbon and Nitrogen based molecules are abundant in the ISM, amounting to about one third of the total detected species. Amongst those, C<sub>n</sub>N molecules, on their neutral and anionic forms, have been detected in ISM (n<5) and also in planetary atmospheres such as Titan [1]. Despite their presence, the reactivity of C<sub>n</sub>N molecules is poorly known experimentally, especially for neutral and cations since the negative species are slightly more documented [2]. In KIDA all reported values concerning photodissociation of C<sub>n</sub>N, dissociative recombination of C<sub>n</sub>N<sup>+</sup> cations, reactions of neutral C<sub>n</sub>N with C, N and C<sup>+</sup> are based on calculations or estimations from results on similar systems [3]. Also the estimations are restricted to the main output channels and a complete picture of the reactivity is missing.

We have studied the fragmentation of neutral, cationic and anionic C<sub>n</sub>N molecules (n=1-3). The tool is the high velocity collision between C<sub>n</sub>N<sup>+</sup> projectiles and helium atoms at high velocity. The dedicated AGAT setup allows to record and identify all fragmentation channels thanks to the use of about ten detectors operating in coincidence. From these measurements it is possible to construct semiempirical Breakdown curves (BDC) which are internal energy dependent branching ratios [4]. The BDC are specific to each molecule and allow to predict its fragmentation induced by any process if the associated energy deposit is known and assuming statistical fragmentation. The method has been applied with success for predictions of branching ratios (BR) in carbon and hydrocarbon molecules submitted to various radiations and chemical reactions [4]. We will present results of fragmentation BR for neutral , cationic and anionic C<sub>n</sub>N and semiempirical BDC of neutral and cationic C<sub>n</sub>N molecule. We will discuss applications of those BDC and compare some of their predictions with existing data.

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\*Speaker

# Laboratory Measurements for Deuterated Astrochemistry

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Deuterated molecules are powerful probes of the cold interstellar medium (ISM). Observations of D-bearing molecules are used to infer the chemistry of the ISM and to trace out physical conditions such as density, ionization fraction, and thermal history. The chemistry of the cold ISM results from a complicated interplay between gas-phase processes, reactions on dust grain surfaces, and chemistry occurring both in and on the icy mantles of dust grains. Our focus here is on an improved understanding of the relevant deuterated gas-phase chemistry. At the low densities and temperatures typical of the cold ISM, much of this chemistry is driven by binary ion-neutral reactions, which are typically barrierless and exoergic (as compared to neutral-neutral reactions which often have significant activation energies).

One of the biggest challenges in generating a reliable deuterated gas-phase astrochemical network is the uncertainty of the necessary rate coefficients. The vast majority of available chemical kinetic data are for H-bearing species. For those D-bearing reactions where no laboratory data are available, two approaches have been adopted for converting the H-bearing data into partial- and fully-deuterated species. The first approach simply "clones" the H-bearing reactions into D-bearing reactions and assumes that the rate coefficients are the same. The second approach uses a simple mass scaling relationship based on the Langevin formalism.

We have initiated a series of laboratory measurements aimed at resolving this issue. For this we use our novel dual-source, merged fast-beams apparatus, which enables us to study reactions of neutral atoms and charged molecules. Using co-propagating beams allows us to achieve collision energies corresponding to temperatures as low as 25 K, limited only by the divergences of the two beams. Recently we have measured the reaction C on H<sub>2</sub><sup>+</sup> forming CH<sup>+</sup> and C on D<sub>2</sub><sup>+</sup> forming CD<sup>+</sup>. We are now studying D on H<sub>3</sub><sup>+</sup> forming H<sub>2</sub>D<sup>+</sup> and D on D<sub>2</sub>H<sup>+</sup> forming D<sub>3</sub><sup>+</sup>. Here we report on these results and discuss their astrochemical implications.

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# Collisional Excitation of NH molecules by He and H<sub>2</sub>

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We present fine and hyperfine resolved collisional rate coefficients for the NH(ND)-He and NH(ND)-H<sub>2</sub> systems. NH and ND molecules play a very crucial role in the prestellar chemistry as they act as intermediate during the formation of the ubiquitous ammonia. Hence there is a need for the accurate modelling of their abundances in space to better understand the physical conditions and the chemical evolution of the prestellar core. We consider H<sub>2</sub> and He as the colliding partners as they are dominant species in the interstellar medium and significantly contribute to the excitation of both NH and ND.

The earlier studies [1][2] on the NH-He system were performed using the potential energy surface (PES) of the Cybulski et al. [3], which was proved to be relatively accurate. However, they did not consider the vibration of the NH bond which can impact the magnitude of the collisional data. Hence, in the present calculations, we take into account the vibration of the N-H molecules. The calculated rate coefficients are compared with the previous available theoretical data and the experimental measurements at room temperature. From the comparison we can observe that there significant difference between the new and the old rate coefficients. We also observe a good agreement with the experiments. It confirms that inclusion of NH vibration is needed to accurately model the energy transfer in the NH(ND)-He system. Hence the new set of data could be used to redefine the earlier observations and their interpretations.

We also present the first ever computed PES for the NH-H<sub>2</sub> system and preliminary rate coefficients. These results would be of particular interest because they are first for this system and they should contribute significantly impact the astrophysical modelling by allowing an accurate determination of the NH abundance in the space.

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# An analytical fit of adiabatic potential energy surface

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Astrochemical models at the molecular level deals with chemical reactions described as

collision between two molecules. The conditions in the interstellar medium (ISM) are extreme and mostly the chemistry can be viewed as a collision with interest in the abundances of surface species through the use of rate equations by giving the reaction rate coefficients for chemical reactions.

In order to obtain a better description of the collision between two molecules, a form for the molecular interaction potential should be assumed. Usually, a Lennard Jones potential is employed. The first theory of ion-molecule reactions was proposed by P. Langevin.

Determining theoretically a rate coefficient first one focuses on electronic calculations for calculating potential energy surfaces (PES), in BO approximation, further used to study the motion of the nuclei (collision dynamics).

In this work an analytical expression of potential energy surface is derived and used to describe especially the cases where the present data fully support a model [sor94] that assumes that

there are potential barriers or bottle necks.

The figure 1 shows some combinations of parameters for the analytical expression of potential [iac15]. The evaluation of energies in Schrodinger dynamics has been made (figure 2).

It is an open question whether one can classify reactions with nonstandard temperature dependences with a few simple reaction mechanisms based on simple properties of the potential energy surface such as barriers or wells. Low temperature experiments have shown [asv04a] that there can be significant deviations from such simple models. This may be due to subtle details of

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the potential energy surfaces such as small barriers or bottle necks which are not yet known with the accuracy required for low temperature reactions. In addition it is rather sure although not yet understood quantitatively with exception of simple systems [ger90] that symmetry selection rules play a pivotal role in replacing in a group of identical atoms just one by an isotope or vice versa.

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# Modeling volatile depletion in protoplanetary disks

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It has been found that carbon- and oxygen-bearing species are depleted relative to dust in some protoplanetary disks, e.g. in TW Hya and DM Tau. This could be due to the overall reduction of the disk gas mass, or, it could be that the disk gas mass (mainly contributed by H<sub>2</sub> molecule) is not reduced but the carbon and oxygen elements are depleted (and by a different degree for different elements). Another line of reasoning comes from observations of C<sub>2</sub>H and C<sub>3</sub>H<sub>2</sub> molecules in TW Hya and DM Tau, which exhibit ring structures. To explain their strong ring features, we propose that oxygen is depleted relative to carbon in the outer part of the disk, caused by the formation of ice-covered grains followed by the sedimentation and aggregation processes. We model this effect in a parametric approach. Future work need to couple the dust processes with the chemical processes (work in progress).

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\*Speaker

# Photochemistry of Fe:H<sub>2</sub>O adducts in argon matrices

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The ISM is a very disparate environment, within which molecular clouds play an important role by sheltering interstellar dust from irradiation, and thus allowing the development of a very rich chemistry. Observations combined with elemental abundance calculations show that iron is severely depleted in molecular clouds, which in turn could indicate that this key element may be in interaction with water, PAHs, or both, on dust grain surfaces. This study consisted of the deposition and spectral characterisation of binary systems of atomic iron with H<sub>2</sub>O in cryogenic argon matrices. In this way, we were able to obtain information about the interaction of the two species; we observed the formation of adducts of iron monomers and dimers with water molecules in the MIR and UV-visible spectral domains. Upon irradiation with a UV radiation source, the iron species were inserted into the water molecules to form HFeOH, leading in some cases to the formation of FeO possibly accompanied by the production of H<sub>2</sub>. DFT and ab-initio calculations confirmed our attributions, and this combination of IR and UV-visible spectroscopy with theoretical calculations allowed us to determine, for the first time, the spectral characteristics of iron adducts and their photoproducts in the UV-visible and in the OH stretching region of the MIR domain. These results combined with our previous work on PAH: H<sub>2</sub>O represent a strong benchmark for further experimentation on ternary systems including Fe, PAH and H<sub>2</sub>O.

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\*Speaker

# Influence of the basis set on the branching ratios for mutual neutralization in Li and D-collisions

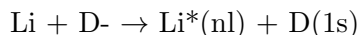
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Modelling of stellar atmospheres requires various detailed and accurate data on different processes such as the mutual neutralization (MN) of cation-anion pairs that can affect atomic species of interest. Among all the possible reactions, neutralization plays an important role in atmospheric and astrophysical processes. Furthermore, due to the difficulty to accurately obtain experimental and theoretical data, there is a strong demand for information on the low energy cross section of processes involving H- (or D-).

Our merged-beam setup [1] was modified in order to be able to study the mutual neutralization between Li and D- and determine which states of the neutral lithium atom are predominant in the total cross section:



Preliminary measurements at 7 meV average collision energy have been performed and compared with theoretical calculations [2]. Our apparatus gives access to the branching ratio among accessible neutral channels of the lithium atom and could discriminate between the Li(3p) and Li(3d) channels which are separated by only 44 meV. The measured total cross section of this study agrees with the results of Croft et al. However, our measured branching ratio suggests higher proportions of the 3d (by approximately 6%) and 3s (by approximately 5%) channels at the expense of the Li(3p).

In order to explain this difference, new theoretical calculations using the MRCI+Q methodology have been performed and cover various basis sets, i.e. Slater Type Orbitals (STOs) or even-tempered basis sets, in order to look at their influence on the avoided crossings and the non-adiabatic coupling matrix elements.

Thus, using a multi-channel Landau-Zener methodology, partial and total cross sections have been computed, showing a good agreement with the experimental values using STO basis set. Dramatic influence of the basis set on the branching ratios is shown and can completely change the dynamic.

Further experiments at higher collision energies are still needed to compare our results with the experimental study of Pear and Hayton [3] which was restricted to higher collision energies in the range of 0.7 to 316 eV or with the new calculations.

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# UV photodesorption of CH<sub>4</sub> from pure and CO-rich ices

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In cold and dense regions of the interstellar medium (ISM), molecules are found either in gas phase or accreted at the surface of interstellar dust grains. UV irradiation of the ice mantle of these grains is the motor for a rich solid-phase chemistry, but also provides a non-thermal pathway for the desorption of molecules. This photodesorption process is believed to account for a significant part of the gas-to-ice abundance ratio of some molecules. In recent years, laboratory studies have aimed at determining absolute photodesorption rates of molecules commonly found in the ISM (CO, H<sub>2</sub>O, N<sub>2</sub>, CO<sub>2</sub>...) and at understanding the underlying desorption mechanisms (Bertin et al 2013, Fayolle et al 2013, Fillion et al 2014).

Here we report an experimental study of the photon-induced desorption of CH<sub>4</sub> (Dupuy et al 2017), one of the most abundant molecules in ice mantles. We obtained the energy-resolved photodesorption rates between 7 and 13.6 eV for both a pure, thick CH<sub>4</sub> ice and for CH<sub>4</sub> deposited on top of a thick CO ice. The photodesorption of CH<sub>4</sub> from pure ice in various interstellar environments is around  $2.0 \pm 1.0 \times 10^{-3}$  molecules per incident photon. Results on CO-induced indirect desorption of CH<sub>4</sub> confirms the ability of CO to induce desorption of other molecules as already observed in Bertin et al (2013), significantly changing the energy-resolved profile and overall photodesorption yield of CH<sub>4</sub> compared to the case of the pure ice.

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\*Speaker

# Experimental study of collisions of $2\text{H}^+$ , $\text{He}^+$ , and $\text{He}2^+$ with complex interstellar molecules at keV energies

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Several complex organic molecules have already been detected in various regions of the interstellar medium. Namely, dimethyl ether, methyl formate, ethanol, formic acid, methyl cyanide, and ethyl cyanide were detected in several star-forming regions and cold molecular clouds. [1] The current scenario of their formation is based on the recombination of radicals at the surface of interstellar grains. [2] Recently, possible mechanisms for their destruction also became a subject of laboratory studies. [3]

In this paper, laboratory experiments aimed at interactions of selected interstellar molecules with stellar wind particles such as  $\text{H}^+$  ( $2\text{H}^+$ ),  $\text{He}^+$  and  $\text{He}2^+$  at keV collision energies will be reported. The experiments were performed on a modified sector-type mass spectrometer having a quadrupole mass analyzer attached to a collision chamber located between the magnetic and the electrostatic sector. The incident particles were formed by electron ionization of hydrogen (deuterium) and helium gases, accelerated to 5 – 10 keV, mass-selected by the magnetic sector and directed through the collision chamber. The slow secondary ions stemming from the neutral molecules admitted to the collision chamber were analyzed by the quadrupole mass analyzer.

Pressure inside the collision chamber, as well as projectile and secondary ion currents, were measured absolutely so that we were able to determine collision cross sections for the formation of positive ions from studied molecules.

As follows from Fig.1, the abundances of both the parent and fragment ions strongly depend on the nature of incident particles. Various aspects of these high-energy processes such as relative cross sections, internal energy depositions, projectile recombination and collision energy dependencies, and comparisons with analogous processes at thermal energies will be discussed.

## Acknowledgement

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# O<sub>2</sub> interaction with water ice surfaces for desorption modelling in astrochemical applications

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Desorption is the fundamental process through which frozen-out molecules on icy dust grains can be freed to the gas phase where they can remotely be identified in the interstellar medium (ISM). Although many efforts have been made to study thermal desorption processes experimentally, it remains difficult to obtain unimolecular (photo)desorption rates, *i.e.* at  $\sim 0$  surface coverage, which is more representative of scarce molecules in the ISM. This is however not a problem for theoretical simulations, where the interaction of a single molecule with its environment can be studied precisely. The O<sub>2</sub>-water ice system is studied as a benchmark for the development of the method. The interaction configuration of molecular oxygen with a slab of amorphous water ice is studied using classical molecular dynamics and QM/MM in order to determine the ground and excited states potential energy surfaces (PES) of the system. From these, desorption cross sections will be determined through wave packet propagation. The obtained desorption rates will be included in chemical reaction network models for comets or molecular clouds, where the different desorption processes have an important impact for the interpretation of remote observations. Cessateur *et al.* have already set up a minimal model of comet 67P/Churyumov-Gerasimenko (67P) for the study of atomic oxygen line emissions, while De Keyser *et al.* have already documented the presence of distributed sources – essentially, desorption from icy grains in the cometary atmosphere – in the coma of comet 67P specifically. The goal of this work is ultimately to use more comprehensive software packages such as KIDA in order to assess the impact of distributed sources on the overall chemistry of comae. The input parameters for the model, such as neutral densities in the coma of 67P, will be provided by ROSINA/DFMS mass spectrometry measurements aboard the ESA Rosetta spacecraft.

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# Forming ozone: A kinetic study of the irradiation of water and carbon dioxide ices

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Water and carbon dioxide ices are found throughout the Solar System, from the polar ice caps of Mars to the distant moons of Uranus (Ariel, Umbriel and Titania), and they often occur as a mixture. Water and carbon dioxide ice is also found in the interstellar medium on dust grains. Galactic cosmic rays exist in both the Solar System and further afield, as well as UV photons and these can influence the composition of the ices. Additionally, outer Solar System moons are subjected to their host planets magnetosphere which also contain ions. From previous laboratory studies, it is well known that when a mixture of water and carbon dioxide ice is processed, ozone is formed amongst other products, but when pure water ice is processed, ozone production is inhibited. In these studies, several processing techniques are used (e.g. electrons, UV photons, ion bombardment) and the mixing ratios of the water : carbon dioxide mixture ranges from 1:1 to 1:0.2 to 10:1 to 1:5. Here, I present a systematic study of the effect that mixing ratios have on the formation of ozone from processed water : carbon dioxide ice mixtures using mid-IR spectroscopy to monitor the formation. Also, I will present the effect that two different processing techniques, electrons and UV photons, have on the formation rates of ozone.

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# Ion-induced Ionization and Dissociation of Polycyclic Aromatic Hydrocarbons by keV Ions

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Polycyclic aromatic hydrocarbons (PAHs) are known carcinogens with fairly wide natural abundance. Most surprisingly, their presence was detected in the interstellar medium or in the upper atmosphere of Saturn's moon Titan [1, 2] and are anticipated in the atmosphere of Jupiter [2, 3]. The PAHs emerge as a result of ion-molecule reactions of simpler organic species, however, they are also subjected to collisions with the "water group ions" (H<sub>2</sub>O<sup>+</sup>, OH<sup>+</sup>, and O<sup>+</sup>) and with ions formed by ionization of sulphur dioxide (S<sup>+</sup>, O<sup>+</sup>, SO<sup>+</sup>, SO<sub>2</sub><sup>+</sup>, S<sub>2</sub><sup>+</sup>, and O<sub>2</sub><sup>+</sup>) in Titan's [4] and Jupiter's [5, 6] atmospheres respectively.

In this study the effects of mass, charge and chemical structure of projectile ions on the ionization cross section and the amount of internal energy deposited in nascent secondary ions are investigated using a modified sector type mass spectrometer.

The modifications include collision chamber and quadrupole mass analyser which is to analyse secondary ions stemming from the collisions of projectiles with neutrals. The PAHs are introduced into the collision chamber using a heated direct insertion probe. The projectile ion current is measured absolutely, however the pressure of PAH vapours cannot be measured, therefore we are not able to determine absolute cross sections. Mass spectra reflecting the amount of internal energy deposited into the emerging PAH molecular ions will be presented.

## Acknowledgements

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# Modélisation périodique *ab initio* de processus non-réactifs et réactifs à la surface de grains

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La compréhension de la formation et de la réactivité des molécules organiques complexes (COMs) détectées dans le cosmos reste parcellaire et sujet à polémique. Longtemps les processus réactionnels en phase gazeuse ont été considérés comme les seules voies de synthèse de ces molécules. Mais, jusqu'à présent, la réactivité en phase gazeuse seule n'a pas permis d'expliquer toutes les observations, loin s'en faut.

Dès lors, les processus chimiques hétérogènes à la surface des grains de poussière interstellaires constituent une piste sérieuse de réactions catalysées dans le MIS.

Dans ce contexte, la réactivité chimique de molécules et de radicaux, soit à la surface du solide, soit au cœur du solide, doit être examinée grâce à des simulations numériques basées sur des méthodes de Chimie théorique de type DFT périodique "premier principe" et *ab initio*. La périodicité du modèle est particulièrement indispensable à cette modélisation.

Le cas des surfaces de glace, de loin les plus répandues dans le MIS servira d'illustration. Plusieurs exemples de problématiques astrochimiques reliées au solide seront détaillés.

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# ALMA observations of oxygen-bearing complex organic molecules towards the low-mass protostellar binary IRAS 16293-2422

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Many questions remain concerning the formation of complex organic molecules and their presence in the inner regions close to solar-type protostars. The low-mass Class 0 protostellar binary IRAS 16293-2422, located only 137 pc away, is an excellent object to study these species on solar system scales. Unprecedented levels of detail in such star forming regions can be studied using the high spectral and spatial resolution of ALMA (Atacama Large Millimeter/sub-millimeter Array). We use the observations from the Protostellar Interferometric Line Survey (PILS), an ALMA survey of IRAS 16293-2422, to analyse oxygen-bearing complex organic molecules in both IRAS16293A and IRAS16293B. A comparative analysis of the two sources shows differences in abundances for some of the species, and their isotopologues. For example, acetaldehyde ( $\text{CH}_3\text{CHO}$ ) shows an abundance towards IRAS16293A one order of magnitude lower in abundance towards IRAS16293B, with respect to methanol, whereas ethylene oxide (*c*- $\text{H}_2\text{COCH}_2$ ), one of its isomers, is present in similar proportions towards both sources. Such differences between isomer species, that share some formation pathways, lead to a better understanding of the chemistry that takes place in low-mass star forming region.

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\*Speaker

# Study of chemical evolution in cold clouds using Nautilus grain size distribution model

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ABSTRACT:

Many chemical reactions occur at the surface of interstellar dust grains, producing a large diversity of molecules more or less complex. Most current astrochemical models include a single size of grains (0.1 micron representing most of the mass of silicate grains). We have studied the effect of considering a distribution of grain sizes on the chemical evolution of various complex molecules in cold clouds in the ISM

We used two different types of grain size distributions, MRN and WD. Each grain has its own grain number density which comes from either MRN or WD distribution. Other parameters such as grain temperature or cosmic ray desorption also varies with grain size. We present abundance of various molecules including some complex molecules in gas phase and also on the surface of dust grains at different time interval during the simulation.

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# X-ray radiolysis of solid and matrix isolated C2 hydrocarbons

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The C2 hydrocarbons (ethane, ethylene, and acetylene) were detected on Titan and Pluto as well as in cometary ices, and therefore, the investigation of radiation effects on these compounds is of significant interest for astrochemistry [1-3]. In the present study, we focused on the X-ray radiolysis of the C2 hydrocarbons in solid media.

The radiation-chemical experiments were performed at cryogenic temperatures with both pure C2 hydrocarbons and C2H<sub>x</sub>/Ng mixtures (x = 2, 4, or 6; Ng = Ar, Kr, or Xe; typical concentration is 1/1000). Gases (or gaseous mixtures) were deposited onto a cold KBr substrate mounted in a closed-cycle helium cryostat and then irradiated with X-rays (effective energy ca. 20 keV). Radiation-induced products were detected using FTIR spectroscopy.

Our observations of the radiation-induced products in the solid C2 hydrocarbons are mainly in line with the previous reports on the radiation processing of pure hydrocarbon ices [1-3]. In the case of ethane (C2H6), the principal radiation-induced products are C2H5 and C2H4, and formation of C2H2, CH4, and C4H10 is observed at higher doses. X-ray radiolysis of solid ethylene (C2H4) leads to the production of C2H2 and C2H5, whereas the irradiation of solid acetylene (C2H2) results mainly in the formation of some conjugated hydrocarbons.

Results of the matrix-isolation experiments bring some new information about the radiation chemistry of C2 hydrocarbons at a molecular level concerning primary degradation channels of a single molecule. In the case of matrix-isolated acetylene, the C2H2 → C2H + H is the only primary reaction and further dissociation C2H → C2 + H occurs at higher doses. It was found that primary radiation-induced decomposition of matrix-isolated ethylene included both C2H4 → C2H3 + H and C2H4 → C2H2 + H2 (or 2H) reactions, and prolonged radiolysis leads to the decomposition of the primary radiation-induced products. In the case of ethane, we also observed the involvement of "deep dehydrogenation" channels, i.e. effective formation of C2H2 and C2H4 (in addition to C2H5). From the quantitative measurements of the radiation-induced decay of different C2 hydrocarbons isolated in noble gas-matrices we may conclude that radiation resistance of these molecules increases in a row C2H6 – C2H4 – C2H2.

We believe that the results of the present studies make an original contribution to the laboratory simulations of the hydrocarbons chemistry in the space environment. This work was supported by the Russian Foundation for Basic Research (grant 16-33-00859-mol.a).

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# Energy dependence of effective destruction rates of CH<sub>4</sub>- and N<sub>2</sub>-rich ices - I: Experimental approach considering ions, photons, and electrons.

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In this work we present an experimental study on the determination of effective destruction rate  $k_d$  of molecular methane and nitrogen by cosmic rays in CH<sub>4</sub>- and N<sub>2</sub>-rich ices at very low temperature. The ice samples were produced inside a high-vacuum chamber and bombarded by swift ions (15 MeV O<sup>(+5)</sup>) at the IRSSUD beam line of the GANIL heavy ion accelerator at Caen, France. The chemical changes in the samples were monitored by IR spectroscopy at different ion fluences. The effective destruction rate of solid samples were derived from the measurement of effective destruction cross section combined with typical ion flux in space environments (interstellar medium). The value obtained of  $k_d$  for both solid species in the presence of 15 MeV oxygen ions were around  $10^{-14}$  -  $10^{-13}$  s<sup>-1</sup>. Additionally, we combined the current measurement with the available data from the literature and derive a power law dependence of  $k_d$  with the electronic stopping power ( $S_e$ ) of the incoming ions. The obtained relation were  $k_d \propto S_e^n$  with  $n=1.3$  and  $2.1$  for CH<sub>4</sub> and N<sub>2</sub> destruction respectively (See figure). This equation help us to understand influence of different incoming cosmic rays (with different energies) in the destruction of astrophysical ices and should be included in future astrochemical models of ices exposed to space radiation. For comparison purpose we add additional data of ices irradiated by ionizing photons (UV and X-rays) and electrons and compare the results with the ones obtained with ions. **Acknowledgments:** We thank the Brazilian financial agencies FAPESP, CNPQ and the technical help of GANIL staff.

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\*Speaker

# From crystalline to amorphous water ices simulations: The case study of atomic and molecular embedding.

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The origin of volatiles observed in different environments in the solar system, such as comets, and atmospheres of giant planets satellites, rises important problems still unsolved. We investigated different types of scenarios that all require the trapping of the volatiles of interest inside the ice bulk. Using first principle periodic DFT simulations, we calculated the stability of these volatiles as a function of their location inside the ice.

The strategy to obtain cavities inside the bulk will be presented. It is shown that a continuous path exists that allows to pass progressively from a pure crystalline network to an porous structure by appropriate modifications of the size and composition of the unit cells of the periodic calculations.

It will be seen that the stabilization energies may vary with the size and shape of the cavities present within the solid host; we have found also that the role of the distance of the embedded species to the surface may be a non negligible factor.

Illustrative examples of atomic (Na,K) and diatomic molecules (O<sub>2</sub>, S<sub>2</sub>, ...) will be presented.

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# Energy dependency of effective destruction rates of CH<sub>4</sub>- and N<sub>2</sub>-rich ices – II: Astrophysical implications on PPDs employing the ProDiMo code

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Astrophysical ices are ubiquitous in the Interstellar Medium as have been shown by ground- and space based telescopes in the IR. In this sense, the increasing in the sensitivity of detection of the instruments, has led to detection of large and complex molecules both in gas- and solid-phase. In this scenario laboratory experiments and theoretical models have work together to address the chemistry of dense molecular clouds and star-forming regions. In this work we report some results obtained with the state-of-art ProDiMo code by comparing simulations with and without surface chemistry in the Protoplanetary Disks (PPDs). Specifically, in the models with surface reactions, we study the energy dependency of effective destruction rates ( $k_{eff}$ ) of CH<sub>4</sub>- and N<sub>2</sub>-rich ices obtained from the effective photodissociation cross-sections from UV to X-rays (6 – 2000 eV). The preliminary results have shown the formation of several complex molecules such as CH<sub>3</sub>OH, CH<sub>3</sub>CHO, as well as, a large amount of ions, which retards the star formation process due to ambipolar diffusion.

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# Reactive collisions of electrons with molecules of astrochemical interest: application to hydride cations and to neutral oxygen

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New cross sections and rate coefficients for dissociative recombination, elastic scattering and ro-vibrational excitation of molecular ions relevant for the interstellar molecular clouds and for the early Universe [1] will be presented. They have been obtained using a stepwise method based on the Multichannel Quantum Defect Theory (MQDT) [2], accounting for the interference between direct and indirect process, the latter occurring via strongly resonant captures into highly excited bound Rydberg states.

The reaction dynamics calculations rely on recently-obtained molecular structure data – potential energy curves and Rydberg-valence interactions – produced by the use of either the R-matrix [3], or the block-diagonalization [4] method.

Rotational excitation rate coefficients for H<sub>2</sub><sup>+</sup> [5] and HD<sup>+</sup> [2] will be shown, as well as rotationally-resolved dissociative recombination rate coefficients for these ions and for CH<sup>+</sup> [6]. The rotational effects diminish above 1000 K, but the dissociative excitation plays an important role, as shown in extensive computations on H<sub>2</sub><sup>+</sup>. Core-excited-bound-Rydberg-states effects will be illustrated for SH<sup>+</sup> [4] and CH<sup>+</sup>, and the recombination of ArH<sup>+</sup>, poorly studied so far, will be discussed.

Our state-to-state calculations will be compared with measurements performed in the TSR (Heidelberg), TARN (Tokyo) and CRYRING (Stockholm) magnetic storage rings.

Finally, recently obtained results on electron-impact vibrational excitation, dissociative attachment and dissociative excitation of O<sub>2</sub> [7] will be illustrated.

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# Simplified model for estimating inelastic heavy-particle-hydrogen collision data.

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A simplified model for estimating atomic data on inelastic processes in low-energy collisions of heavy-particles with hydrogen is derived. The model gives reliable estimates for the inelastic processes with high and moderate rate coefficients, that are known to be important for non-LTE modeling of cool stellar atmospheres.

The proposed model is based on the asymptotic method for electronic structure calculations and the Landau-Zener model for nonadiabatic transition probability determination.

The rate coefficients are expressed via statistical probabilities and reduced rate coefficients. Reduced rate coefficients for mutual neutralization and ion-pair formation processes depend on single electronic bound energies of an atom, while the reduced rate coefficients for excitation and de-excitation processes depend on two electronic bound energies.

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# Gas-phase and grain surface chemistry in hydrodynamic simulations

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Observational studies find different spatial distributions of molecules in individual prestellar cores (e.g. CH<sub>3</sub>OH and carbon chain molecules in L1544). The interpretation of these features using pseudo-time dependent gas-grain chemical models, that assume single zone or spherically symmetric geometries, is limited. However, self-consistent, three-dimensional hydro-chemical simulations of molecular clouds cores, which include these species and their gas phase, gas-grain and grain surface formation/destruction mechanisms are computationally challenging and to date lacking.

We present a computationally cost-efficient method to model the gas-grain chemistry of molecular clouds, in particular focusing on low mass prestellar cores. A relatively small chemical network of the most important chemical coolants (e.g. C<sup>+</sup>, O, CO) is used in our hydrodynamic simulation to follow the formation of prestellar-cores and to obtain time dependent physical conditions. The time evolving physical conditions are fed to a gas-grain chemical code, based on the KIDA reaction network. The resulting abundances are combined with the hydrodynamic quantities (i.e. density, temperature, velocity field) to obtain column density maps and radial abundance profiles of the prestellar cores.

We find morphologies similar to observations, e.g. shifted column density peak of CH<sub>3</sub>OH compared to the H<sub>2</sub> column density peak, and similar degrees of depletion. We investigate the role of direction dependent irradiation, non-symmetric matter distribution and gas dynamics in producing these features.

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# Efficient chemical pathway for the synthesis of formamide on cold interstellar dust grains

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# The reactions of electronically excited atomic nitrogen, N(2D), with small aromatic compounds and their relevance in the prebiotic chemistry of Titan

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Gas-phase reactions involving atomic nitrogen in the ground 4S and first excited 2D electronic states with simple hydrocarbons or hydrocarbon radicals lead to the formation of prebiotic N-containing organic molecules. These reactions are now active in the upper atmosphere of Titan (a massive moon of Saturn) and might have played an important role in nitrogen fixation in the primitive upper terrestrial atmosphere, assuming that it was similar to the present atmosphere of Titan. The products of these reactions (nitriles, imines and radicals) are the precursors of larger N-containing molecules, which form the dense haze aerosols that completely cover Titan. If anything similar to Titan's haze has ever existed on our planet, it is reasonable to imagine that, once deposited on the surface of the oceans, further chemical evolution might have transformed these molecules into amino acids and nucleobases [1].

In our laboratory we have investigated several bimolecular reactions involving N(2D) and aliphatic hydrocarbons by means of the crossed molecular beam technique with mass spectrometric detection. According to our experimental data, the reactions of N(2D) with hydrocarbons lead to an inventory of complex N-containing organic molecules (see, for instance, Refs. [2,3]). In this contribution new experimental data on the reactions with small aromatic compounds (also present in the upper atmosphere of Titan) will be presented. Experimental data are interpreted in the light of electronic structure calculations of the relevant potential energy surface performed ad hoc.

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# Laboratory experiments for the interaction of complex organic molecules with cold surfaces of interstellar interests

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Formamide and methylamine are known to be the most abundant amine-containing molecules in many astrophysical environments. The presence of these molecules in the gas phase may result from thermal annealing of interstellar ices. The aim of this work is to determine the accurate values of the desorption energies of formamide and methylamine from analogues of interstellar dust grain surfaces, and to understand their interaction with the water ice. Thermal programmed desorption (TPD) experiments of formamide and methylamine ices have been performed in the submonolayer and monolayer regimes on graphite (HOPG) and on amorphous solid water (ASW) ice surfaces using the FORMOLISM (FORMation of MOlecules in the ISM) set-up. The desorption energy distributions of NH<sub>2</sub>COH and NH<sub>2</sub>CH<sub>3</sub> are derived from TPD measurements in the submonolayer regime using the Polanyi-Wigner equation. The desorption of solid formamide from both graphite and ASW ices surfaces occurs 18 K after the onset of the H<sub>2</sub>O water desorption. Whereas, the desorption profile of methylamine depends on the substrate, and the derived binding energies of NH<sub>2</sub>CH<sub>3</sub> are very different from those obtained from pure multilayer experiments. The desorption energy distribution of formamide from the graphite surface is (7460 K-9380 K), while the desorption energy distribution of methylamine from the np-ASW ice surface is found to be (3900 K-4810 K). Such desorption energies are far from multilayer desorption energies. More information and details about the interaction of these two COMs molecules with the substrates are given in the poster.

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# Non-Detection of HC11N toward TMC-1: Constraining the Chemistry of Large Carbon-Chain Molecules

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Bell et al. (1997) reported the first detection of the cyanopolyne HC11N toward the cold dark cloud TMC-1; no subsequent detections have been reported toward any source. Additional observations of cyanopolyynes and other carbon-chain molecules toward TMC-1 have shown a log-linear trend between molecule size and column density, and in an effort to further explore the underlying chemical processes driving this trend, we have analyzed GBT observations of HC9N and HC11N toward TMC-1. Although we find an HC9N column density consistent with previous values, HC11N is not detected and we derive an upper limit column density significantly below that reported in Bell et al. (1997). Using a state-of-the-art chemical model, we have investigated possible explanations of non-linearity in the column density trend. Despite updating the chemical model to better account for ion-dipole interactions, we are not able to explain the non-detection of HC11N, and we interpret this as evidence of previously unknown carbon-chain chemistry. We propose that cyclization reactions may be responsible for the depleted HC11N abundance, and that products of these cyclization reactions should be investigated as candidate interstellar molecules.

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\*Speaker

# H13CO+ and HN13C toward massive protostellar envelopes

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The physical conditions in massive dense cores (MDCs) leading to high-mass star formation are poorly constrained. We carried out an extensive study of the most massive and youngest clumps selected from the ATLASGAL (APEX Telescope Large Area Survey of the GALaxy) survey in the frame of the SPARKS project (Survey for high-mass Protostars with ALMA Revealed up to Kpc Scales). We studied the physical properties of the dense gas associated with the envelope of 35 protostars identified by SPARKS. To determine whether the kinematics of the protostellar envelope is dominated by supersonic turbulence or by organised dynamical flows, we present ALMA data from dense gas tracers (H13CO+ (J=4-3) and HN13C (J=4-3)) at high angular resolution. The data reveal the kinematics of the molecular gas forming the envelope at small scales (3000 AU). We analysed the line-widths and the velocity field of the sample and found a high degree of organised motions in the immediate vicinity of high-mass protostars likely associated with accretion flows.

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# On the reservoir of sulphur in dark clouds : chemistry and elemental abundance reconciled

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Sulphur-bearing species are often used to probe the physical structure of star forming regions of the interstellar medium, but the chemistry of sulphur in these regions is still poorly understood. In dark clouds, sulphur is supposed to be depleted under a form which is still unknown despite numerous observations and chemical modeling studies that have been performed. In order to improve the modeling of sulphur chemistry, we propose an enhancement of the sulphur chemical network using experimental and theoretical literature. We test the effect of the updated network on the outputs of a three phases gas-grain chemical model for dark cloud conditions using different elemental sulphur abundances. More particularly, we focus our study on the main sulphur reservoirs as well as on the agreement between model predictions and the abundances observed in the dark cloud TMC-1 (CP). Our results show that depending on the age of the observed cloud, the reservoir of sulphur could either be atomic sulphur in the gas-phase or HS and H<sub>2</sub>S in icy grain bulks. We also report the first chemical model able to reproduce the abundances of observed S-bearing species in TMC-1 (CP) using as elemental abundance of sulphur its cosmic value.

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\*Speaker

# Tomography of the thermal and density gas structure of the edge-on protoplanetary disk the Flying Saucer

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# Introduction to surface processes

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This presentation is a tutorial lecture on aspects of surface science and how they can be applied to laboratory astrophysics. Examples will be taken from the presenter's own work and fully referenced.

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\*Speaker



# Discovery of new interstellar molecules: expected and unexpected

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The great improvement achieved in last years in the sensitivity of radioastronomical receivers is allowing nowadays to detect interstellar molecules down to unprecedented abundance levels. In this talk I will present the detection of various organic molecules in cold dense clouds. The ketenyl radical (HCCO) and protonated cyanogen (NCCNH<sup>+</sup>) have been detected for the first time in space in various dark clouds down to abundance levels as low as 1e-12-1e-11 relative to H<sub>2</sub>, while other molecules such as the HCO radical and propylene (CH<sub>2</sub>CHCH<sub>3</sub>), which were known to be present in just a few cold dense clouds, have been detected in a wide sample of such sources. I will discuss the implications of these detections for our current understanding of the chemistry of cold dense clouds.

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\*Speaker

# Tunneling of hydrogen transfer reactions on and in interstellar ices

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The darkness readily observed between the stars on a clear night is far from empty. The low temperatures ( $T \approx 10$  K) in dark molecular clouds combined with the low particle densities ( $n = 10^4 \text{ cm}^{-3}$ ) make it seem unlikely for chemistry to take place efficiently. The chemistry that occurs can be partly explained by the presence of ice-coated dust grains on which molecules freeze out and, when they find each other, react. These grains act both as a molecule reservoir and as an energy sink for exothermic reactions. As such they allow a rich chemistry to occur. Barriers at cryogenic temperatures can only be overcome, however, when tunneling is invoked as a crucial component of the reaction mechanism. Hydrogen is very abundant in the interstellar medium and many surface reactions involve H transfer reactions, ultimately leading to the formation of saturated species like H<sub>2</sub>O and C<sub>2</sub>H<sub>6</sub> [1]. Furthermore, tunneling can also affect the D/H ratio of the products that are finally formed [2]. Rate constants for tunneled reactions are calculated with the use of instanton theory, while the ice surface is taken into account via, e.g., small clusters or multiscale modeling approaches (QM/MM). We elaborate on the influence of an ice environment on reaction rate constants, how and when an ice can be approximated without taking into account all degrees of freedom, and how the rate constants are to be interpreted in the light of astrochemical mean-field models and observations. References [1] T. Lamberts et al., *Phys. Chem. Chem. Phys.* 18 (2016), 33021, H. Kobayashi et al., *Astrophys. J.* 837 (2017), 155, T. Lamberts and J. Kästner *subm. Astrophys. J.* [2] J. Meisner et al. *J. Chem. Phys.* 144 (2016), 174303, J. Meisner et al., *subm. Earth and Space Chem.*, T. Lamberts et al. *Astron. Astrophys.* 599 (2017), A132

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# Destruction of interstellar COMs by collisions with He<sup>+</sup>: the case of dimethyl ether and methylformate

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Collisions with He<sup>+</sup> are an important pathway for the decomposition of complex organic molecules in the interstellar medium (ISM). Using a Guided-Ion Beam Mass Spectrometer we have explored the reactions of He<sup>+</sup> with two O-bearing organic molecules, ubiquitous in star-forming regions, but whose kinetics has never been studied experimentally: dimethyl ether CH<sub>3</sub>OCH<sub>3</sub> (DME) and methyl formate HCOOCH<sub>3</sub> (MF). Absolute reactive cross sections and product branching ratios have been measured as a function of the collision energy and the DME and MF radical cations are never detected, speaking for completely dissociative charge transfer processes. A semiclassical model based on an improved Landau-Zener approach [1], an analytical representation of the PES for the entrance and exit channels [2] and taking into accounts electron densities of the molecular orbitals from which electron is removed, has been developed to interpret experimental results and extract rate constant values as a function of temperature. Interestingly, our modelling shows that the large interaction anisotropy among colliding partners induces a pronounced orientation of the polar DME and MF, confining them, especially at low collision energies, into configurations ("pendular states") that are inefficient for charge-transfer due to poor orbital overlap. Hence the reaction is increasingly driven by the Coriolis coupling rather than by the orbital overlap. Our dynamical study casts light on some new and general guidelines to be properly taken into account for an appropriate evaluation of kinetics of ion-molecule reactions that goes beyond simple capture models, often adopted to estimate temperature dependent rate coefficients [3].

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# The Green Bank Ammonia Survey (GAS): First results of NH<sub>3</sub> mapping the Gould Belt

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We present an overview of the first data release (DR1) and first-look science from the Green Bank Ammonia Survey (GAS). GAS is an ambitious Large Program at the Green Bank Telescope to map all Gould Belt starforming regions with  $A_V$  & 7 visible from the northern hemisphere in emission from NH<sub>3</sub> and other key molecular tracers. This first release includes the data for four regions in Gould Belt clouds: B18 in Taurus, NGC 1333 in Perseus, L1688 in Ophiuchus, and Orion A North in Orion. We find that the NH<sub>3</sub> emission is generally extended beyond the typical 0.1 pc length scales found in dense cores. Thanks to these observations we can finally explore the sharp transition between the supersonic turbulence in molecular clouds and the subsonic turbulence inside cores in a systematic fashion across different environments. We also present the initial analysis of the abundance variation of NH<sub>3</sub> at different column densities, a comparison of the gas and dust temperatures across the clouds different clouds in this release and how they vary with increasing star formation activity.

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\*Speaker

# Study of the $\text{CF}^+$ formation from the $\text{HF} + \text{C}^+ \rightarrow \text{CF}^+ + \text{H}$ reaction at energies of astrophysical interest and the interaction of vibrating $\text{CF}^+$ with He.

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The recent detections of the carbon monofluoride cation ( $\text{CF}^+$ ) in galactic and extragalactic regions have increased the interest in the chemistry of this system. This species considered the second reservoir of fluorine in regions where  $\text{C}^+$  is abundant, has been proposed as a tracer of  $\text{C}^+$  in photo-dissociation regions and dense core environments [1, 2]. Furthermore, a correct interpretation of the astronomical observations requires the rate coefficients with the most common colliders in the ISM (e.g. He,  $\text{H}_2$ , H). The  $\text{CF}^+$  molecule can be formed from the reaction of HF with  $\text{C}^+$  [3]. However, in exothermic reactions like  $\text{HF} + \text{C}^+ \rightarrow \text{CF}^+ + \text{H}$ , even from the ground vibrational state of the reactant diatomic molecule (e.g. HF), the product diatom (e.g.  $\text{CF}^+$ ) can be in an excited vibrational state [4]. Therefore, this work focuses on the study of the  $\text{CF}^+$  formation from the  $\text{HF} + \text{C}^+$  reaction and the interaction of vibrating  $\text{CF}^+$  with He. First, we develop a potential energy surface (PES) for the  $\text{HF} + \text{C}^+$  at the MRCI+Q/aug-cc-pVQZ level of theory, where the correct R-4 asymptotic behavior is taking into account in the fitting procedure. The dynamics of the system is studied using quasi-classical trajectory and time-independent quantum reactive scattering calculations. The results using both, classical and quantum methods, are compared. Second, the He +  $\text{CF}^+$  interaction in full dimensionally at the close-coupling level is investigated. A set of CCSD(T)/aug-cc-pv5z ab-initio interaction energies was computed, and a new three-dimensional potential energy surface (PES) is represented using a reproducing kernel Hilbert space (RKHS). The vibrational quenching cross sections were found to be at least six orders of magnitude lower than the pure rotational cross sections at collision energies lower than 1000  $\text{cm}^{-1}$ . Finally, the hyperfine rate coefficients are explored. The data here computed can be useful for the determination of the interstellar conditions where this molecule has been detected.

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<sup>\*</sup>Speaker

# Astrochemical modeling of protoplanetary disks and new challenges from high resolution observations

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Protoplanetary disks exhibit rich diversity in their physical structure as traced by dust, including gaps, asymmetries, and now fine rings. More recently, advances in sensitivity with the Atacama Large Millimeter/Submillimeter Array have uncovered equally rich structure in the molecular composition of disks, including symmetric and asymmetric features, vertically layered structure, and more. These new observations offer a unique opportunity to probe compositional properties across vastly different environments within a single source, from the icy midplane to the warm surface, and the optically shielded dense material to the irradiated layers. In this talk, I will review recent results regarding the molecular inventory of disks with ALMA, and how these efforts are uncovering new challenges for chemical models, including the impact of differential evolution of gas and ice-coated dust.

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\*Speaker

# Introduction to astrochemical modeling

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It has been almost 45 years since the first chemical simulation of the chemistry of dense interstellar clouds was published. This simulation involved 100 gas-phase reactions between 35 molecules with up to 5 atoms. The gas phase was assumed to be homogeneous and time-independent. Since that time, astrochemical modelling has become far more detailed, with networks of many thousands of chemical reactions involving both the gas phase and dust surfaces, and thermal and non-thermal physical processes involving the exchange of molecules between the two phases. Moreover, models with heterogeneous conditions, such as those treating photon-dominated regions and protoplanetary disks, have become common, and time-dependence of the physical conditions in the formation of disks and other objects included with approaches that vary in complexity from semi-empirical methods to full three-dimensional magneto-hydrodynamical treatments. The enlargement of chemical networks has been helped by both experimental and theoretical treatments of reaction rate coefficients in both the gas and on dust particles or the mantles that surround them. Sensitivity methods have been employed to determine which reactions are most important to understand better. For a time it was thought that chemical simulations of cold interstellar cloud cores were so accurate as to be predictive, but the detection of more saturated "complex" organic molecules, previously thought to exist only in hot cores, in the gas phase of these objects has complicated matters and led to more complex treatments of the formation of such species, involving both gas and dust. Indeed, new and improved treatments of surface reactions have led to a transformation of this subject, while the inclusion of processes involving tunneling and radiative association has similarly transformed the use of gas-phase chemistry. Although chemical simulations are normally treated by solutions of kinetic rate equations, such treatments are only approximate because of the small number of reactive species per dust particle. More detailed stochastic treatments, involving master equations or Monte Carlo simulations of master equations, are more accurate, but still very computer intensive. Chemical simulations currently exist for all evolutionary periods in the formation of low-mass stars and planets (diffuse clouds, translucent clouds, cold cores, pre-stellar cores, hot corinos, winds, shocks, protoplanetary disks, and even planetary atmospheres, with the simulations for high-temperature regions such as hot corinos the most problematical. In the talk, both the history of astrochemical modeling, and the current level of the subject will be discussed.

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\*Speaker

# Molecular richness around protostars: the ALMA/NOEMA revolution

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The gas associated with the early stages of star formation contains traces of a large variety of molecular species, many of which are organic in nature. Thanks to last generation (sub-)millimetre interferometers such as ALMA and NOEMA, we are currently witnessing huge progress in our understanding of molecular complexity in star forming regions. In this context, I will introduce our most recent interferometric results in two different objects: (i) the protostellar binary and hot corino source NGC1333 IRAS4A, which is a beautiful example of how the level of chemical richness attained in protostellar cores can vary drastically between neighbouring sources, and (ii) the intriguing protostellar cluster OMC-2 FIR 4, which constitutes so far the best known analogue of the formation environment of the Solar System. The data I will present include ALMA observations and the very first results of the IRAM NOEMA Large Program SOLIS (Seeds Of Life In Space), whose goal is to understand the evolution of organic chemistry across the first phases of formation of solar-mass stars.

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\*Speaker



# Radical-induced chemistry in interstellar ices: intermediates characterization and reactivity

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Astrophysical observations led to the identification of numerous organic molecules. Among them, some have an important number of atoms and are so called Complex Organic Molecules (COMs). COMs are species of interest since they are incorporated in small bodies of the interstellar medium and could have played a role in the emergence of life on Early Earth.

Although their characterization in the interstellar medium is confident, their formation mechanism is still under investigation. The particular conditions – UV photons, hydrogen bombardments, thermal effects – makes formation mechanisms hard to be clearly identified. We focus here on radical reactivity in astrophysical conditions. Interstellar ice analogues are made in laboratory and submitted to ISM-like processes -hydrogenation, VUV irradiation, heating effect- while the chemical composition of the ice analogue is monitored by spectroscopic techniques – IR, MS and, if required, GC-MS.

Radical species produced during the experiment are difficult to analyze, due to their short lifespan and high reactivity. To overcome this problem, we use cryogenic matrix isolation technique combined with IR spectroscopy to characterize unstable species and observe their reactivity(1, 2). Nonetheless, this technique detects all species – radical and non-radical molecules – leading to overlapping of some vibration modes from intermediates of interest. By using EPR spectroscopy, we are able to focus only on radical species and to detect them even in low amount.

In this work, we focus on COMs formation from VUV irradiated methanol CH<sub>3</sub>OH or formaldehyde at low temperature, from radical intermediates identification (HCO, CH<sub>2</sub>OH, CH<sub>3</sub>O) to their recombination products(4, 5, 6) (glycolaldehyde, ethylene glycol, methylformate). Quantum calculations were also performed to explain particular chemical pathways(1, 2, 3). We show that HCO dimerization does not produce glyoxal and identified a possible way to form more complex molecules from radical-initiated polymerization. Results from this study could be used to understand data from spatial mission – such as Rosetta mission – or to direct observations towards new organic molecules.

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# Complex molecules in PDRs and protoplanetary disks

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Complex molecules are commonly detected in high- and low-mass star forming regions. In the past years, however, complex species have been detected in unexpected environments like photo-dominated regions (PDRs). The great sensitivity and resolution power of ALMA has also allowed us to start detecting and resolving complex species in protoplanetary disks.

I will first show results from the WHISPER line survey in the famous Horsehead nebula. We detect the complex organic molecules H<sub>2</sub>CO, CH<sub>3</sub>OH, HCOOH, CH<sub>2</sub>CO, CH<sub>3</sub>CHO and CH<sub>3</sub>CCH, with similar abundances in the UV-exposed PDR and the UV-shielded dense core. This shows the importance of the interplay between the solid and gas phase chemistry in the formation of (complex) organic species, and confirm that ice photo-processing is an efficient mechanism to release frozen species in the gas phase. We also detect CH<sub>3</sub>CN and its isomer CH<sub>3</sub>NC in the PDR. In contrast to the other complex molecules, CH<sub>3</sub>CN is 30 times more abundant in the PDR than in the core, suggesting a specific formation mechanism.

In the second part, I will show recent observations of complex organic molecules in protoplanetary disks. CH<sub>3</sub>CN and HC<sub>3</sub>N have been detected in at least two disks, MWC 480 and V4046 Sgr, and CH<sub>3</sub>OH been detected towards the TW Hya disk. I will also discuss observations of H<sub>2</sub>CO, a key intermediate in the formation of more complex species in ices. Contrary to CH<sub>3</sub>OH, H<sub>2</sub>CO is readily observable in disks and could thus be used to trace the cold organic reservoir in disks.

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\*Speaker

# Demonstration of the KIDA database and Nautilus astrochemical model

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The KIDA database is a collection of kinetic data for astrochemistry that has now been used by a large community. Last year, we have entirely changed the online interface and extended it to surface reactions. There are still more questions that arise time to time about the way to use the database. In parallel, our group in Bordeaux have been developing an astrochemical model called Nautilus that can compute gas and grain composition in the interstellar medium under many different conditions. This code is available upon request and starts to be used by several groups. In this presentation, I will present user cases of the use of the KIDA database and the Nautilus astrochemical model to help potential users.

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\*Speaker

# The role of an ice surface's structure in determining the orientation and subsequent reactivity of adsorbed small molecules.

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The chemistry occurring on the surface of an ice-covered dust grain plays a key role in modifying the composition of both the solid and gas phases in astrophysical environments. This presentation will discuss the role of the structure of the ice surface in both physical (adsorption/desorption) and chemical (reaction) processes. In the first part, the structure of the amorphous solid water surface, and its reorganisation upon thermally- or photon-driven processing, will be discussed. Secondly, the interaction of polycyclic aromatic hydrocarbons with water clusters and ices will be used as an illustration of the critical role played by molecular orientation in chemical reactivity.

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\*Speaker

# Chemistry of cold dense cores: On the observed abundance gradients in dense clouds

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Observations of cold and dense interstellar clouds have revealed an extraordinary molecular richness but also a large dispersion in the inferred abundances between and within them. Understanding these differences is a difficult task because (1) the chemistry is out of equilibrium in most of these objects and, (2) molecular observations provide us only a snapshot of what their state are. Although a considerable theoretical work has been done to understand the chemistry at work in such regions, most of the time dependent chemical modeling of dense clouds rely on simple approximation that reflect these difficulties. Based on the lack of information on their dynamical state, dense clouds are often considered as very simple objects in which the physical conditions are homogeneous and fixed.

In this talk, I will discuss this assumption and show how the past physical conditions of dense clouds can impact their molecular composition. I will show that the physical history from the diffuse interstellar medium to the birth of dense clouds could be important in establishing their chemical composition and account for the observed abundance gradients.

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\*Speaker

# Temperature fluctuations and surface processes : a statistical modeling approach

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The surface of interstellar dust grains hosts crucial physico-chemical processes, from the formation of H<sub>2</sub>, initial step of all interstellar chemistry, to the formation of complex organic molecules in ice mantles inside dark clouds. Most of these processes are very sensitive to the grain temperatures (Pauly & Garrod 2016) and are controlled by binding energies or reaction barriers which are often poorly known. These grain temperatures are subject to wide fluctuations in most environments, from stochastic UV heating of small grains in exposed environments such as PDRs, to cosmic-ray-induced fluctuations affecting much bigger grain deeper inside clouds (Kalvans 2016).

I will present a statistical modeling approach of this problem and its application to two of the simplest surface processes (H<sub>2</sub> formation and ortho-para conversion) in UV-rich environments (PDRs) where small grains are subject to large temperature fluctuations, successfully explaining ISO and Spitzer observations (Bron et al. 2014, 2016). These results exhibit two general effects of temperature fluctuations : smoothing out threshold effects thought to sharply limit certain processes to a limited range of conditions, and reducing the impact of uncertainties on binding energies and other microphysical parameters. Finally, I will discuss the implications of these results for, and their extension to, surface chemistry in dark clouds.

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# Introduction to observational astrochemistry

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In this presentation I will provide some general information on how observations carried out at telescopes can be converted into abundances of chemical species towards an astronomical source. I will explain the general methods and will emphasise not only the machinery behind this, but also the assumptions and the limits of what we can and do derive.

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# Low temperature gas-phase kinetics studies related to molecular growth in space

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The CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme, or Reaction Kinetics in Uniform Supersonic Flow) technique has enabled us to show that many neutral-neutral reactions may be rapid down to the temperatures of dense interstellar clouds (10-20 K), as well as proving an exacting test for theory [1,2]. Rate coefficients have been measured as low as 6 K for the reaction  $S(1D) + H_2$  [3] and 11 K for the prototypical reaction  $F + H_2 \rightarrow HF + H$  [4]. A series of fast barrierless reactions related to the formation of long chain cyanopolyne molecules  $H(C_2)_nCN$  [5] of interest in both interstellar clouds and Titan's atmosphere, have been studied both experimentally and theoretically, and our latest results involving reactions of CN, C<sub>2</sub>H and C<sub>3</sub>N radicals to yield HC<sub>5</sub>N will be presented.

One of the current principal challenges in chemical kinetics is the determination of absolute product-channel specific rate constants for elementary reactions. This is particularly the case at low temperatures, and I will also present current efforts in Rennes (ERC CRESUCHIRP project) in collaboration with leading groups (Arthur Suits, U. Missouri, Robert Field, MIT) to use a promising new technique to determine product branching ratios at low temperatures in combination with the CRESU technique, namely Chirped Pulse microwave spectroscopy in Uniform supersonic Flow (CPUF) [6].

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# Introduction to gas phase processes

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TBD

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# Effects of cosmic rays on grains chemistry

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