

# “Physique et Chimie du Milieu Interstellaire” National Program Symposium

## MARSEILLE 2018

June 25 – 29 2018

The interstellar Medium from the Milky Way to the far  
External Galaxies

From Molecular Clouds to the Protoplanetary Systems

On The Origin of Matter Complexity

<https://pcmimarseille18.sciencesconf.org>



Société Française d'Exobiologie





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## Foreword

Understanding the interstellar medium is one of the keys to understand the most diverse objects of our universe, near and far, small and large. The challenges are huge to answer the related astrophysical questions: for instance, the formation and evolution of the Giant Molecular Clouds, the efficiency of star formation and its link with the galactic environments, the formation of the first stars in the primordial universe, the formation and properties of protoplanetary disks, the emergence and the robustness of the molecular and dust complexity (up to pre-biological molecules), ... Solving these questions requires the use of the world-class astronomical facilities, state-of-the-art simulations to model the observations, advanced statistical analyzes to relate observations and models, and cutting-edge experiments that produce analogous of interstellar matter and that study in-depth the fundamental physical and chemical processes at play.

Only a multi-disciplinary approach, linking astrophysicists, physicists, chemists, statisticians, ..., can overcome these challenges. That's what PCMI has learned to do over decades, in particular, during its biennial conferences. These have proved to be instrumental in gathering researchers from different fields to envisage solutions during fruitful discussions. Once again, the PCMI community is heavily invested in this conference with more than 120 participants for a community of about 350 researchers. Invited reviewers kindly agreed to synthesize broad and sometimes technical field in short and pedagogical talks. Because of time constraints, we were able to only retain 37 oral presentations among the many propositions. But the 82 posters that will be exhibited during the conference testify of the liveliness of the community and the four discussion workshops will be the occasion to deepen several topics. We thank our institutional sponsors (Université Aix Marseille, CNRS, CNES, IRAM, SFC, SFE) whose support is essential to organize this conference. We also thank the local organizing committee for having worked out all the practical details in an efficient way. Finally, we wish you all a convivial conference. Jérôme, Karine, et Jean-Hugues at the behalf of the PCMI scientific council.

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## Rational

During this meeting, we will discuss recent advances in key PCMI science themes (we list below some of the topical issues that will be addressed during the meeting). The conference will also be the occasion to discuss the renewal of PCMI mandate: A dedicated session will be organized to foster discussions on the direction to follow during the next five years (from 2019 to 2023), in the context of the development of NOEMA, ALMA, JWST, and SOLEIL and of future instruments such as SKA, ATHENA, XFEL... In addition to the plenary sessions, there will also be 4 discussion workshops dedicated to specific topics proposed by the PCMI community:

- databases in astrochemistry
- dust from the diffuse ISM to proto-planetary discs: Where do we stand?
- new perspectives in millimeter astronomy with IRAM telescopes
- primordial chemistry

These workshops aim to gather specialists and interested people to engage in active discussion of the proposed topic.

### **The interstellar medium (ISM) from the Milky Way to far external galaxies:**

We can first ask how giant molecular clouds (GMC) form and evolve: How to infer information about the matter distribution along the line of sight ? Are the ISM mass/density tracers such as CII, HI, CO, HCO<sup>+</sup>, HCN, quantitatively understood in the Milky Way? How to take into account the stochastic nature of turbulence in ISM models? What is the impact of anisotropic FUV field on the ISM structure and progresses of star formation? What is the size distribution of dust in dense gas? Are gas and dust well-coupled? What is the typical lifetime of a GMC? Are GMCs mostly isolated structures or accreting/loosing matter from/to their environment? Are molecular cloud properties and star formation efficiencies affected by the galactic environment (e.g., arm/inter-arm, mergers)? How do energetic phenomena (cosmic rays, SNs, ...) affect the structure of the ISM? Moreover, the study of molecular gas in galaxies near and far requires the use of indirect tracers of the molecular mass: What are the best molecular tracers of dense gas that can be detected in nearby galaxies? What are the dust properties in nearby galaxies? How does dust evolve in the ISM? Can we build dust models parameterized as a function of the physical conditions (UV field, density)? How

different are the dust properties in nearby galaxies (LMC, SMC, M31, etc.)? What does the detection of molecules tell us about the first galaxies? What's the impact of chemistry on the first generation of stars?

**From molecular clouds to protoplanetary systems:** Many questions arise about the formation of stars and proto-planetary disks: Is the core mass function universal? Are filament properties universal, and if so, why? Are filaments sub-structured in fibers? What's the role of the magnetic field at different spatial scales in the ISM and different stages of the star formation process? Does the kind of turbulence affect the star formation efficiency? How does the grain size distribution vary in proto-planetary disks? What traps dust in disks? What are the properties of snow lines? What is the limit of chemical complexity in disks?

**On the origin of matter complexity:** Recent observations, and laboratory experiments have renewed long-standing issues: What are the most stable carbonaceous structures in space? Are all DIBs associated with fullerenes? Are branched alkyl molecules a first step towards aromatic cycles? How does chirality appear? What's the relative importance of top-down and bottom-up chemistry on the global molecular budget? Why are complex organic molecules (COMs) detected in unexpected environments (cold cores, PDRs, etc...)? Why are COMs difficult to detect in comets? What is the limit of molecular complexity in gas or ices? Do we understand the link between isotopic ratios in the Solar System and in the local ISM? What can we learn from pre-solar grains? How representative are they of ISM dust? How does dust form and evolve in circumstellar shells around evolved stars? Can refractory dust be formed in the ISM? In what forms are iron and sulfur incorporated into dust grains? What explains the relative abundances of organic isomers? How to trace the ortho/para ratio? What needs to be measured first about state-to-state chemistry? What are the key molecular compounds that need to be studied in space and laboratory to understand interstellar chemistry? Can we realistically model surface chemistry? Do molecular excited states play a role in the chemistry of PDRs?

PCMI is an "action sur projet" from CNRS-INSU (Sciences de l'Univers), also supported by the CNRS-INP (Institute of Physics), the CNRS-INC (Institute of Chemistry), CNES (Centre National d'Études Spatiales), and CEA (Commissariat à l'énergie atomique et aux énergies alternatives).

## PCMI scientific board

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**Ysard, Nathalie**, Institut Astrophysique de Paris (IAP), Paris

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**Parent Philippe**, Centre Interdisciplinaire de Nanoscience de Marseille (CINAM), Marseille

**Paroutaud Emilien**, Laboratoire de Physique des Interactions Ioniques et Moléculaires (PIIM), Marseille

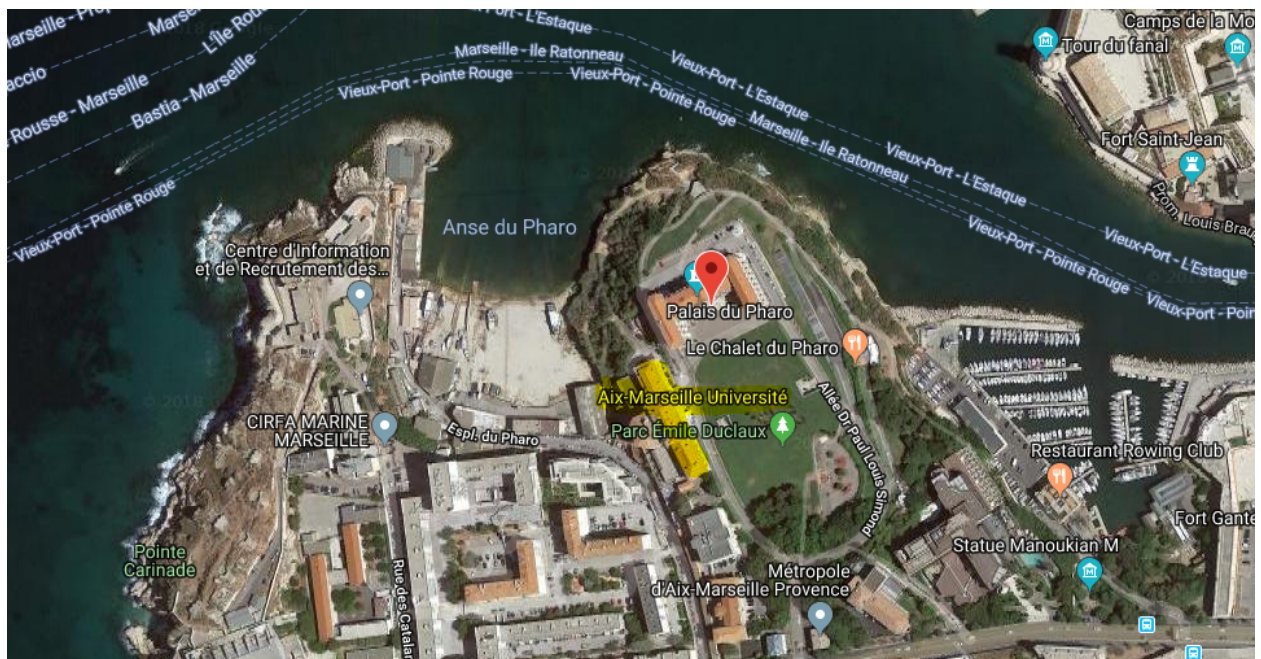
**Pietri Nathalie**, Laboratoire de Physique des Interactions Ioniques et Moléculaires (PIIM), Marseille

**Rostand Eric**, Laboratoire de Physique des Interactions Ioniques et Moléculaires (PIIM), Marseille

**Theulé Patrice**, Laboratoire de Physique des Interactions Ioniques et Moléculaires (PIIM), Marseille

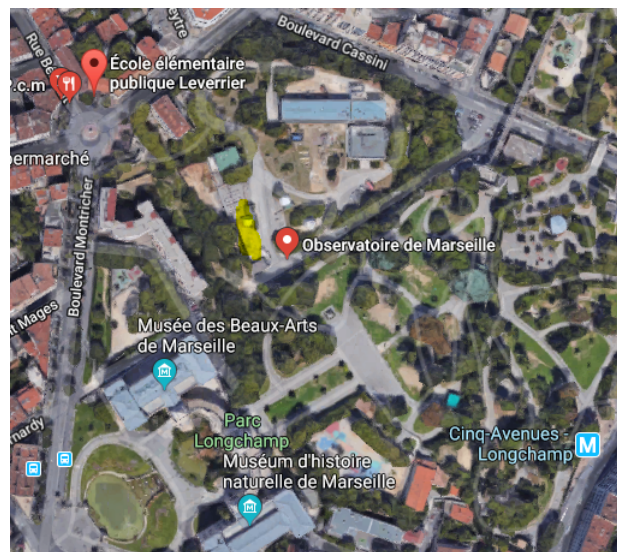
# Symposium locations

from Monday to Wednesday:



Gastaut amphitheatre at the Pharo Aix-Marseille University headquarters

**Tuesday 26<sup>th</sup> 8:30 pm:**



Marseille historical observatory, 2 place Leverrier, Association Andromède

**from Thursday to Friday:**



Ponte and Rouard amphitheatres at the Saint-Jérôme Campus + PIIM laboratory visit

Directions to Saint-Jérôme Campus:

take metro line 1 to Malpassé, then bus B3A to Saint-Jérôme

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Monday June 25<sup>th</sup>

Pharo Palace, Gastaut amphitheatre

09:00 - 09:45		<i>Welcome and registration</i>
09:45 - 10:00	<b>P. Theulé</b>	<i>Opening - Opening</i>
		<b><i>ISM in external Galaxies</i></b>
10:00 - 10:20	<b>G. Lagache</b>	<i>The [CII] 158 micron line emission in high-redshift galaxies</i>
10:20 - 10:40	<b>Q. Salome</b>	<i>Inefficient jet-induced star formation in Centaurus A: High resolution ALMA observations of the northern filaments</i>
10:40 - 11:00	<b>D. Cormier</b>	<i>The EMPIRE Survey : Dense Gas and Star Formation across Nearby Galaxy Disks</i>
11:00 - 11:20	<b>V. Leboutteiller</b>	<i>CO-dark molecular gas and the origin of [CII] emission in metal-poor galaxies</i>
11:20 - 11:45	<b>P. Guillard</b>	<i>Molecular Hydrogen in the Universe</i>
		<b><i>Ices and molecular complexity from the ISM to protostars (session 1)</i></b>
11:45 - 12:10	<b>S. Bontemps</b>	<i>The fate of COMs during high mass star formation</i>
12:10 - 12:30	<b>A. Lopez Sepulcre</b>	<i>Seeds Of Life In Space: An IRAM-NOEMA large programme to investigate organic chemistry in solar-type star forming regions</i>
12:25 - 14:00		<i>lunch break (salle des voûtes - Pharo palace)</i>
		<b><i>Poster session 1</i></b>
14:00 - 14:15		<i>flash poster presentations 1 (Gastaut amphitheatre)</i>
14:15 - 15:30		<i>poster session 1 (vaults room)</i>
15:30 - 16:00		<i>coffee break</i>
		<b><i>Ices and molecular complexity from the ISM to protostars (session 2)</i></b>
16:00 - 16:20	<b>M.-A. Martin-Drumel</b>	<i>Investigating transient species in the millimeter domain using spectral taxonomy</i>
16:20 - 16:45	<b>M. McCoustra</b>	<i>Laboratory Studies of Thermal and Non-thermal Processes on and in Growing Icy Grain Mantles</i>
16:45 - 17:05	<b>P. Ghesquière</b>	<i>Reactivity in interstellar ice analogues: role of the structural evolution</i>
17:05 - 17:25	<b>F. Dulieu</b>	<i>Formation of complex molecules on cold surfaces</i>
17:25 - 17:50	<b>D. Talbi</b>	<i>Theoretical approaches for gas-phase and ice surface processes</i>
18:00 - 20:00		<i>Welcome drinks party</i>

# MARSEILLE 2018

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**Tuesday June 26<sup>th</sup>**

Pharo Palace, Gastaut amphitheatre

09:00 - 10:50		<b><i>ISM Structures: Statistical views and modelling</i></b>
09:00 - 09:25	<b>J. Montillaud</b>	<i>ISM in 3D: methods and astrophysical consequences</i>
09:25 - 09:45	<b>I. Grenier</b>	<i>The gamma-ray view on the HI-H<sub>2</sub>-CO interface in nearby clouds</i>
09:45 - 10:10	<b>F. Le Petit</b>	<i>Stochastic modeling of the ISM processes</i>
10:10 - 10:30		<i>coffee break</i>
10:30 - 10:55	<b>E. Allys</b>	<i>Novel statistical tools to characterize interstellar magnetized turbulence</i>
10:55 - 11:20	<b>E. Bron</b>	<i>The dynamics of photodissociation regions: from the observed tracers to a dynamical model</i>
11:20 - 11:45	<b>G. Laibe</b>	<i>Simulating the ISM</i>
		<b><i>Cosmic cycle of matter/dust: Session 1</i></b>
11:45 - 12:10	<b>E. Dartois</b>	<i>Carbonaceous matter: from ISM to protoplanetary disks</i>
12:10 - 12:30	<b>I. Ristorcelli</b>	<i>Dust properties in Galactic Cold Cores: intensity and polarization</i>
12:30 - 12:50	<b>N. Cox</b>	<i>Gas and dust in the diffuse interstellar medium: new surveys of diffuse interstellar bands and dust polarisation</i>
12:50 - 14:20		<i>picnic (Pharo palace)</i>
		<b><i>Cosmic cycle of matter/dust: Session 2</i></b>
14:20 - 14:40	<b>J. Chastenet</b>	<i>Polycyclic Aromatic Hydrocarbon fraction at 20pc scale in the Magellanic Clouds</i>
14:40 - 15:00	<b>R. Berard</b>	<i>Probing the impact of the C/O ratio and metals on the properties of dust particles in a cold plasma reactor</i>
15:00 - 15:20	<b>E. Michoulier</b>	<i>PAHs adsorbed on interstellar ice : structures, energetics and IR spectra from a multi-method theoretical study</i>
		<b><i>Poster session 2</i></b>
15:20 - 15:35		<i>flash poster presentations 2 (Gastaut amphitheatre)</i>
15:35 - 16:05		<i>coffee break</i>
16:05 - 17:00		<i>poster session 2 (vaults room)</i>

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## Tuesday June 26<sup>th</sup>

Pharo Palace, Gastaut amphitheatre

<i><b>Magnetic field and star formation: Session 1</b></i>		
17:00 - 17:25	<b>P. André</b>	<i>The ArTéMiS submillimeter continuum camera on APEX: Capabilities and first scientific results on the structure of dense star-forming complexes</i>
17:25 - 17:45	<b>A. Mangilli</b>	<i>PILOT magnetic field in the Milky Way and Star Forming Regions</i>
<i><b>Outreach conference (Marseille historical Observatory, 2 place Leverrier)</b></i>		
20:30 - 21:30	<b>T. Chiavassa</b>	<i>Du Milieu Interstellaire aux Systèmes Planétaires : Evolution de la Matière Organique vers le Vivant</i>
21:30 - 22:00	<b>Unistellar</b>	<i>Unistellar telescope presentation and drinks party</i>
22:00 - 24:00	<b>Andromède</b>	<i>sky observations</i>

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**Wednesday June 27<sup>th</sup>**

Pharo Palace, Gastaut amphitheatre

09:00 - 10:10		<b><i>Magnetic field and star formation: Session 2</i></b>
09:00 - 09:25	<b>F. Boulanger</b>	<i>Interstellar magnetic fields</i>
09:25 - 09:45	<b>M. Galametz</b>	<i>ALMA and SMA observations of magnetic fields in the youngest solar-type protostars</i>
09:45 - 10:10	<b>S. Cabrit</b>	<i>Shocks, jets and star formation with NOEMA and ALMA</i>
10:10 - 10:40		<i>coffee break</i>
10:40 - 12:20		<i>Présentation et discussion du renouvellement du PN (J.Pety, K.Demyk, J.H.Fillion)</i>
12:20 - 13:50		<i>lunch break</i>
13:50 - 15:20		<b><i>From disks to planets</i></b>
13:50 - 14:15	<b>E. Chapillon</b>	<i>Protoplanetary disks and planet formation</i>
14:15 - 14:35	<b>P. Hily-Blant</b>	<i>The origin of nitrogen in planetary systems: recent findings from observational studies of prestellar cores, protostars, and disks</i>
14:35 - 14:55	<b>O. Ozgurel</b>	<i>Which origin for molecular oxygen and sulfur in Comet 67P/Churyumov-Gerasimenko?</i>
14:55 - 15:20	<b>P. Tremblin</b>	<i>Modeling exoplanet atmospheres</i>
15:20 - 19:00		<i>boat trip to Marseilles calanques (meeting at the quai des Belges pier)</i>
20:00 - 23:00		<i>conference dinner at le Palais de la Major)</i>

« Physique et Chimie du Milieu Interstellaire » symposium

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**Thursday June 28<sup>th</sup>**

Saint-Jérôme Campus (Rouard and Ponte amphitheatres)

09:00 - 10:30	<i>workshops "Databases in astrochemistry" &amp; "Dust from the diffuse ISM to protoplanetary discs: where do we stand?" in parallel</i>
10:30 - 11:00	<i>coffee break</i>
11:00 - 12:30	<i>workshops "Databases in astrochemistry" &amp; "Dust from the diffuse ISM to protoplanetary discs: where do we stand?" in parallel</i>
12:30 - 14:00	<i>lunch break</i>
14:00 - 15:30	<i>workshops "New perspectives in millimeter astronomy" &amp; "Primordial Chemistry" in parallel</i>
15:30 - 16:00	<i>coffee break</i>
16:00 - 17:30	<i>workshops "New perspectives in millimeter astronomy" &amp; "Primordial Chemistry" in parallel</i>
18:30 - 20:00	<i>visit of PIIM &amp; drinks party</i>

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**Friday June 29<sup>th</sup>**

Saint-Jérôme Campus (Ponte amphitheatre)

09:00 - 10:40		<i>Workshops summary and conclusion</i>
09:00 - 09:25	<b>P. Gratier, A. Faure</b>	<i>Bases de données en astrochimie</i>
09:25 - 09:50	<b>D. Puy</b>	<i>Primordial Chemistry</i>
09:50 - 10:15	<b>B. Commerçon</b>	<i>Dust from the diffuse ISM to protoplanetary discs: where do we stand ?</i>
10:15 - 10:40	<b>M.Y. Gérin</b>	<i>New perspectives in millimeter astronomy</i>
10:40 - 11:10		<i>coffee break</i>
		<b><i>Molecular signatures in cold ISM</i></b>
11:10 - 11:35	<b>A. Bergeat</b>	<i>State-to-state collisional rates and characterization of products at low temperature</i>
11:35 - 11:55	<b>J. Laureau</b>	<i>An efficient statistical method to compute molecular collisional rate coefficients</i>
11:55 - 12:15	<b>L. Biennier</b>	<i>Anion chemistry at low temperature in the interstellar medium: insights from the laboratory</i>
12:15 - 12:35	<b>R. Georges</b>	<i>Nuclear spin symmetry conservation in H<sub>2</sub>O water vapor cooled in a supersonic expansion</i>
12:35 - 12:55	<b>T. Putaud</b>	<i>Ortho-to-Para Ratio of Water in the Orion Bar</i>
12:55 - 13:00	<b>LOC</b>	<i>conference closing</i>



## ISM in external Galaxies

**Monday June 25<sup>th</sup> 10:00**

## The [CII] 158 micron line emission in high-redshift galaxies

Guilaine Lagache<sup>1</sup>, Morgane Cousin<sup>1</sup>

<sup>1</sup> LAM, UMR7326 du CNRS, Laboratoire d'Astrophysique de Marseille, 38 rue Frédéric Joliot Curie, 13013, Marseille – France

Gas is a crucial component of galaxies, providing the fuel to form stars, and it is impossible to understand the evolution of galaxies without knowing their gas properties. The [CII] fine structure transition at 158 microns is the dominant cooling line of cool interstellar gas. With the advent of ALMA and NOEMA, capable of detecting [CII]-line emission in high-redshift galaxies, there has been a growing interest in using the [CII] line as a probe of the physical conditions of the gas in galaxies, and as a star formation rate (SFR) indicator at  $z > 4$ .

We have used a semi-analytical model of galaxy evolution combined with the photoionisation code CLOUDY to predict the [CII] luminosity of a large number of galaxies (25,000 at  $z = 5$ ) at  $4 < z < 8$ . The model takes into account the effects of CMB heating and attenuation that are important at such high redshifts. I will present the model, its predictions and comparisons with observations at  $z > 4$ . In particular, the model allowed us to study in detail the L[CII]–SFR L[CII]–metallicity relations and their evolution with redshift. It reproduces the L[CII]–SFR relation observed for  $\sim 50$  star-forming galaxies at  $z > 4$  and it is used to understand the observed dispersion, which is large and due to combined effects of different metallicities, ISRF, gas contents in the high-redshift galaxies, as well as timescales that are implicitly assumed when measuring the SFR in galaxies. I will also show that the model naturally produces the [CII] deficit which appears to be strongly correlated with the intensity of the radiation field in our simulated galaxies. Finally, I will discuss how such models are important in the framework of future observations with NOEMA and ALMA, as well as experiments targeting the [CII] line deep into the reionisation era (CONCERTO and Time).

### Références

- [1] Lagache G., Cousin M., Chatzikos M., A&A 609, 130 (2018)
- [2] Lagache G., IAU Symposium 333 "Peering towards Cosmic Dawn", eds. Vibor Jelic and Thijs van der Hulst, arXiv:1801.08054 (2018)

## **Inefficient jet-induced star formation in Centaurus A: High resolution ALMA observations of the northern filaments**

Quentin Salomé<sup>1</sup>, Philippe Salomé<sup>2</sup> Marc-Antoine Miville-Deschênes<sup>3</sup>,  
Françoise Combes<sup>2</sup>, Stephen Hamer<sup>4</sup>

<sup>1</sup>*Instituto de Radioastronomía y Astrofísica, UNAM, Morelia 58089 – México*

<sup>2</sup>*LERMA, Observatoire de Paris, 75014 Paris - France*

<sup>3</sup>*Département d'Astrophysique, CEA-Saclay, 91191 Gif sur Yvette – France*

<sup>4</sup>*CRAL, Observatoire de Lyon, 69561 Saint-Genis Laval Cedex - France*

Star formation is one of the key mechanisms driving the evolution of galaxies across cosmic times. The physical properties and the multi-scale dynamics of the molecular gas influence the star formation efficiency, therefore looking at large scales is essential to understand the physics of star formation. The environment certainly plays a role in star formation. In particular, recent studies suggest that AGN can regulate the gas accretion and thus slow down star formation. However, evidence of AGN positive feedback is also invoked in a few radio galaxies.

The northern filaments of Centaurus A are a testbed region for positive feedback, here through jet-induced star formation. These filaments extend on scales up to 15 kpc, aligned with the radio-jet, and show evidence of recent star formation [1]. At the intersection of the radio jet and one of the HI shells that surround the galaxy [2], CO emission in the shell has been detected with SEST [3]. With APEX, we mapped the CO emission along the FUV filaments that lie at the jet-HI interaction. In particular, we discovered a large amount of molecular gas outside the HI gas [4], that we interpreted as the result of the HI-to-H<sub>2</sub> transition triggered by the jet-gas interaction.

By confronting the CO emission to archival Herschel-FIR and GALEX-FUV data, we determined that the gas in the filaments is very inefficient to form stars compared to star-forming disc galaxies [4,5]. To understand why star formation is inefficient while the molecular gas reservoir is important, we recently obtained ALMA observations to map the <sup>12</sup>CO emission along the filaments, at a resolution of ~20 pc [6]. Such resolution enabled us to separate giant molecular clouds and study their physical properties (mass, size, velocity dispersion). While the properties of the molecular clouds in the filaments are very similar to those of molecular clouds in the inner Milky Way, we found that the virial parameter is slightly higher than in the Milky Way.

We concluded that the strong CO emission is an indication that the energy injected by the jet acts positively in the formation of molecular gas. On the other hand, the relatively high virial parameter of the molecular clouds suggests that the injected kinetic energy is too strong for star formation to be efficient. The filaments of Centaurus A are the first evidence of inefficient AGN positive feedback.

### **Références**

- |  |                                       |
|--|---------------------------------------|
| [1] Rejkuba et al. 2001, A&A, 379, 781       | [4] Salomé et al. 2016, A&A, 595, A65 |
| [2] Schiminovich et al. 1994, ApJ, 423, L101 | [5] Salomé et al. 2016, A&A, 586, A45 |
| [3] Charmandaris et al. 2000, A&A, 356, L1   | [6] Salomé et al. 2017, A&A, 608, A98 |

## The EMPIRE Survey : Dense Gas and Star Formation across Nearby Galaxy Disks

Diane Cormier<sup>1</sup>, Frank Bigiel<sup>2</sup>, María Jesús Jiménez-Donaire<sup>2</sup>, et al.

<sup>1</sup> *Laboratoire AIM, CEA/DSM - CNRS - Université Paris Diderot, Irfu/Service d'Astrophysique, CEA Saclay, 91191, Gif-sur-Yvette, France*

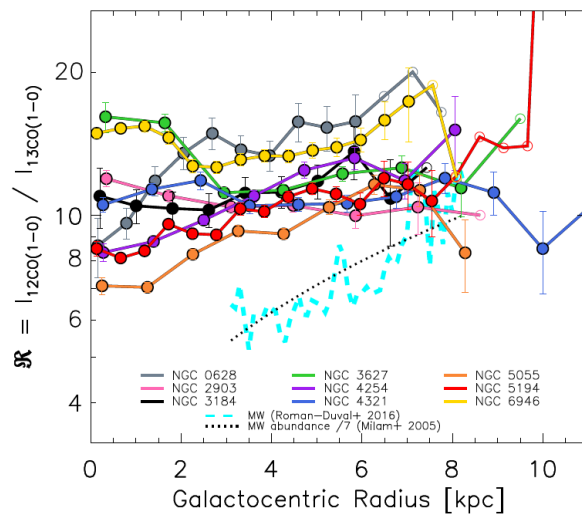
<sup>2</sup> *ITA, ZAH, University of Heidelberg, Albert-Ueberle Str. 2, D-69120 Heidelberg, Germany*

While stars are formed in the cold, dense parts of molecular clouds, extragalactic studies have mainly focused on  $^{12}\text{CO}$  emission to study star formation in galaxies. To make a significant step forward, with the EMPIRE survey, an IRAM 30m large program ( $\sim 500\text{h}$ ; [1,2]), we have obtained sensitive observations of dense gas tracers such as HCN,  $\text{HCO}^+$ , HNC,  $^{13}\text{CO}$ ,  $\text{C}^{18}\text{O}$ , across the entire disks of 9 nearby spiral galaxies. The key goals of the survey are to characterize the emission properties of the dense gas, the ISM physical conditions that they trace (densities, opacities, etc.), and how those relate to the star-formation activity and environment within galaxies.

I will present the first results from the survey. 1/ We find that, contrary to galaxy-integrated studies, dense gas fractions ( $\text{HCN}/\text{CO}$ ) and star formation efficiencies ( $\text{HCN}/\text{IR}$ ) vary within galaxies. Dense gas is abundant but particularly inefficient at forming stars in the galaxy centers, which are high-pressure environments ([2]). 2/ Analysis of the isotopologues of CO and the dense gas provide important new constraints on the optical depths, filling factors, and evidence for abundance variations in our sample of galaxies ([3,4,5], figure). In particular, we find that,  $^{13}\text{CO}$  does not appear to be a better predictor of the bulk molecular gas mass than  $^{12}\text{CO}$  because it does not measure diffuse molecular gas that seems to be important (though less so in the galaxy centers).

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## CO-dark molecular gas and the origin of [CII] emission in metal-poor galaxies

V. Lebouteiller<sup>1</sup>

<sup>1</sup> *Laboratoire AIM, UMR7158, Sorbonne Paris Cité, CEA, CNRS, 91191, Gif-sur-Yvette – France*

The difficulty to detect cold H<sub>2</sub> in metal-poor galaxies ([1]) has led to the hypothesis that atomic gas could contribute to the star-forming gas reservoir ([2]). However, there is growing evidence that a significant fraction of the molecular gas may not be detectable in CO transitions ([3]). This is especially true in low-metallicity environments where the low dust abundance results in enhanced far-UV photon penetration and CO photodissociation within a zone where H<sub>2</sub> is self-shielded and where IR/sub-mm tracers such as [CI] and [CII] may emit. Therefore, the total amount of H<sub>2</sub> in metal-poor galaxies and the fraction that lies in a cold dense phase is largely unknown. I will present two new results that shed a new light on the tracers of the CO-dark molecular gas and on the distribution of dense clouds in low-metallicity galaxies.

First, I will present a study of the star-forming region N11 in the moderately metal-poor (1/2 Z<sub>⊙</sub>) Large Magellanic Cloud. Using SOFIA/GREAT observations, we examined the velocity components of [CII], CO, HI, and H-alpha in order to isolate CO-dark and atomic gas components that are bright in [CII]. We find that most of the [CII] emission traces the CO-dark molecular gas and that most of the molecular gas toward and between CO clouds is CO-dark, either as layers around CO clumps or as interclump medium.

Second, I will describe the multi-phase and multi-sector ISM modeling of the extremely metal-poor (1/30 Z<sub>⊙</sub>) nearby galaxy IZw18 [4]. We infer that the [CII] cooling line emits in an X-ray dominated region (XDR) and traces an almost purely atomic gas. We also derive stringent upper limit on the size of H<sub>2</sub> clumps that may be detected in the future with JWST and IRAM/NOEMA.

By drawing on these two examples and others, I will then conclude by defining a paradigm of enhanced photodissociation and prevalence of XDRs at low metallicity partly due to the low dust-to-gas mass ratio. I will also discuss the diagnostics held by [CII] and other IR tracers in different environments.

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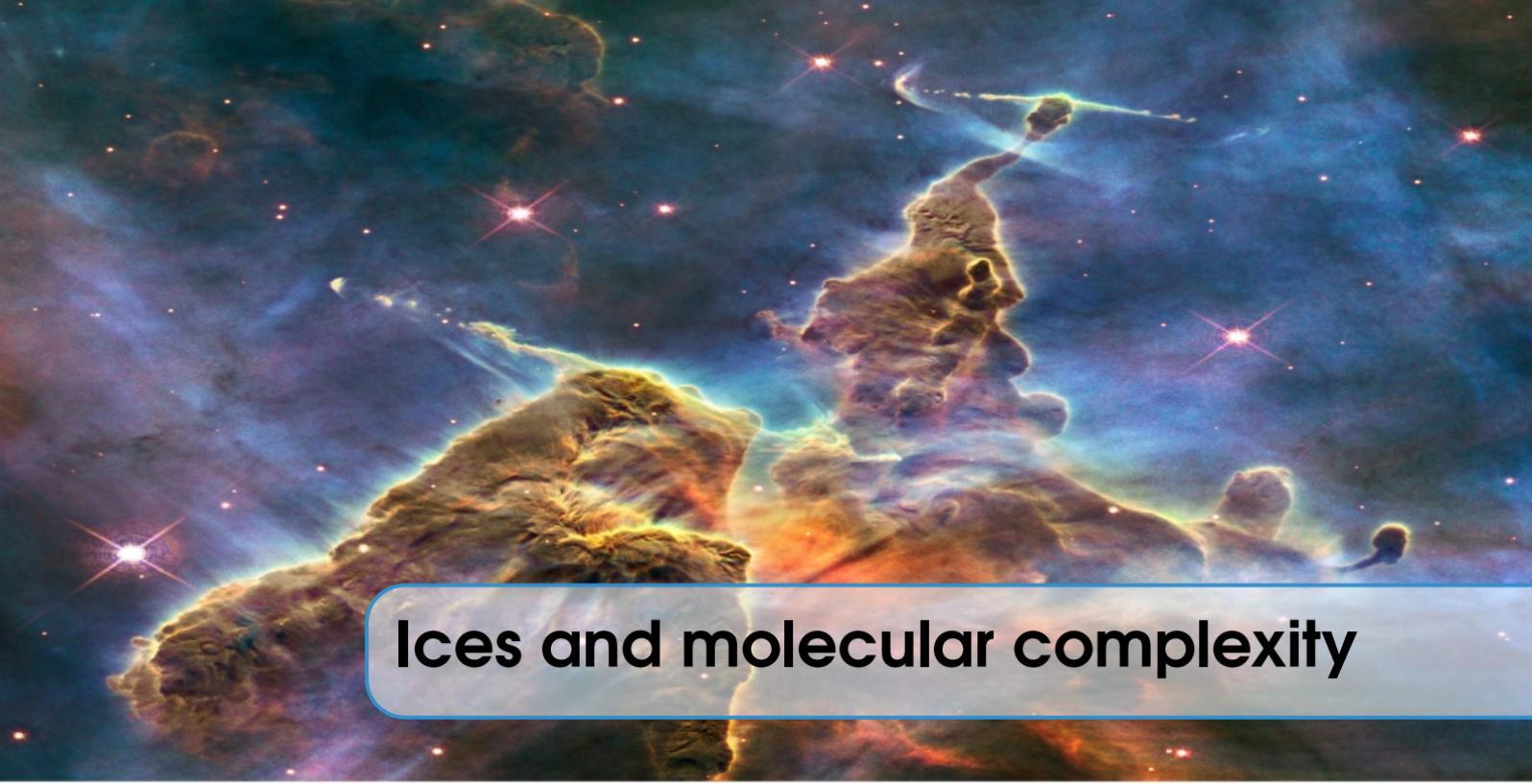
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## Molecular Hydrogen in Space

Pierre Guillard<sup>1</sup>

<sup>1</sup> *Sorbonne Université, Institut d'Astrophysique de Paris, UMR 7095*

The physics and chemistry of molecular gas are key to three fundamental questions in astrophysics: the formation of galaxies, stars and planets. Progress in these areas depends critically on our ability to observe the molecular gas in galaxies, especially  $\text{H}_2$ .  $\text{H}_2$  initiates complex interstellar chemistry by bonding with heavier elements.  $\text{H}_2$  is a tracer of the low-metallicity molecular material in the outskirts of galaxies, but also a tracer of the energetic processes that shape the structure of the interstellar matter, from galactic scales to the scales of turbulent dissipation. In that sense,  $\text{H}_2$  is very complementary to CO. I will review what we learned from extragalactic  $\text{H}_2$  observations, the perspectives with JWST, and some critical points that remain to be achieved on modelling and lab experiments.



**Ices and molecular complexity**

**Monday June 25<sup>th</sup> 11:45**

## The fate of COMs during high mass star formation

Sylvain Bontemps<sup>1</sup>

<sup>1</sup> *Laboratoire d'Astrophysique de Bordeaux, Université de Bordeaux*

*Allée Geoffroy Saint-Hilaire - 33615 Pessac*

High-mass stars become extremely luminous while reaching the main sequence as still accreting objects, i.e. as protostars. These large luminosities are believed to trigger dust surface and gas phase chemistry during the so-called hot core phase. In the past, emblematic sources such as SgrB2 (collection of hot cores) or classical hot cores such as G31.41 have proven to be indeed important targets to search for the rarest species found in the interstellar medium with for instance the detection of amino acetonitrile by Belloche et al. (2008) [1] in SgrB2(N) or glycolaldehyde by Beltran et al. (2009) [2] in G31.41. These sources are prime targets for astro-chemistry studies and complex organic molecules (COMs) hunts as they offer both large column densities of gas (often reaching more than  $10^{24} \text{ cm}^{-2}$ ) and large fractions of gas at temperatures above ice sublimation and desorption from the dust grains leading to warm/hot gas chemistry and large gas phase abundances of rare species. In order to progress on the precise origin (formation processes) of COMs in hot cores, it is of high importance to fully understand the physical evolution and its interplay with chemistry of young high-mass protostars. I will review the recent results on this topic with a particular emphasis on the earliest phases of the evolution of high-mass protostars which are now at reach with interferometers such as ALMA. These early phases may provide ways to probe the early chemical evolution before complete ice sublimation and desorption, ie at the time of chemistry dominated by dust surface processes. The comparison of young and evolved hot cores could for instance help to discriminate dust surface from gas phase products and help to recognize main formation path for most important COMs. I will also mention recent ALMA results which may challenge the classical view of hot cores as mostly warmed up by radiation.

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## **Seeds Of Life In Space (SOLIS): An IRAM-NOEMA large programme to investigate organic chemistry in solar-type star forming regions**

A. López Sepulcre<sup>1,2</sup>, C. Ceccarelli<sup>1</sup>, P. Caselli<sup>3</sup>, F. Fontani<sup>4</sup>, R. Neri<sup>2</sup>, C. Codella<sup>4</sup> and the SOLIS team

<sup>1</sup> *Univ. Grenoble Alpes, CNRS, IPAG, F38000, Grenoble – France*

<sup>2</sup> *Institut de Radio Astronomie Millimétrique, 300 rue de la piscine, 38406, Saint-Martin d'Hères – France*

<sup>3</sup> *Max Planck Institut für Extraterrestrische Physik, Giessenbachstrasse 1, 85748 Garching – Germany*

<sup>4</sup> *INAF-Osservatorio Astrofisica di Arcetri, Largo E. Fermi 5, I-50125, Florence – Italy*

Terrestrial life is based on organic chemistry, which appears to originate in interstellar clouds, the progenitors of Solar-like systems. Indeed, a large number of organic molecules are present in the interstellar medium. These are referred to as iCOMS (interstellar Complex Organic Molecules), and are typically defined as carbon-bearing molecules with six or more atoms.

How did organic chemistry develop during the formation our Solar System and Earth, where chemical complexity has reached its highest known level, i.e life? Addressing these two major questions is the main goal of SOLIS (Seeds Of Life In Space), an IRAM large program that makes use of NOEMA (NOthern Extended Millimetre Array) interferometer to systematically study a set of key iCOMs in a well-known sample of sources that covers the early phases of solar-type star formation. In this contribution, I will give an overview of SOLIS [1] and present a selection of its first results, which mainly regard the growth of cyanopolyynes (HC<sub>3</sub>N, HC<sub>5</sub>N) [2] and the formation of the prebiotic precursor formamide (NH<sub>2</sub>CHO) [3].

Finally, while sensitive spectral observations are a crucial ingredient to meet our goals, I will also stress the importance of joining efforts with experts on both theoretical and experimental chemistry in order to make progress.

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## Investigating transient species in the millimeter domain using spectral taxonomy

Marie-Aline Martin-Drumel<sup>1</sup>, Olivier Pirali<sup>1</sup> et Michael McCarthy<sup>2</sup>

<sup>1</sup> ISMO, UMR8214 du CNRS, Institut des Sciences Moléculaires d'Orsay, rue André Rivièrè, Université Paris-Sud, Université Paris-Saclay, 91405, Orsay Cedex – France ;

<sup>2</sup>Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, 02138 Cambridge, MA – United States

With their unprecedented performances in terms of spectral resolution and sensitivity, spectral survey currently recorded using the new generation of observational platforms (ALMA, NOEMA) reveal unsurprisingly many molecular features that are currently absent from spectroscopic databases as JPL or CDMS [1, 2] and thus arise from so far unknown species (U-lines). The determination of the carriers of these features, which will enable a better understanding of the physical conditions and chemical evolution of the ISM, requires deep investigations from laboratory spectroscopy especially in the spectral range covered by these instruments, at millimeter and sub-millimeter wavelength. Several types of compounds are of high interest as potential carriers for the U-lines: already identified stable interstellar species but in excited vibrational states or isotopic variants (owing to the increased sensitivity and signal-to-noise ratio of the new astronomical instruments) or entirely new compounds. Of particular interest are transient, highly reactive species, as they remain widely understudied in the laboratory compared to stable molecules.

Currently, most of the laboratory studies on astronomical species are highly biased: a target molecule, thought to be present in the ISM, is selected and experiments are performed to detect its rotational lines by recording spectra in very narrow spectral ranges matching the predictions for this species. We recently developed a new approach, spectral taxonomy, that allows investigation of complex mixtures and identification of new species without a priori knowledge of their elemental composition or molecular structure [3]. Spectral taxonomy involves acquiring a broadband rotational spectrum of a rich mixture and subsequently categorizing each individual line based on its relative intensity under series of assays: dependence over one precursor or another is an indication of atomic composition, disappearance in absence of the excitation source (e.g., discharge) implies a transient species, and influence of an external magnetic field on the line shape points out an open-shell molecule. Initially developed in the centimeter domain, spectral taxonomy is now extended to the millimeter domain. We will present recent results obtained on several transient species, as  $c\text{-C}_3\text{H}_2$  and HCCSH.

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## **Laboratory Studies of Thermal and Non-thermal Processes on and in Growing Icy Grain Mantles.**

D. Marchione, A. Rosu-Finsen, A. G. M. Abdulgalil, J. D. Thrower, V.

Frankland, M. P Collings and M. R. S. McCoustra<sup>1</sup>

*Institute of Chemical Science, Heriot-Watt University, EDINBURGH, EH14 4As,  
UK.*

A synthesis observations from laboratory studies on the thermal and non-thermal physics and chemistry of dust grains as they evolve from diffuse to dense environments in the interstellar medium will be presented. We will specifically report on (1) thermal desorption and the impact of surface heterogeneity; (2) agglomeration of water (H<sub>2</sub>O) on an amorphous silica (aSiO<sub>2</sub>) surface; (3) highly efficient electron-promoted desorption of weakly bound adsorbates from H<sub>2</sub>O ice surfaces; (4) photo-desorption from H<sub>2</sub>O ice surfaces at ultraviolet wavelengths in the 200 to 300 nm range; and (5) efficient molecular hydrogen (H<sub>2</sub>) generation from ionisation of reduced carbon-containing species. The conclusion drawn from this synthesis is that the onion model of icy grain mantles needs revision.

## Reactivity in interstellar ice analogs : role of the structural evolution

Ghesquiere P.<sup>1</sup>, Noble J. A. <sup>2</sup>, Ivlev A.<sup>3</sup> et Theulé P.<sup>4</sup>

<sup>1</sup> *Institut de Chimie Moléculaire de l'Université de Bourgogne, UMR 6302 CNRS, Université de Bourgogne Franche-Comté, 9 Av. A. Savary, BP 47 870, 21078 Dijon*

<sup>2</sup> *Laboratoire de Physique des Lasers, Atomes et Molécules (UMR CNRS 8523), Université Lille 1 Sciences Technologies*

<sup>3</sup> *Max-Planck-Institut für Extraterrestrische Physik, Giessenbachstr. 1, D-85748 Garching, Germany*

<sup>4</sup> *Aix-Marseille Université, PIIM UMR-CNRS 7345, 13397 Marseille, France*

The synthesis of interstellar complex organic molecules in ice involves several types of reactions between molecules and/or radicals, which are usually considered to be diffusion controlled [1]. We aim to understand the coupling between diffusion and reactivity in the interstellar ice mantle, using a model binary reaction in the diffusion-limited regime.

We performed isothermal kinetic laboratory experiments on interstellar ice analogues at low temperatures, using the NH<sub>3</sub>:CO<sub>2</sub>:H<sub>2</sub>O model system we previously reported [2] where reactants NH<sub>3</sub> and CO<sub>2</sub> have a low reaction barrier and are diluted in a water-dominated ice.

We found that in the diffusion-limited regime, the reaction kinetics is not determined by the intrinsic bulk diffusivity of reactants. Instead, reactions are driven by structural changes evolving in amorphous water ice, such as pore collapse and crystallization. Diffusion of reactants in this case likely occurs along the surface of (tiny) cracks generated by the structural changes [3].

The reactivity driven by the structural changes breaks the conventional picture of reactant molecules/radicals diffusing in a bulk water ice. This phenomenon is expected to lead to a dramatic increase of the production rates of interstellar complex organic molecules in star forming regions.

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## Formation of complex molecules on cold surfaces

F. Dulieu<sup>1</sup>, T. Nguyen<sup>1</sup>, E. Congiu<sup>1</sup>, S. Baouche<sup>1</sup>, A. Sow<sup>1</sup>, M. Minissale<sup>1,2</sup>, J.C. Loison<sup>3</sup>, D. Talbi<sup>4</sup>.

<sup>1</sup> *LERMA, Université de Cergy-Pontoise, Sorbonne Université, Observatoire de Paris, PSL University, CNRS, LERMA, F-95000, Cergy-Pontoise*

<sup>2</sup> *PIIM, Institut Fresnel, Aix-Marseille Université, F-13013 Marseille*

<sup>3</sup> *ISM – Université de Bordeaux – CNRS, UMR 5255, F-33405 Talence Cedex,*

<sup>4</sup> *Laboratoire Univers et Particules de Montpellier, UMR 5299 - Université Montpellier 2, F-34095 Montpellier cedex 05*

Interstellar Complex Organic Molecules (iCOMs) are considered as the building blocks of more complex pre-biotic compounds. In particular, formamide (NH<sub>2</sub>CHO), widely observed in different astrophysical media, is thought to be the starting point of some emblematic metabolic and genetic species (Saladino et al. 2012). Formamide formation through Gas Phase route exists (Barone et al 2015, Codella et al 2017), even if it is still debated, but solid-state chemistry should also be a vector of the molecular complexity observed in later phases of the matter evolution, such as in comets and meteorites.

Our group aims at understanding how the molecular complexity may increase on cold surfaces, from atoms or molecules, without the help of others external energetic agents (photons, electrons, ions...). During the last few years we have developed a new experimental facility (named VENUS) to study the different non-energetic pathways of solid-state astrochemistry.

During my presentation I will show how we can constrain the penetration depth of H and O through molecular ices (e. g. H<sub>2</sub>O, NO, H<sub>2</sub>CO). Penetration actually occurs at a negligible rate in comparison with other surface processes (diffusion and self reaction) (Minissale et al, Sow et al in prep.). Thus, I will present evidence that formamide can also be formed very efficiently following solid-state chemical pathways (Nguyen et al, in prep.).

Finally, I will give few example of how we can nowadays determine the chemical networks (including the evaluation of barriers, and type of reaction) of specific chemical solid state systems, such like the hydrogenation of NO (Nguyen et al, in prep.), combining complete sets of experiments with state-of-the-art calculations of quantum chemistry.

## **Theoretical approaches for gas-phase and ice surface processes**

Dahbia Talbi

*LUPM, UMR5299 du CNRS, Université de Montpellier, Place Eugene Bataillon,  
34095, Montpellier Cedex 5 – France*

It is nowadays an evidence that both gas phase reactive collisions and heterogeneous chemistry involving interstellar grains/ices, play a fundamental role in the formation of molecules in space. For the last processes, in addition to understanding the catalytic role of the solid phase, there is also the problem of understanding the adsorption, diffusion and desorption of the reactants and/or products as well as the thermal exchanges between the products and the solid phase. Theoretical chemistry is able to address both chemistries with more or less accuracy and success but always bringing useful information for astrochemical modelling. I will through this talk, try to address in a manner accessible to an interdisciplinary audience, the approaches used by the theoretical chemists/physicists of the PCMI community to understand both this gas phase and solid state chemistry.



# ISM Structures

**Tuesday June 26<sup>th</sup> 9:00**

## ISM in 3D: methods and astrophysical consequences

J.Montillaud<sup>1</sup>

<sup>1</sup> *Institut UTINAM, CNRS UMR 6213, Univ de Bourgogne Franche-Comté,  
OSU THETA*

Determining distances is a longstanding issue in astrophysics, limiting our ability to build an accurate and reliable three-dimensional picture of our Galaxy. Because interstellar gas and dust are often optically thin and generally consist of diffuse emissions, our knowledge of the 3D structure of the interstellar medium (ISM) is even more uncertain than the spatial distribution of stars.

Numerous strategies have been developed to circumvent those difficulties utilising a variety of observations. The observation of gas line emission (CO rotational emission, HI hyperfine emission, ...) has proven fruitful to separate ISM components according to their kinematic properties, and to estimate cloud distances based on assumptions on the Galactic dynamics. Several ambitious surveys were recently published (e.g. the HI4PI all-sky 21cm survey) or are still being conducted (e.g. the Mopra Southern Galactic Plane CO Survey) which increase by orders of magnitude the amount of data available to study the 3D structure of the ISM, and make statistical, automated methods unavoidable. But presently, the best potential to progress on our knowledge of the 3D ISM comes from the recent large stellar surveys like SDSS, Pan-starrs and, even more importantly, Gaia and its spectroscopic follow-up surveys, which trace the distribution of interstellar dust extinction. Analysing these large (>1 billion stars) and heterogeneous (magnitudes, parallaxes, spectra, ...) data sets raises numerous challenges both in terms of methods and physical knowledge of the ISM (e.g. the extinction curve and its variations).

In this presentation, I will review the methods that were developed to deal with the wealth of available data and the recent advances in the characterisation of the ISM 3D structure, with an emphasis on scales from giant molecular clouds to Galactic scales.

## The $\gamma$ -ray view on the HI-H<sub>2</sub>-CO interface in nearby clouds

Grenier I. A.<sup>1</sup> and Remy Q.<sup>2</sup>

<sup>1</sup> *Laboratoire AIM, CEA-IRFU/CNRS/Université Paris Diderot, Département d'Astrophysique, CEA Saclay, F-91191 Gif sur Yvette – France*

<sup>2</sup> *Laboratoire Univers et Particules de Montpellier, Université de Montpellier, CNRS/IN2P3, Montpellier– France*

The interstellar gamma-ray emission can be used to infer the column densities of optically-thick HI, diffuse CO-dark H<sub>2</sub>, and dense CO-bright H<sub>2</sub> in a cloud. We have used observations by the Fermi Large Area Telescope and by Planck, together with HI and CO line data to probe the HI-H<sub>2</sub>-CO transitions in a sample of nearby clouds in the Chamaeleon and anticentre regions. We will show how the gas mass in the dark neutral medium (DNM) present at the atomic-molecular interface relates to the mass observed in the other bright phases [1]. The DNM fraction by mass varies with the diffuse character and peak CO intensity of the cloud [1].

We will also discuss how the average CO-to-H<sub>2</sub> conversion factor per cloud,  $X_{\text{CO}}$ , tends to decrease from diffuse to more compact CO clouds, in qualitative, but not quantitative agreement with theoretical predictions [2].

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## Stochastic modeling of the ISM processes

Franck Le Petit<sup>1</sup>, Emeric Bron<sup>2,1</sup> et Jacques Le Bourlot<sup>1</sup>

<sup>1</sup> *Sorbonne Université, Observatoire de Paris, Université PSL, CNRS, LERMA, F92190 Meudon, France*

<sup>2</sup> *ICMM, Consejo Superior de Investigaciones Científicas (CSIC). E-28049. Madrid, Spain.*

Our understanding of the physical and chemical processes in interstellar gas has made significant progress thanks to increasingly sophisticated numerical models. However, key problems remain while their resolution is essential to answer the major questions in the field. Examples are the modelling of chemical processes on grain surfaces or the impact of interstellar turbulence on gas chemistry. Partial answers have been provided, but the quantitative jump in modeling quality needed to fully answer the questions seems to face barriers that are difficult to overcome.

In this presentation, I will show that one of the blocking points is the very formalism used to simulate processes. Indeed, the approach adopted since the 1980s for modelling processes in interstellar gas is often based on the classical deterministic approach, whereas a number of fundamental physical and chemical processes are by nature probabilistic. Therefore, significant progress can probably only be made by reconsidering traditional approaches and inventing new ones, based on stochastic approaches. I will illustrate this on grain surface chemistry and turbulence [1,2,3].

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## **Novel statistical tools to characterize interstellar magnetized turbulence.**

E. Allys<sup>1</sup>, C. Colling<sup>2</sup>, S. Zhang<sup>5</sup>, F. Boulanger<sup>1</sup>, E. Falgarone<sup>1</sup>,  
P. Hennebelle<sup>1,2</sup>, F. Levrier<sup>1</sup> et S. Mallat<sup>4,5</sup>.

<sup>1</sup> *Sorbonne Université, Observatoire de Paris, Université PSL, Ecole Normale Supérieure, CNRS, LERMA, F-75005, Paris, France*

<sup>2</sup> *IRFU, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France*

<sup>3</sup> *Université Paris-Diderot, AIM, Sorbonne Paris Cité, CEA, CNRS, F-91191 Gif-sur-Yvette, France*

<sup>4</sup> *Collège de France, 11 place Marcelin Berthelot, F-75005 Paris, France*

<sup>5</sup> *Ecole Normale Supérieure, Université PSL, F-75005 Paris, France*

The structures of matter formed in the interstellar medium are the result of a complex interplay of physical processes, acting on many connected spatial and temporal scales. Among these processes, magnetized turbulence is thought to play a major role, and numerical simulations are now able to reproduce qualitatively the complex, filamentary structures observed, e.g., in thermal dust emission, but the non-linear nature of the processes at work hinders our ability to precisely compare these simulations to observations and thus assess the characteristics of interstellar turbulence.

To overcome this difficulty, we have initiated a collaboration with data scientists who have developed an analysis framework, the wavelet scattering transform (WST), which is able to capture the essential statistical properties in any given image, beyond the standard power spectrum estimation [1]. Applying the WST to numerical simulations of interstellar turbulence with various levels of turbulent forcing and magnetic field intensity, we demonstrate that it is able to efficiently discriminate between different physical settings, even though the structures appearing in these simulations look very similar to the naked eye.

The WST thus promises to open a fruitful new avenue of research to quantitatively assess the properties of magnetized interstellar turbulence based on a morphological analysis of the structures appearing in emission maps.

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## The dynamics of photodissociation regions: from the observed tracers to a dynamical model.

Bron E.<sup>1,2</sup>, Agúndez M.<sup>1</sup>, Goicoechea J. R.<sup>1</sup>, Cernicharo J.<sup>1</sup>, Joblin C.<sup>3</sup>, Wu R.<sup>2</sup>

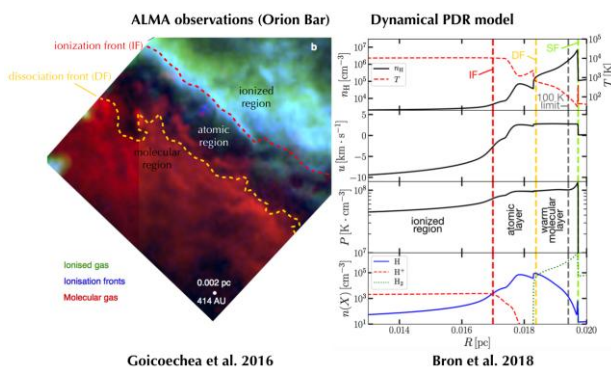
<sup>1</sup> Instituto de Física Fundamental-CSIC, Calle de Serrano 123, 28006 Madrid, Spain

<sup>2</sup> LERMA, Observatoire de Paris, PSL Research University, CNRS, Sorbonne Universités, UPMC Univ. Paris 06, F-92190, Meudon, France

<sup>3</sup> IRAP, Université de Toulouse, CNRS, UPS, CNES, 9 Av. colonel Roche, BP 44346, 31028 Toulouse Cedex 4, France

Photodissociation regions (PDR) constitute the skin layer of molecular clouds in star forming regions, where dense molecular gas is submitted to dissociating and ionizing UV photons. The rich emission spectrum emitted in this warm, partially molecular layer (numerous ionic, atomic and molecular lines, PAH emission) dominates large parts of the infrared and submm spectrum of a whole galaxy. Tracers emitted in these regions (e.g.  $C^+$ ,  $C$ , mid/high-J CO) are increasingly used in extragalactic observations to trace the star formation cycle in other galaxies, but result from a complex interplay of physical and chemical processes: chemistry in the gas and on grain surfaces, (de)excitation processes of the atoms and molecules, heating and cooling balance, etc. Their interpretation thus requires detailed astrochemical models.

I will present how recent Herschel [1,2] and ALMA [3,5] observations have changed our understanding of the processes governing the emission of these regions, and have in particular revealed the important role of gas dynamics in shaping these interfaces. In order to answer the new questions raised by these observations, we have developed a new hydrodynamical PDR code, the *Hydra* PDR code [4]. I will show how taking the photoevaporation dynamics into account naturally explains several problematic aspects of the observations, such as a strong and recurrent correlation between the gas pressure in the PDR and the UV field intensity illuminating it, or the strong density gradients at the edge of the PDR.



### Références :

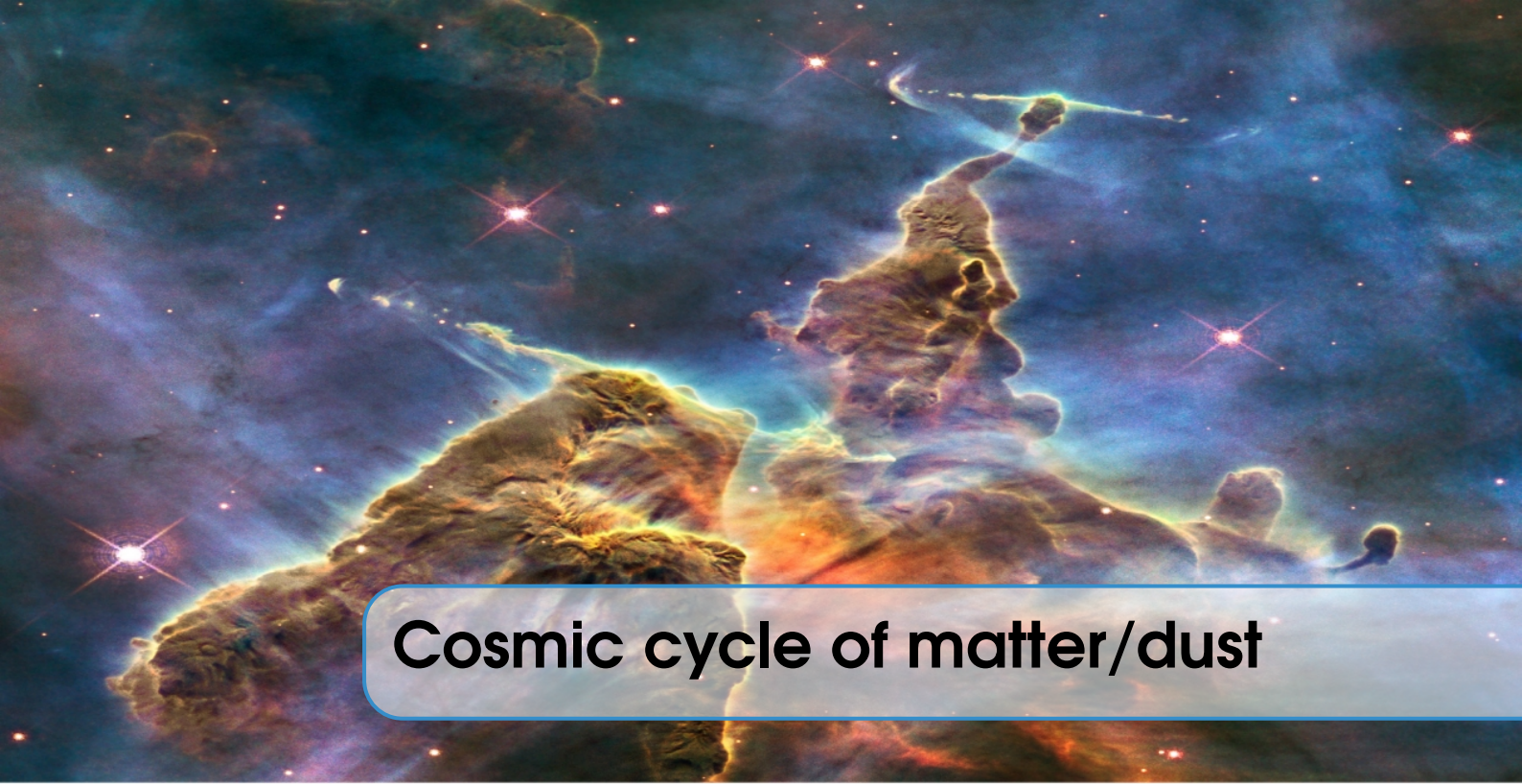
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- [5] Goicoechea J. R., Pety J., Cuadrado S., Cernicharo J., Chapillon E., Fuente A., Gerin M., Joblin C., Nuria M., Pilleri P., Nature, 537, 7619, p207 (2016)

## **Simulating the ISM**

Guillaume Laibe

*Ecole Nationale Supérieure de Lyon*

We will illustrate some difficulties inherent to the numerical simulation of the Interstellar Medium on the concrete example of the treatment of the dynamics of the grains. In particular, we will present the advantages of the MULTIGRAIN monofluid approach in this context.



## Cosmic cycle of matter/dust

**Tuesday June 26<sup>th</sup> 11:45**

## Carbonaceous matter: from ISM to protoplanetary disks.

E. Dartois

*ISMO, Institut des Sciences Moléculaires d'Orsay, UMR8214 du CNRS, Bât. 520,  
Rue André Rivière, 91405 Orsay Cedex.*

The interstellar medium carbonaceous dust grains and their observed spectral signatures reveal a great diversity of allotropes. Astronomical observations give access to the molecular functionality of these solids, setting constraints on the composition of organic solids and molecules in the cycling of matter in the Galaxy. Some of them can be reproduced in the laboratory. Other signatures still await for their carriers definitive identifications and laboratory analogues help in constraining their physico-chemical composition and evolution under the harsh radiation environments.

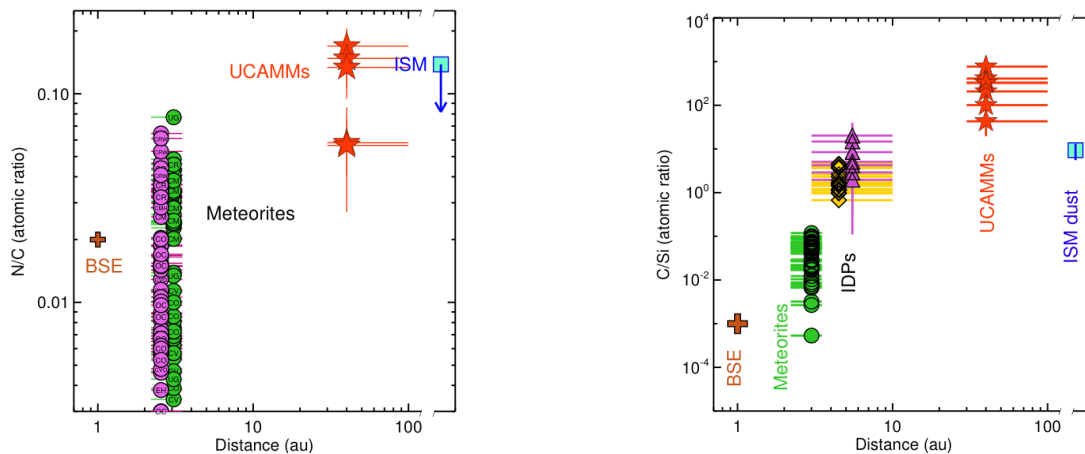


Figure 1: *Left, Nitrogen abundances relative to carbon (atomic ratio) are compared to solar system solids (Earth-BSE, meteorites, Ultracarbonaceous micrometeorites, ISM), in function of heliocentric distance. Right, same for carbon abundances relative to silicon, including Interplanetary dust particles (IDPs) (atomic ratio), compared to solar system solids (Dartois et al., A&A 609, A65, 2018).*

This talk will particularly focus on carbonaceous dust materials from the far space environments, from diffuse ISM to protoplanetary disks and in our neighbourhood (Solar System) extraterrestrial collected dust. One objective will be to draft some commonalities and differences between materials found in the Solar System, protoplanetary disks and Interstellar dust.

## Dust properties in Galactic Cold Cores: intensity and polarization

I.Ristorcelli<sup>1</sup>, M.Juvela<sup>2</sup> on behalf of  
the *Galactic cold cores* collaboration

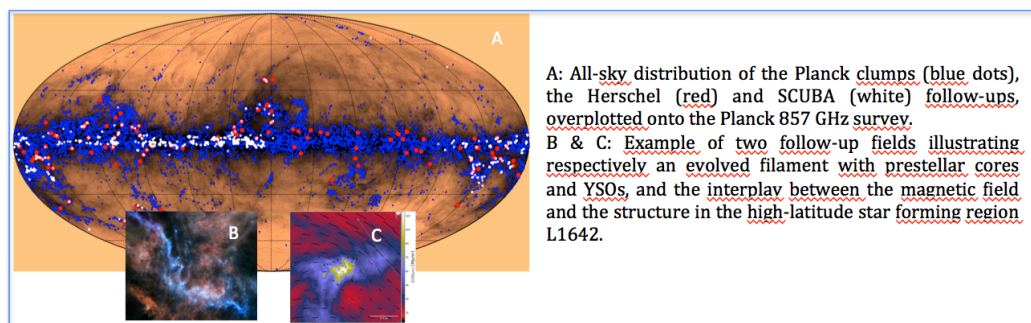
<sup>1</sup> IRAP, Université de Toulouse, CNRS, UPS, CNES, Toulouse, France

<sup>2</sup> University of Helsinki, Department of Physics, Finland

The Planck satellite provided the first all-sky survey of the interstellar medium with a sensitivity, wavelength coverage and resolution well suited to detect cold clumps at arc minute scales. This survey allowed us to build a catalogue of more than 13000 sources [1], covering a wide range of Galactic environments and physical conditions, and making this sample unique for statistical investigation of star formation in the Milky Way. In the Galactic Cold cores program, the properties of the Planck clumps are being investigated with data from various follow-up surveys, including higher angular resolution continuum data (Herschel key programme, SCUBA-2 legacy program, NIKA) and molecular spectroscopy of dense-gas tracers (IRAM, Effelsberg, TRAO, etc.).

We have investigated the dust emissivity variations indicative of processes like grain growth [2,3,4], the filament characteristics with links to the environment [4,5], and the physical clumps and cores properties (morphology, mass, size, temperatures, evolutionary stage) [6, 7]. In parallel, the Planck dust polarized emission has allowed us to analyse the magnetic field morphology in the clump environment and to study its interplay with structures such as filaments and striations [8,9]. We also have performed a statistical study of the polarization fraction variations and their column-density dependence, discussing their origin in terms of magnetic field geometry and grain alignment efficiency [10].

I will review the main results of these analyses, focusing on dust properties in intensity and polarization, and present our perspectives for future studies.



### References

- |  |   |
|--|---|
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## Gas and dust in the diffuse interstellar medium: new surveys of diffuse interstellar bands and dust polarisation

Nick Cox<sup>1</sup>, and the EDIBLES and LIPS consortia

<sup>1</sup> *ACRI-ST, Route du Pin Montard, 06904, Sophia-Antipolis – France*

The composition and nature of interstellar dust grains and the molecular composition of interstellar gas are important factors in understanding the chemistry and physics of the diffuse interstellar medium and its role in star formation and galaxy evolution. In this contribution we present the first results from two VLT surveys studying in detail the nature and properties of interstellar gas and dust in diffuse clouds.

The ESO diffuse interstellar band large exploration survey (EDIBLES<sup>[1]</sup>) focusses on the atomic and molecular content of the diffuse ISM by probing the lines-of-sight towards ~120 bright OB stars. This survey provides a deep census of interstellar atomic and molecular abundances and diffuse interstellar band (DIB) absorptions in the diffuse/translucent ISM. The goal of EDIBLES is to ‘reverse-engineer’ the physical properties of the carriers of the enigmatic unidentified diffuse interstellar bands as a contribution towards their identification. I will present the first results related to DIB profiles, interstellar hydrides, and the C60 fullerene.

The large interstellar polarisation survey (LIPS<sup>[2]</sup>) is a medium-resolution spectropolarimetry study with FORS2 to measure the wavelength-dependent polarisation of starlight by aligned interstellar dust grains in ~100 lines-of-sight (a large fraction overlapping with EDIBLES). We investigate the variations (evolution) of dust grains through a parametrised Serkowski-law fitting of these curves. The polarisation spectra are combined with UV extinction curves and modelled simultaneously with a physical dust grain model. We present the first observational results in terms of the Serkowski-parameters as well as the dust modelling of a sub-set of the targets, in particular our study of “single-cloud” sightlines.

Together, EDIBLES and LIPS provide a comprehensive examination of the molecules and dust properties in a statistically large sample of nearby Galactic sightlines.

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## Polycyclic Aromatic Hydrocarbon fraction at ~20 pc scale in the Magellanic Clouds

Jeremy Chastenet<sup>1</sup>, Karin Sandstrom<sup>1</sup>, Caroline Bot<sup>2</sup>, Karl  
Gordon<sup>3</sup>

<sup>1</sup>*Center for Astrophysics & Space Sciences, University of California San Diego,  
9500 Gilman Drive La Jolla, CA 92093, USA*

<sup>2</sup>*Universite de Strasbourg, CNRS, Observatoire astronomique de Strasbourg,  
UMR 7550, F-67000 Strasbourg, France*

<sup>3</sup>*Space Telescope Science Institute, 3700 San Martin Drive, Baltimore, MD  
21218, USA*

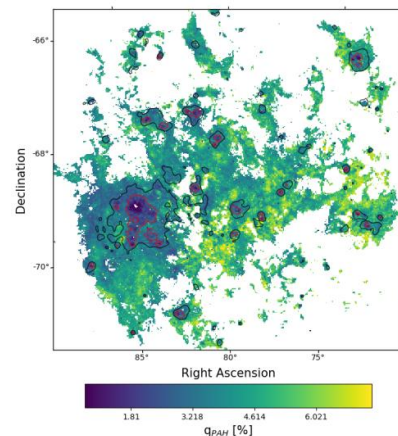
The spatial variations of dust properties within a galaxy and their correlation with local environment provide critical insights into the life cycle of dust. Low metallicity galaxies, in particular, let one study the dust life cycle in environments relevant for galaxies earlier in the history of the Universe.

In this work, we present maps of the dust properties in the Small and Large Magellanic Clouds (SMC, LMC), two nearby, highly resolved, low metallicity galaxies, fit with the Draine & Li (2007; DL07)<sup>[1]</sup>, Compiegne et al. (2011)<sup>[2]</sup> and THEMIS (Jones et al. 2017)<sup>[3]</sup> dust grain models (Chastenet et al. 2017)<sup>[4]</sup>. We use *Spitzer* and *Herschel* infrared observations of the clouds to derive the spatial distribution of the dust properties, in particular the abundance of the small carbonaceous grain (or polycyclic aromatic hydrocarbons; PAH) component. Overall, the average PAH fraction is

smaller in the SMC than in the LMC, which is lower than that of the Milky Way. In particular, we find an anti-correlation between the DL07  $q_{\text{PAH}}$  fraction and the H $\alpha$  intensity (Figure 1). This is an indication that the smallest dust grains could be destroyed in high-ionization regions. We provide maps of the  $q_{\text{PAH}}$  fraction at resolved scales (16 pc in the SMC, 13 pc in the LMC). We also compare our final maps with previous modeling (LMC: Paradis et al. 2009<sup>[5]</sup>, using the Désert et al. 1990<sup>[6]</sup> model; SMC: Sandstrom et al. 2010<sup>[7]</sup>, using the DL07 model). This helps us identifying the most model-dependent dust properties, and how they vary with resolution and wavelength coverage. We use these results to constrain the drivers of the PAH lifecycle in low metallicity environments.

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## Probing the impact of the C/O ratio and metals on the properties of dust particles in a cold plasma reactor

R. Berard<sup>1,2</sup>, K. Makasheva<sup>2</sup>, H. Sabbah<sup>1,3</sup>, and C. Joblin<sup>1</sup>

<sup>1</sup>IRAP, Université de Toulouse, CNRS, UPS, CNES, 9 Av. du Colonel Roche, 31028 Toulouse Cedex 4, France

<sup>2</sup>LAPLACE (Laboratoire Plasma et Conversion d'Energie), Université de Toulouse, CNRS, UPS, INPT, 118 route de Narbonne, Toulouse cedex 9, France

<sup>3</sup>LCAR-IRSAMC, Université de Toulouse UPS, CNRS, 118 Route de Narbonne, Toulouse cedex 9, France

The formation of dust in the envelopes of evolved stars is still poorly understood. Nucleation theories and thermodynamic models predict two main different dust families depending on the C/O ratio in the envelope. C-rich stars would lead to carbonaceous nanograins possibly including polycyclic aromatic hydrocarbons (PAHs) whereas O-rich stars would lead to oxide or silicate nanograins. Our aim is to get insights into the impact of the C/O ratio and the presence of metals on dust properties. To that end we carry experiments in a cold plasma reactor to generate dust analogues and perform *ex-situ* molecular mass analysis of the collected dust.

The advantage of experiments in plasma reactors is that one can play on the gas-phase chemical composition by using different gas precursors and also, in our case, sputtering of a metal target to release metal atoms in the plasma gas phase [1]. More specifically we use an axially asymmetric radiofrequency argon discharge with pulsed injection of hexamethyldisiloxane (HMDSO, C<sub>6</sub>H<sub>18</sub>OSi<sub>2</sub>) that contains key elements present in the envelopes of evolved stars. This configuration allows to study the impact of two specific parameters on the dust formation: -(i)- the C/O ratio by enriching the mixture with oxygen by O<sub>2</sub> injection and -(ii)- the metal atoms by sputtering of Ag and, currently, Fe.

To probe the impact of the C/O ratio and metals, we investigate the molecular composition of the collected dust using the AROMA (Astrochemistry Research of Organics with Molecular Analyzer) set-up. The instrument combines laser desorption/ionisation, in a single or two-steps scheme, with an ion trap mass spectrometer [2]. Diagrams are built from the obtained mass spectra and some first considerations on chemical pathways are provided.

### Acknowledgement

We acknowledge support from the European Research Council under the European Union's Seventh Framework Programme ERC-2013-SyG, Grant Agreement n. 610256 NANOCOSMOS and from the UMS Raymond Castaing of the University of Toulouse for the SEM and TEM observations.

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## PAHs adsorbed on interstellar ice : structures, energetics and IR spectra from a multi-method theoretical study

E. Michoulier<sup>1,2</sup>, C. Toubin<sup>2</sup>, A. Simon<sup>1</sup>

<sup>1</sup> Laboratoire LCPQ, Université Paul Sabatier 31062 Toulouse Cedex 09, France  
aude.simon@irsamc.ups-tlse.fr

<sup>2</sup> Laboratoire PhLAM, UMR CNRS 8523, Université de Lille, 59655, Villeneuve d'Ascq  
Cedex-France

Polycyclic Aromatic Hydrocarbons (**PAHs**) have had an astrophysical interest since they were proposed, in the mid-eighties, to be the carriers of 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). 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], studies of ices containing PAHs are scarcer and have been reported recently [3]. To shed light on the unexpected role played by PAHs in cosmic ice chemistry, IR spectroscopy experiments on the cryogenic codeposition [4] of PAH and water are achieved at "Institut des Sciences Moléculaires" (Université de Bordeaux). In connection with these experiments, we are modeling **PAHs of various sizes and shapes** interacting with **various icy environments** (amorphous and crystalline) using a **multi-method approach** :

- \* **Molecular dynamics/force-field (MD/FF) simulations** were performed to determine the adsorption sites of PAH on ice and draw binding energy maps characterizing the variations of the PAH-ice interaction over the surface [5a].

- \* From the MD/FF configurations, a finite PAH-ice system was built, that can be described within the Density Functional based Tight Binding (DFTB) scheme, providing an explicit electronic structure description for such a large system. This allowed the determination of the **influence of ice interaction on the PAH ionization potential (IP)** at the DFTB level. Besides, a **relationship between interface structures** (number of interacting dangling OH) **and IP variation** was established. The theoretical results are discussed in the light of experimental data [5b].

- \* IR spectra of the previously determined PAH-ice structures were computed within the harmonic approximation at the DFTB level : the **influence of the adsorption of the PAH on the dangling OH mode** at the ice surface is quantified and compared to the experimental shifts.

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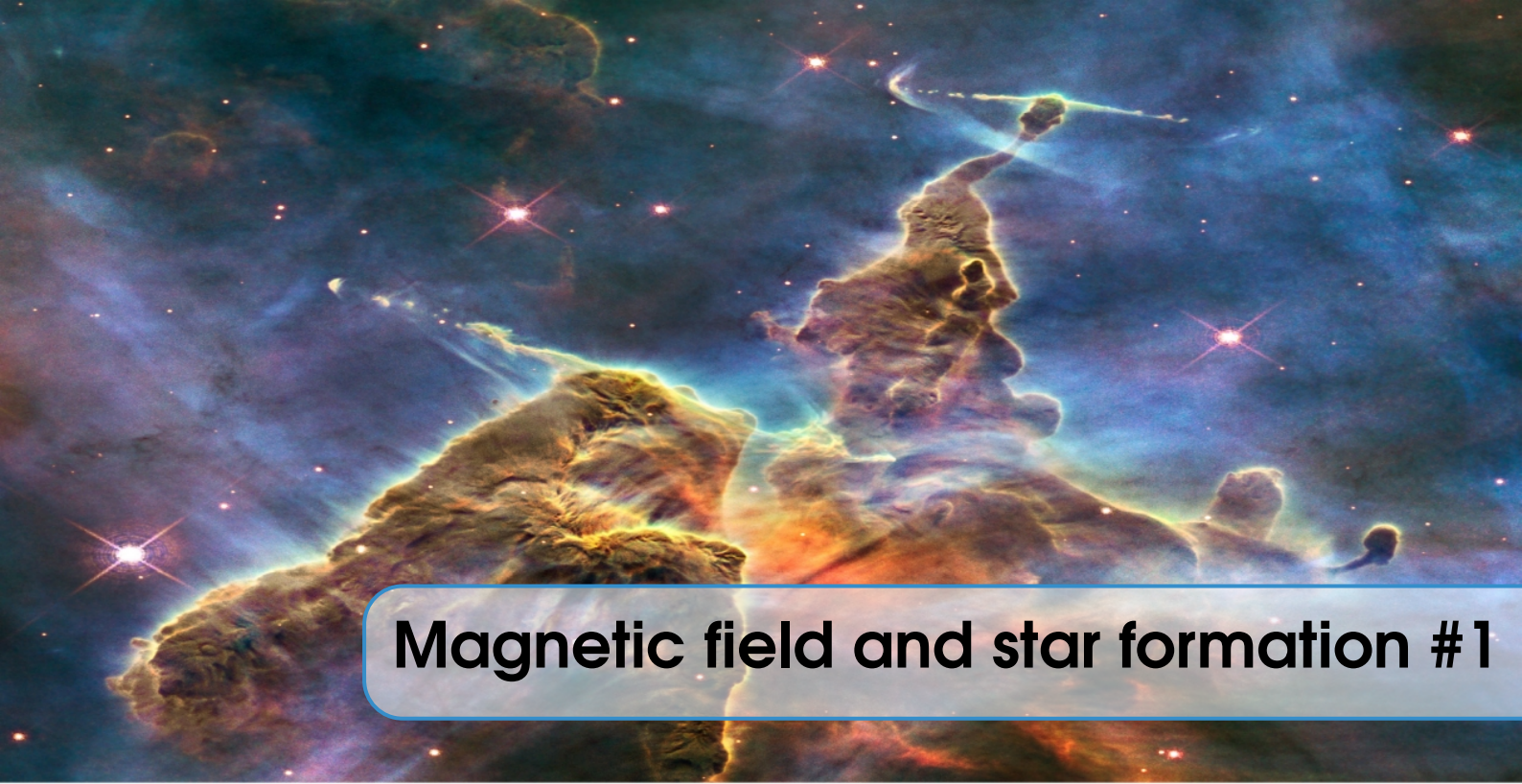
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**Funding** : ANR PARCS : ANR-13-BS08-0005



# Magnetic field and star formation #1

**Tuesday June 26<sup>th</sup> 17:00**

## **The ArTéMiS submillimeter continuum camera on APEX: Capabilities and first scientific results on the structure of dense star-forming complexes**

Ph. André<sup>1</sup>, F. Schuller<sup>1</sup>, A. Zavagno<sup>2</sup>, V. Revéret<sup>1</sup>, H. Roussel<sup>3</sup>, N. Peretto<sup>4</sup>

<sup>1</sup>*AIM, Laboratoire d'Astrophysique-Instrumentation-Modélisation, UMR7158  
CEA-Université Paris-Diderot-CNRS, C.E. Saclay, Orme des Merisiers - Bât. 709, 91191  
Gif-sur-Yvette Cedex – France*

<sup>2</sup>*LAM, Laboratoire d'Astrophysique de Marseille, UMR7326 Aix Marseille  
Université-CNRS, 13388 Marseille – France*

<sup>3</sup>*IAP, Institut d'Astrophysique de Paris, UMR7095, 75014 Paris – France*

<sup>4</sup>*School of Physics and Astronomy, Cardiff University – UK*

ArTéMiS is a new large-format bolometer camera, built by CEA/Saclay, with two focal planes and 10 sub-arrays of 16x18 bolometric pixels operating at 350  $\mu\text{m}$  and 450  $\mu\text{m}$  simultaneously in the Cassegrain cabin of the APEX 12m telescope in Chile [1]. It has been open to proposals from the ESO and OSO communities since 2014. The APEX telescope is itself expected to remain available until at least 2022. ArTéMiS provides an angular resolution of  $\sim 8''$  at 350  $\mu\text{m}$  and  $\sim 10''$  at 450  $\mu\text{m}$ , comparable to *Herschel*/PACS at 70/100  $\mu\text{m}$  and a factor of 3.5 higher than *Herschel*/SPIRE at 350/500  $\mu\text{m}$ . It can image much wider fields than ALMA and is a factor  $\geq 4$  faster than the earlier-generation camera SABOCA on APEX.

Following a summary of the instrument capabilities and currently available data reduction tools (including a tailored version of the Scanamorphos software [2]), we will discuss the first results of an on-going long-term project with ArTéMiS to image the structure of the densest molecular gas at  $< 0.1$  pc resolution out to  $d \sim 3$  kpc in the Milky Way. This ArTéMiS project is motivated by the findings of *Herschel* imaging surveys of nearby Galactic clouds, which support a filamentary paradigm for solar-type star formation. Our main scientific goals are 1) to investigate whether fragmentation of 0.1-pc wide filaments remains the dominant mode of star formation beyond the Gould Belt, and 2) to clarify whether and how a transition between a “core-fed” and a “clump-fed” regime of protostellar mass growth occurs for intermediate-mass and high-mass star formation. Initial ArTéMiS results on NGC6334 (see [3]), NGC6357, M17, W48, and a few IRDCs will be presented.

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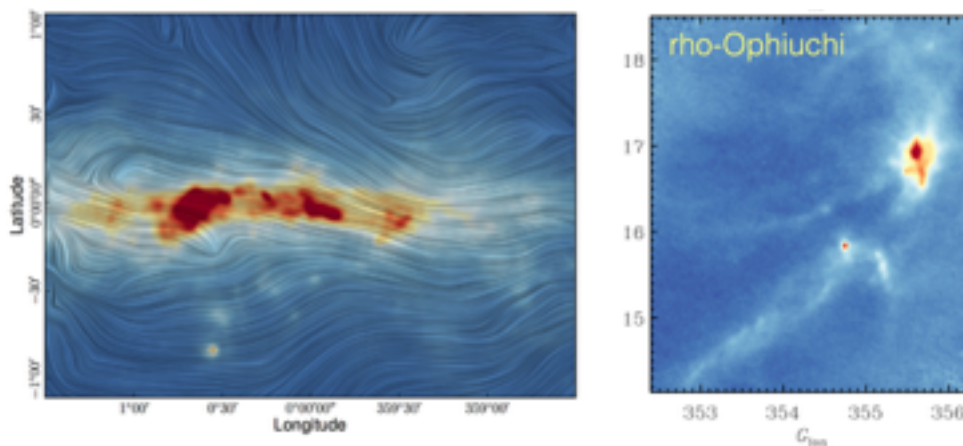
## PILOT magnetic field in the Milky Way and Star Forming Regions

A. Mangilli<sup>1</sup>, on behalf of the PILOT collaboration<sup>2</sup>.

<sup>1</sup> IRAP, UMR5277 du CNRS, 9 Avenue du colonel Roche, 31028, Toulouse France

<sup>2</sup> <http://pilot.irap.omp.eu>

The PILOT balloon-borne instrument is dedicated to measure the linear polarization of the faint interstellar diffuse dust emission in the Far-Infrared in our Galaxy and nearby galaxies. We present dust polarization measurements Galactic regions observed with the PILOT balloon-borne experiment, during its second flight from Alice Springs, Australia in April 2017 ([1]). The Galactic center area was chosen as the first target for PILOT data processing, since it is very bright but very weakly polarized (e.g. [2]), and is therefore a good target to check that the response calibration of the detectors is accurate. We measured the response flat-field using the residual atmospheric emission and the time-variations of the response using the PILOT Internal Calibration Source (ICS). This calibration is accurate at the 3% level. The polarization angles measured toward the Galactic center are consistent with a magnetic field globally aligned with the MW plane, and with angles measured using the Planck satellite at longer wavelengths. We will also present preliminary results obtained towards nearby star forming regions Orion, rho-Ophiuchi and in the Large Magellanic Cloud. The PILOT data will be combined with previous polarization measurements at other frequencies to discuss polarization dust properties.



Right: Preliminary map of the total intensity (color) and magnetic field direction (striations) as derived from polarization PILOT measurements at 240 microns, towards the Galactic center region. Left: Preliminary PILOT total intensity map in Rho-Ophiuchi at 240 microns.

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# Outreach conference

**Tuesday June 26<sup>th</sup> 20:00**



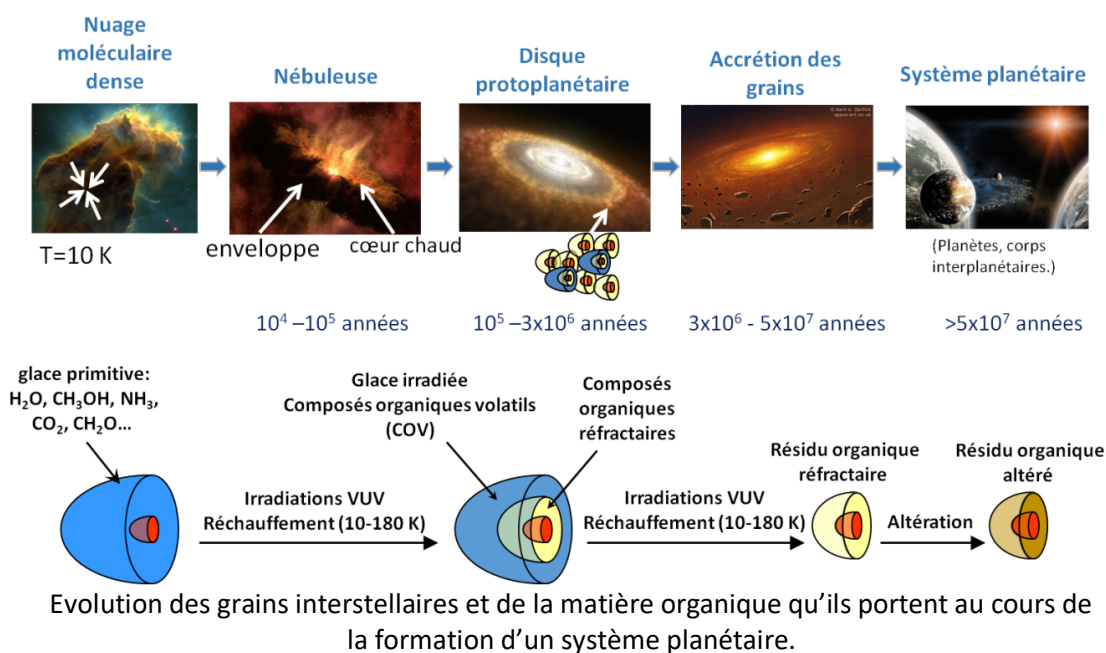
## Du milieu interstellaire aux systèmes planétaires : Evolution de la matière organique vers le vivant ?

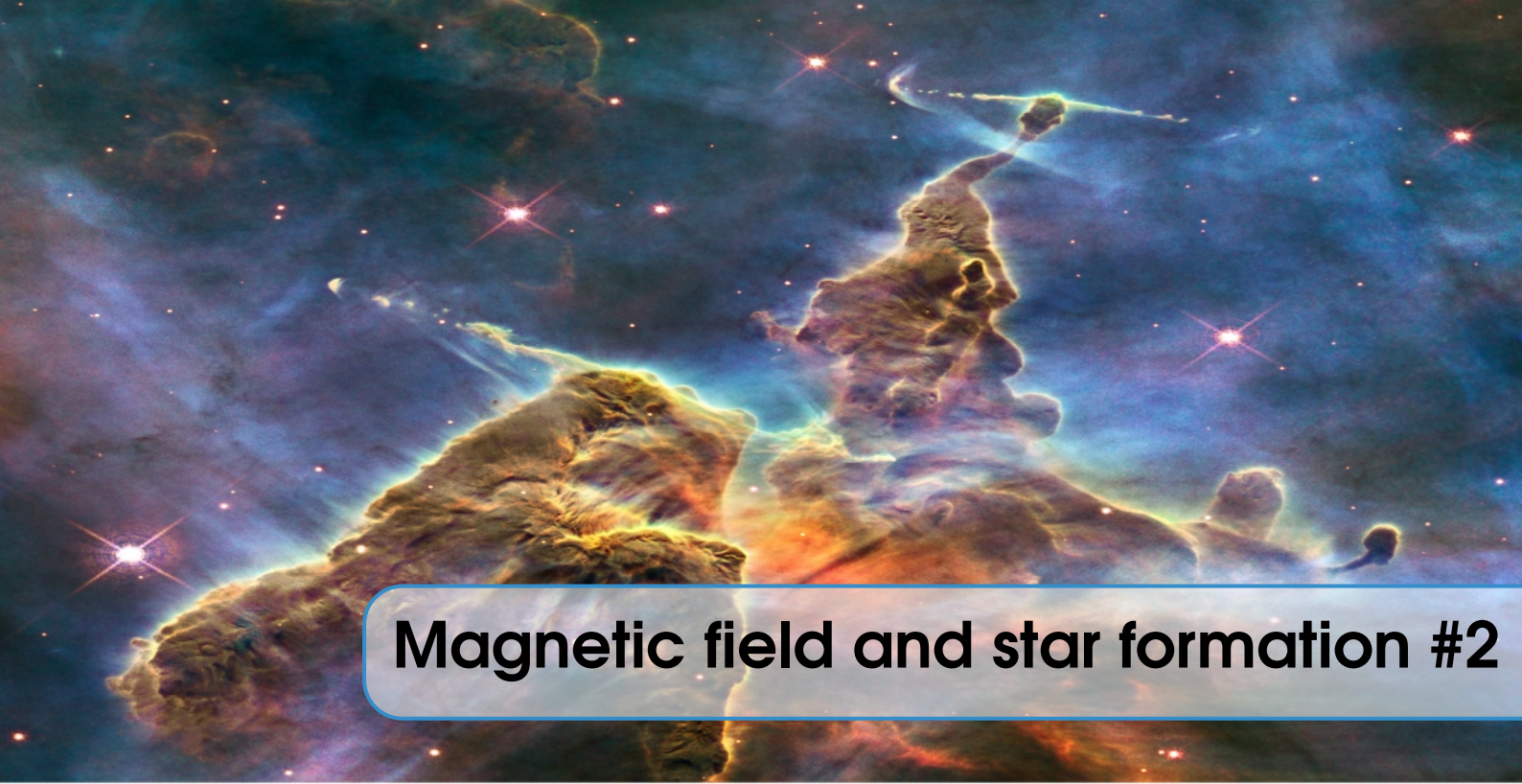
**Thierry Chiavassa,**

**Laboratoire PIIM Service 252 - ST JEROME - Avenue Escadrille Normandie Niemen -  
13013 Marseille**

Email : [thierry.chiavassa@univ-amu.fr](mailto:thierry.chiavassa@univ-amu.fr)

Les observations réalisées depuis plus de 50 ans par des télescopes ont permis de révéler la richesse moléculaire du milieu interstellaire. Ce milieu est constitué de gaz mais aussi de poussières formées par des étoiles en fin de vie, qui vont être par la suite recyclées pour former des planètes mais aussi des comètes/astéroïdes. Les analyses réalisées sur des météorites issues de corps parents astéroïdaux mais aussi plus récemment sur la comète 67P/Tchourioumov-Guérassimenko montrent la présence d'une grande diversité de molécules. L'apport à la terre primitive de matière organique et d'eau par de tels objets, a pu jouer un rôle important dans une chimie conduisant à l'émergence du vivant, il y a un peu plus de 3 milliards d'années. Au cours de cette conférence nous aborderons un certain nombre de questions sur l'origine et la caractérisation de ces molécules en particulier celles qui peuvent avoir une importance pour la chimie du vivant, sur les expériences d'astrochimie qui sont réalisées en laboratoire pour rendre compte de l'évolution et de la complexification de cette matière mais aussi sur le lien entre astrochimie et exobiologie.





## **Magnetic field and star formation #2**

**Wednesday June 27<sup>th</sup> 9:00**

## Interstellar magnetic fields

François Boulanger

<sup>1</sup> *LERMA/LRA Ecole Normale Supérieure, Observatoire de Paris,  
Université PSL, CNRS F-75005, Paris, France*

Magnetic fields are an essential piece of the interstellar puzzle, entangled with the structure, dynamics, and energetics of interstellar matter. However, despite of their importance, due to the paucity of data, magnetic fields have long been the least studied component of the interstellar medium (ISM). This situation is rapidly changing thanks to major steps forward in observational capabilities.

Radio polarization observations have delivered data that have been used to map magnetic fields on galactic scales. More recently, Planck provided us with all-sky maps of dust polarization characterizing the structure of the turbulent component of interstellar magnetic fields and their coupling with interstellar matter, with unprecedented sensitivity and statistics. Today, the precursors to the Square Kilometre Array (SKA), especially the low frequency array (LOFAR) in Europe, reveal an array of newly discovered structures in the diffuse magnetized ISM, through Faraday tomography. At the same time, the Atacama Large Millimetre Array (ALMA) is opening the path to studies of magnetic fields along the star-formation sequence from pre-stellar cores to proto-stars and their proto-planetary disks.

I will review these different perspectives on interstellar magnetic fields, highlighting key results and prospects of on-going and future research.

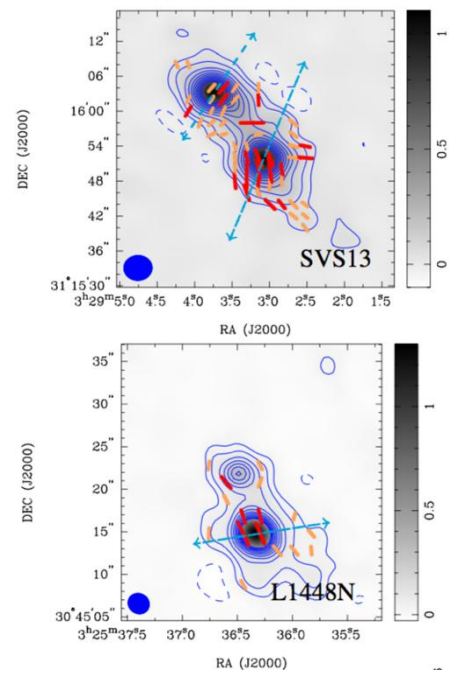
## ALMA and SMA observations of the magnetic fields in the youngest solar-type protostars

M. Galametz<sup>1</sup>, A. Maury<sup>1</sup>, J.-M. Girart<sup>2</sup> et al.

<sup>1</sup> *Astrophysics department, CEA/DRF/IRFU/DAP, Université Paris Saclay, UMR AIM, F-91191 Gif-sur-Yvette, France*

<sup>2</sup> *Institut de Ciències de l'Espai, (CSIC-IEEC), Campus UAB, Facultat de Ciències, C5p 2, 08193 Bellaterra, Catalonia*

Magnetic fields are believed to redistribute angular momentum efficiently during the collapse and could explain the order-of-magnitude difference observed between the large angular momentum of the protostellar envelope and that of a zero-age main sequence star. The Class 0 phase is the main accretion phase during which most of the final stellar material is being collected into the protostellar embryo: the role of the magnetic fields during that key stage is still unclear but might very well have a key impact on the later evolution of the young star and its surrounding protoplanetary disk before it reaches the main sequence. The position angle of linearly polarized submm dust emission is often used to probe the magnetic field. In order to study the structure of B from 50 to 2000 AU scales, we have acquired polarization observations of 9 low-mass protostellar cores with the SMA and for one of the objects, B335, with ALMA. Our sample contains 9 Class 0 protostars and includes single objects as well as close and wide multiples. Polarization is detected in all objects, with polarization degrees ranging from 1-10%. I will discuss how the polarization fraction varies with the source intensity. I will also analyze how the magnetic field lines align or not with the object outflow and show that a relation might exist between the orientation of the magnetic field and the rotational energy at the envelope scale. I will finally show how the magnetic field orientation varies with wavelength. On the small scales traced with ALMA in B335, we detect a large-scale poloidal magnetic field in the outflow direction and a strongly pinched B in the equatorial direction. Our results suggest that the magnetized collapse has a high level of organization from the 2000 AU down to 50 AU scales. Our approach, confronting the most state-of-the-art observations of B at various resolutions allows us to directly address the phenomenon of magnetic braking during protostar formation and give key clues on the pristine properties of B fields in star-forming material.



SMA 850um continuum maps of two Class 0 protostars. The blue arrows indicate the outflow orientations. B-field vectors are overlaid with red (3- $\sigma$  detections) and orange (2- $\sigma$ ) vectors.

## **Shocks, jets and star formation with NOEMA and ALMA**

Sylvie Cabrit<sup>1</sup>

<sup>1</sup> *LERMA UMR 8112, Observatoire de Paris, 61 Av de l'Observatoire 75014 Paris*



## From disks to planets

**Wednesday June 27<sup>th</sup> 13:50**

## Protoplanetary disks and planet formation

E.Chapillon<sup>1,2</sup>

<sup>1</sup> *Laboratoire d'astrophysique de Bordeaux, Université de Bordeaux, CNRS, B18N,  
Allée Geoffroy Saint-Hilaire, F-33615 Pessac*

<sup>2</sup> *IRAM, 300 rue de la piscine, F-38406 Saint Martin d'Hères*

Understanding the structure and composition of the protoplanetary disks surrounding low to intermediate mass stars is a prerequisite to constrain planets formation mechanisms. On one hand, ALMA produces unprecedented results, revealing fines structures like dust rings and gas spirals thanks to its resolving power. On the other hand, the NOEMA new correlator now enable to observe 4 GHz at 62.5 kHz in a single observation, opening the possibility to do large spectral surveys and thus to constrain the molecular content of the disks. In this talk I will review the latest main results.

## The interstellar heritage of planetary systems: the case of nitrogen

P. Hily-Blant<sup>1</sup>, A. Faure<sup>1</sup>, V. Magalhaes<sup>1</sup>, J. Kastner<sup>2</sup>, T. Forveille<sup>1</sup>, C. Rist<sup>1</sup>, G. Pineau des Forêts<sup>3</sup>, D. Flower<sup>4</sup>

<sup>1</sup> *Université Grenoble Alpes, IPAG, Grenoble 3800*

Understanding the formation of the solar system is a prerequisite to a comprehensive theory of our origins, while providing essential clues for the birth of planetary systems in general. In particular, the total amount of volatile carbon, oxygen, and nitrogen, and their spatial distributions, in the early protosolar nebula (PSN), and in PSN analogs, is a fascinating issue in our understanding of the primitive chemical composition of exoplanets. A key question from both astrophysical and planetary science perspectives is thus to know to what extent the reservoirs of volatiles (namely, gas and ice) in planetary systems are of interstellar nature or if chemistry was reset in the PSN at the epoch of planet formation. Isotopic ratios are powerful tools to evince the chemical heritage preserved during star and planet formation. Nevertheless, the isotopic ratios of nitrogen in the solar system is an unsolved problem, which is the central question we will adress in this talk.

In this this talk, we present several results obtained with IRAM and ALMA facilities, towards prestellar cores, protostars, and disks. By measuring the CN/C<sup>15</sup>N isotopic ratio in the TWHya protoplanetary disk, we could demonstrate that fractionated reservoirs of nitrogen are present in PSN analogs [1] and propose a new value, 330+/-30, for the elemental isotopic ratio of nitrogen in the solar neighborhood, which agrees with galactic chemical evolution model predictions. The carbon and nitrogen isotopic ratios in HCN towards the L1498 [2] prestellar core confirm some of the most recent chemical model predictions but challenge others. Meanwhile, new results on the HC<sub>3</sub>N/HC<sub>3</sub><sup>15</sup>N in the L1544 core will serve to illustrate the difficulty of isotopic ratios measurements [3]. In parallel, the gas-phase composition of prestellar cores is investigated using our new nuclear spin *University of Grenoble Astrochemical Network* (UGA) which allows us to reproduce the observed ortho-to-para ratios of nitrogen hydrides in prestellar cores [4]. Future works related to the interstellar heritage of planetary systems from theoretical, modelling, and observational perspectives, will be presented.

### Références

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- [2] V. Magalhaes et al, A&A in press (2018)
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- [4] P. Hily-Blant et al MNRAS in press (2018)

## Which origin for molecular oxygen and sulfur in Comet 67P/Churyumov-Gerasimenko?

Ozge Ozgurel<sup>1</sup>, Françoise Pauzat<sup>1</sup>, Yves Ellinger<sup>1</sup> and Alexis Markovits<sup>1</sup>

<sup>1</sup> Sorbonne Université, CNRS, Laboratoire de Chimie Théorique, LCT, F. 75005 Paris, France

The observation of O<sub>2</sub> and S<sub>2</sub> in comet 67P/Churyumov-Gerasimenko<sup>1,2</sup> has led to a new interest regarding the origin of volatiles detected in comets. A priori, the situation seems different for those two volatiles. The former had not been detected in space for years, whereas the latter has been observed for decades in comets.

However, basing on observations, we assume that O<sub>2</sub> and S<sub>2</sub> have a similar primordial origin and we propose that they formed in the ISM, by irradiation (photolysis and/or radiolysis) of the H<sub>2</sub>O molecules of the icy grains precursors of comets, and of the S-bearing molecules embedded in, creating voids in ices simultaneously, within which the produced volatiles can accumulate.

We have investigated the stability of O<sub>2</sub> and S<sub>2</sub> molecules in cavities formed by the irradiation, assuming that the surrounding material is made of pure H<sub>2</sub>O ice in the case of O<sub>2</sub> and a mixed H<sub>2</sub>O/H<sub>2</sub>S ice in the case of S<sub>2</sub>. To support this scenario, we used chemistry numerical models based on first principle periodic density functional theory (DFT). These models are shown to be well adapted to the description of compact ice and are capable to describe the trapping of the volatiles in the ice matrix. We showed that the stabilization energies of both O<sub>2</sub> and S<sub>2</sub> molecules in such voids are close to that of the H<sub>2</sub>O ice binding energy, implying that they can only leave when the icy matrix sublimates. This is consistent with the observations and also supports our scenario of a common origin for both volatiles O<sub>2</sub> and S<sub>2</sub>.

Differences can also be explained within this scenario. Unlike O<sub>2</sub> whose abundance correlates to H<sub>2</sub>O, no global trend should be drawn between the variation of S<sub>2</sub> and H<sub>2</sub>O abundances if S<sub>2</sub> can accumulate in both S<sub>2</sub>-bearing and H<sub>2</sub>O ices. Such results are supported by the ROSINA data collected between May 2015 (equinox) and August 2015 (perihelion), showing that, contrary to O<sub>2</sub>, there is no correlation observed for S<sub>2</sub> with H<sub>2</sub>O or H<sub>2</sub>S in 67P/C-G.<sup>3</sup>

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- [2] Le Roy, L., Altwegg, K., Balsiger, H., Berthelier, J. J., Bieler, A., Briois, C., ... & Fiethe, B., *Astron. Astrophys.*, 583, A1 (2015)
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## Modeling exoplanet atmospheres

Pascal Tremblin<sup>1</sup>

<sup>1</sup> *Maison de la Simulation, CEA Paris-Saclay, France*

The spectral characterization of exoplanet atmospheres started with Spitzer, Hubble Space Telescopes and ground-based observatories (e.g. VLT/Sphere, Gemini/GPI) will be revolutionized by the arrival of the James Webb Space Telescope (JWST). In this talk, I will review the recent efforts, progresses and remaining challenges in the modeling of exoplanet atmospheres in the light of past and upcoming observations. The precision that will be reached with upcoming observations clearly advocates for the need to push for multi-scale (in space and time) and multi-physics (chemistry, radiative transfer, hydrodynamics) modeling approaches in order to correctly infer the chemical composition of exoplanet atmospheres.



# Workshops

**Friday June 29<sup>th</sup> 9:00**

## Bases de données en astrochimie

Alexandre Faure<sup>1</sup> et Pierre Gratier<sup>2</sup>

<sup>1</sup> *Institut de Planétologie et d'Astrophysique de Grenoble (IPAG)*

<sup>2</sup> *Laboratoire d'Astrophysique de Bordeaux (LAB)*

La communauté astrochimique est structurée autour de deux approches complémentaires: observations astronomiques et modélisations physico-chimiques. De nombreuses étapes sont nécessaires pour relier ces deux aspects, mettant en jeux des données de microphysique à l'interface entre les communautés physico-chimique expérimentale/théorique et astrophysique de PCMI. Les bases de données sont des outils qui permettent de centraliser et d'échanger ces données et de nombreuses bases de données existent déjà pour chacune de ces étapes:

\* transfert de rayonnement (spectroscopie (CDMS[1]/JPL[2], CASSIS[3]), taux d'excitation collisionnelle (BASECOL[4], LAMDA[5])),

\* modélisation astrochimique (taux de réactions et chimie de surface (KIDA[6], UMIST[7]))

ainsi que les bases de données spécifique aux modèles (ISMDB[8]) et aux observations (ISA[9])

Cet atelier propose de faire un état des lieux des BDD existantes, de réunir des producteurs et des utilisateurs de ces données pour identifier les besoins et les offres de chacun autour des bases de données existantes ou éventuellement à créer, et de discuter l'articulation de ces bases de données au delà de PCMI dans le cadre du portail VAMDC[10] et du pôle thématique national "diffusion des données de physique atomique et moléculaire.

### Références

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- [5] <http://home.strw.leidenuniv.nl/~moldata/>
- [6] <http://kida.obs.u-bordeaux1.fr>
- [7] <http://udfa.ajmarkwick.net/index.php>
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- [9] <http://isa.obs.u-bordeaux1.fr>
- [10] <http://portal.vamdc.org/>

## Primordial Chemistry

Y. Scribano<sup>1</sup>, A. Faure<sup>2</sup> et D. Puy<sup>1</sup>

<sup>1</sup> LUPM, UMR5299 du CNRS, Université de Montpellier, Place Eugène Bataillon,  
34095, Montpellier Cedex 5 – France ;

<sup>2</sup>IPAG, CNRS, Universités Grenoble Alpes, 38058, Grenoble Cedex 9 – France

Molecules are found in a large variety of astronomical environments. They are now widely used as diagnostic probes of the physical conditions in which they occur, and the diversity of molecular environments has helped to stimulate interest in a variety of different chemical processes [1].

We know that primordial molecules appeared early in the history of our universe. The understanding of molecular formation as a consequence of cosmological recombination is of primary importance, especially regarding molecular cooling. The huge importance of that cooling process on the dynamics of collapsing proto-structures cannot be underestimated since the evolution of primordial fluctuations depends on the capability of the primordial gas to cool down. It is an absolute necessity, therefore, to take this cooling process into account when trying to determine how small the first cosmological objects were. H<sub>2</sub> and HD cooling have been studied in many works [2]. Their role played in the mechanism of condensation or fragmentation in collapsing proto clouds is crucial, particularly on the formation of primordial stars. In this PCMI session we plan to consider these questions with an overview “State of Art” in different domains such as molecular chemistry, molecular cooling capabilities, collapse with molecules, lines of emissivity during the Dark Ages period of the Universe (Period between the cosmological recombination of hydrogen and the formation of the first gravitational structures) and discuss some outlooks relative to possible detections.

### Références

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- [2] M. C. Coppola et al., Astrophys. Journal. Suppl. Series. 199, 16 (2012)

## **Dust from the diffuse ISM to protoplanetary discs: where do we stand ?**

Benoît Commerçon, Guillaume Laibe, Marc-Antoine Miville-Deschênes and Nathalie Ysard

Dust is ubiquitous in the ISM. Contemporary instruments reveal the dust grains with unprecedented details and add continuously new constraints on the dust grain population. Observations, theory, numerical simulations and laboratory experiments related to the ISM physics and chemistry cannot bypass the dust component. Observations rely on the dust emission to infer various properties of the ISM: gas, magnetic field, radiation field. Theory and numerical experiment need realistic dust grain models to study the interactions of the gas and dust mixture with the radiation and the magnetic fields. We aim to discuss the recent developments made by the PCMI community on the dust and to foster interactions on this timely subject.

The workshop will favour discussion around the three following axes:

- 1) Is the dust a good proxy for the gas at all scales in the ISM? What are the different friction regimes?
- 2) How models and experiments compare with observations? What is the most critical parameter to model dust observations: dynamical coupling with the gas, coagulation/fragmentation, dust grain composition/optical properties?
- 3) What is left to be explained? Which physics is missing? How could laboratory experiment help in understanding dust properties?

## **New Perspectives in Millimeter Astronomy with IRAM telescopes**

F. Boulanger<sup>1</sup>, M. Gerin<sup>1</sup>, G. Lagache<sup>2</sup>, R. Moreno<sup>3</sup>.

<sup>1</sup>*LERMA, 75014, Paris – France*

<sup>2</sup>*LAM, Marseille – France*

<sup>3</sup>*LESIA, Meudon, France*

The focus of the workshop is to introduce NOEMA now that phase 1 is completed and to restate the complementarity of the IRAM instruments for achieving major scientific projects. The format of the workshop includes invited presentations and discussion sessions.

The Agenda has been prepared in order to include both general talks describing the state of the art and the near perspectives, and discussion sessions, prepared by all participants.

All participants are invited to provide material for the discussion sessions by preparing short presentations (2 slides maximum, 1 slide preferred) that will be distributed in advance and could be used by the invited speakers. The slides can describe recent results, new science cases, scientific questions or any topic that can contribute to the discussions.

Suggestions using 1(2) slide(s), to contribute to the presentations and discussions can be deposited at <https://mycore.core-cloud.net/index.php/s/cLIhJ061Q7CoVAf>

and downloaded at : <https://mycore.core-cloud.net/index.php/s/LfVGqQB3NKxmmaQ>

14h-14h30 : What is new at IRAM ? (Frédéric Gueth)

14h30-14h50 : Nearby (spatially resolved) galaxies (Cynthia Herrera) (20 min)

14h50-15h10 : Understanding spectral lines from high z galaxies (Matthieu Béthermin) (20 min)

15h10-15h30 : Discussion 1st session, Extragalactic

15h30-16h : Coffee break

16h20-16h40 : Molecular line spectroscopy as diagnostics of the ISM structure, dynamics, and chemistry (Aurore Bacmann) (20 min)

16h-16h20 : Polarization information : continuum & lines (Anaëlle Maury) (20 min)

16h40-17h10 : Discussion 2nd session Galactic (& Extragalactic)

17h10-17h30 : Discussion : actions and Summary

The expected outcome of the workshop is the creation of working groups for science projects using IRAM instruments, and possibly aiming at writing a white paper supporting new developments.



# Molecular signatures in cold ISM

**Friday June 29<sup>th</sup> 11:10**

## State-to-state collisional rates and characterization of products at low temperature

Astrid Bergeat.

*ISM, UMR5255 du CNRS, Institut des Sciences Moléculaires, 351 cours de la Libération, 33405, Talence Cedex – France ;*

To date more than 200 different molecules have been identified in the interstellar medium or in protoplanetary disks. However, the study of the molecular or atomic abundances or their spatial distribution has been so far limited by local thermodynamic equilibrium (LTE) modeling due to the lack of collisional data. The data are indeed necessary to model out-of-equilibrium (non-LTE) spectra or maser action, owing to the complex competition between the radiative and collisional processes. Non-LTE situations are very common in space where the frequency of collisions is low and to determine column densities with accuracy mainly limited by the calibration uncertainties, or to provide abundance ratios, the energy transfer state-to-state collisional rates become crucial.

Nowadays, a variety of theoretical methods is developed and used, from the coupled-channel theory to classical approaches. Experimentally, three main techniques in France produce complementary results: doppler broadening, double resonance in CRESU apparatus or cells and molecular beam technique. I will discuss on the advantages and limitations of these experimental techniques combined with some theoretical results.

However, to fully benefit from the diagnostic power of the molecular lines, the formation and destruction paths of the parent molecules must be quantitatively (and not just qualitatively) understood. Low temperature experimental kinetic data for only a few hundreds (KIDA database <http://kida.obs.u-bordeaux1.fr/>) of neutral-neutral or ion-neutral reactions have been determined while astrochemical networks have 1000s of reactions, forcing modellers to use rate coefficients estimated from various levels of theory when no experimental data are available. Furthermore, little is experimentally known about the products of reactions and their branching ratios. Indeed, experimental measurements require either determining absolute concentrations or using a calibration reaction of known product yield(s) and they are still great experimental challenges. In this contribution, I will present recent advances and perspectives in the detection of products of gas phase reactions through various experimental techniques and methods for a better understanding of the chemistry of cold astrophysical objects.

## An efficient statistical method to compute molecular collisional rate coefficients

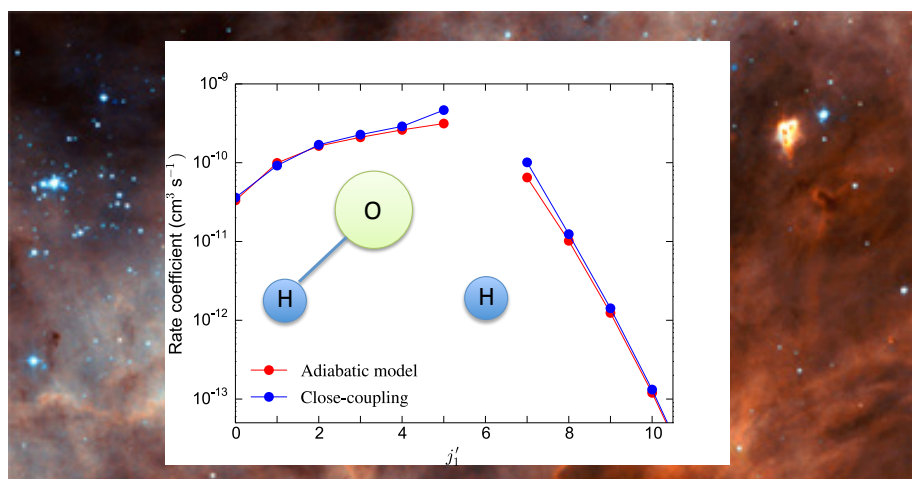
Jérôme Loreau<sup>1,2</sup>, François Lique<sup>1</sup>, and Alexandre Faure<sup>3</sup>

<sup>1</sup>LOMC—UMR 6294, Normandie Université, Université du Havre and CNRS, 25 rue Philippe Lebon, BP 1123-76 063 Le Havre cedex, France

<sup>2</sup>Service de Chimie Quantique et Photophysique, Université libre de Bruxelles (ULB) CP 160/09, B-1050 Brussels, Belgium

<sup>3</sup>Université Grenoble Alpes, CNRS, IPAG, 38000 Grenoble, France

Our knowledge about the “cold” universe often relies on molecular spectra. A general property of such spectra is that the energy level populations are rarely at local thermodynamic equilibrium. Solving the radiative transfer thus requires the availability of collisional rate coefficients with the main colliding partners over the temperature range 10–1000 K. These rate coefficients are notoriously difficult to measure and expensive to compute. In particular, very few reliable collisional data exist for inelastic collisions involving reactive radicals or ions. We have explored the use of a fast quantum statistical method [1] to determine molecular collisional excitation rate coefficients. The method is benchmarked against accurate (but costly) rigid-rotor close-coupling calculations. For collisions proceeding through the formation of a strongly bound complex, the method is found to be highly satisfactory up to room temperature. Its accuracy decreases with decreasing potential well depth and with increasing temperature, as expected. This new method opens the way to the determination of accurate inelastic collisional data involving key reactive species such as  $\text{H}_3^+$ ,  $\text{H}_2\text{O}^+$ , and  $\text{H}_3\text{O}^+$  for which exact quantum calculations are currently not feasible.



### Références

[1] Loreau et al., ApJL, 853, L5 (2018)

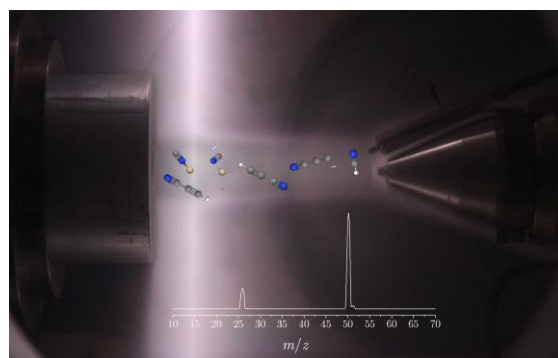
## Anion chemistry in the interstellar medium: insights from the laboratory

L. Biennier<sup>1</sup>, N. Jamal-Eddine<sup>1</sup>, B. Joalland<sup>1</sup>, S. Carles<sup>1</sup>, A. Benidar<sup>1</sup> J.-C. Guillemin<sup>2</sup>, F. Lique<sup>3</sup>

<sup>1</sup> Institut de Physique de Rennes UMR CNRS 6251, Rennes, <sup>2</sup> Institut des Sciences Chimiques de Rennes, Ecole Nationale Supérieure de Chimie de Rennes, UMR CNRS 6226, Rennes, <sup>3</sup> Laboratoire Ondes et Milieux Complexes, UMR CNRS 6294, Le Havre

The molecular diversity of the cold interstellar medium has been recently enriched with the detection of anions,  $C_4H^-$ ,  $C_6H^-$ ,  $C_8H^-$ ,  $C_3N^-$ ,  $C_5N^-$ , and  $CN^-$ , all linear carbon chains [1-7]. The circumstellar envelope of the evolved carbon star IRC +10216 is the only object so far in which all of them have been identified. Despite growing interest, the physical and chemical processes that govern their abundance remain poorly known. A better knowledge of anion reactivity, including chemical kinetics and branching ratios between exit channels at the relevant, low temperature of the interstellar medium, is of crucial importance for properly modeling gaseous cold environments.

To address these questions, we have conducted a series of experiments using the CRESU (French acronym standing for Kinetics of Reactions in Uniform Supersonic Flows) combined with quadrupole mass spectrometry to explore the reactivity of a selection of molecular anions down to 50 K. In our setup, the anions are produced by electron dissociative attachment on a specific precursor directly in the supersonic flow with the help of an electron gun [8-9].



The mode of production of the ions employed under this configuration is however limited to the species, such as  $C_xN^-$  ( $x = 1, 3, 5$ ), whose precursors easily attach low energy electrons and are available or synthesizable. In order to overcome these limitations, we have developed another methodology that relies on the implementation of a mass-selective source of ions on the CRESU chamber. The objective is to extend our study to the reactivity of the ions of the  $C_x^-$  and  $C_xH^-$  families. Preliminary results with this new set-up will be presented.

### References

- |   |  |
|---|--|
| <p>[1] McCarthy, M.C. et al., <i>Astrophys. J.</i> <b>2006</b>, 652, L141.<br/>         [2] Cernicharo, J. et al., <i>A&amp;A.</i> <b>2007</b>, 467, L37.<br/>         [3] Brunken, S. et al., <i>Astrophys. J.</i> <b>2007</b>, 664, L43.<br/>         [4] Thaddeus, P. et al., <i>Astrophys. J.</i> <b>2008</b>, 677, 1132.</p> | <p>[5] Cernicharo, J. et al., <i>Astrophys. J. Lett.</i> <b>2008</b>, 688, L83.<br/>         [6] Agúndez, M. et al., <i>A&amp;A</i> <b>2010</b>, 517, L2.<br/>         [7] Remijan, A.J. et al., <i>Astrophys. J.</i> <b>2007</b>, 664, L47.<br/>         [8] Bourgalais J. et al., <i>Icarus</i> <b>2016</b> 271, 194.<br/>         [9] Joalland B. et al., <i>Journal of Physical Chemistry Letters</i> <b>2016</b> 7, 2957.</p> |
|---|--|

## Nuclear spin symmetry conservation in H<sub>2</sub>O water vapor cooled in a supersonic expansion

R. Georges<sup>1</sup>, X. Michaut<sup>2</sup>, S. Kassi<sup>3</sup>, A. Vigasin<sup>4</sup>, E. Dudas<sup>1</sup>, A. Moudens<sup>2</sup>, M. Goubet<sup>5</sup>, Th. Huet<sup>5</sup>, P. Soulard<sup>6</sup>, P. Asselin<sup>6</sup> and O. Pirali<sup>7</sup>.

<sup>1</sup> *Institut de Physique de Rennes, UMR 6251, Campus de Beaulieu, Université de Rennes 1/CNRS, F-35042 Rennes Cedex, France*

<sup>2</sup> *LERMAA, Sorbonne Universities, UPMC Univ. Paris 06, Université de Cergy-Pontoise, Observatoire de Paris, PSL Research University, CNRS, F-75252, Paris, France*  
*LiPhy, UMR 5588, Université de Grenoble Alpes/CNRS, F-38041 Grenoble, France*

<sup>4</sup> *Obukhov Institute of Atmospheric Physics, Russian Academy of Sciences, 3 Pyzhevsky per, 119017 Moscow, Russia*

<sup>5</sup> *PhLAM, UMR8523 Université Lille, CNRS, F-59000 Lille, France*

<sup>6</sup> *MONARIS, UMR8233, CNRS-UPMC, 4 place Jussieu, 75005 Paris, France*

<sup>7</sup> *Ligne AILES-Synchrotron SOLEIL, L'Orme des Merisiers, 91192 Gif-sur-Yvette, France*

The nuclear spin temperature (NST) deduced from the observation of hydrogenated molecules desorbed from cometary ices seems to disagree with the temperature expected for the environment in which the comets were formed [1]. The measured NST value of ~30 K is not properly understood and several hypotheses have been formulated to explain such a high value [2-4]. The relaxation process of the nuclear spin molecules in the gas phase is probably one of the key problems.

An introduction into the recent studies of nuclear spin isomers conversion (NSC) in water vapor can be found in the recent paper from Manca Tanner et al. [5]. The results reported in this study showed a rapid change in the spin-isomers state in a supersonic expansion of H<sub>2</sub>O water vapor seeded in argon. Whereas at a low water vapor molar fraction the nuclear spin symmetry was conserved, at higher water molar fractions the *ortho* to *para* ratio (OPR) was seen to be completely relaxed, i.e., the measured OPR responded to a low rotational temperature in expansion. This fast relaxation cannot be explained by intramolecular processes in an individual water molecule and was thus interpreted as a result of water cluster formation, which is able presumably to significantly facilitate nuclear spin conversion (NSC).

We performed a new experiment based on the Jet-AILES supersonic-jet apparatus implemented on the AILES beamline at SOLEIL to investigate the water clustering effect on NSC [6]. Despite the presence of the water cluster signatures in our obtained spectra, no transition to a nuclear spin relaxation regime was observed: the OPR derived from the

spectra was conserved on a level characteristic of equilibrium conditions in the stagnation reservoir, that is, the OPR was always equal to 3 irrespective of the extremely low rotational temperature achieved in the supersonic expansion. In addition, no change in OPR was observed when the argon carrier gas was replaced by oxygen. The latter is known to enhance nuclear spin relaxation because of its associated magnetic moment. On the basis of the results obtained, we are in a position to dismiss the hypothesis of a water clustering effect on nuclear spin relaxation and to question the origin of the nuclear spin relaxation reported previously [5].

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## ***Ortho-to-Para Ratio of Water in the Orion Bar.***

T. Putaud<sup>1</sup>, X. Michaut<sup>1</sup>, M. Bertin<sup>1</sup>, R. Dupuy<sup>1</sup>, G. Féraud<sup>1</sup>, P. Jeseck<sup>1</sup>,  
F. Le Petit<sup>1</sup>, L. Philippe<sup>1</sup>, E. Roueff<sup>1</sup>, J.-H. Fillion<sup>1</sup> and D. C. Lis<sup>1</sup>

<sup>1</sup> Sorbonne Université, Observatoire de Paris, Université PSL, CNRS, LERMA, F-75005, Paris, France

The ortho-to-para ratio (OPR) of water has been measured in various astronomical objects, from the Interstellar Medium (ISM) [1,2] to cometary atmospheres [3]. Most of the results are close to 3, which is consistent with water at the thermal equilibrium in warm gas (>50K) [1,3]. However, a very low OPR of 0.1 – 0.4 was derived, based on H<sub>2</sub><sup>18</sup>O observations and Large Velocity Gradient (LVG) modelling, in the Orion Bar [4], a well-studied Photon Dominated Region (PDR). Such a low OPR is equivalent to a spin temperature close to 10K, which is well below the kinetic temperature of this UV-illuminated region [5].

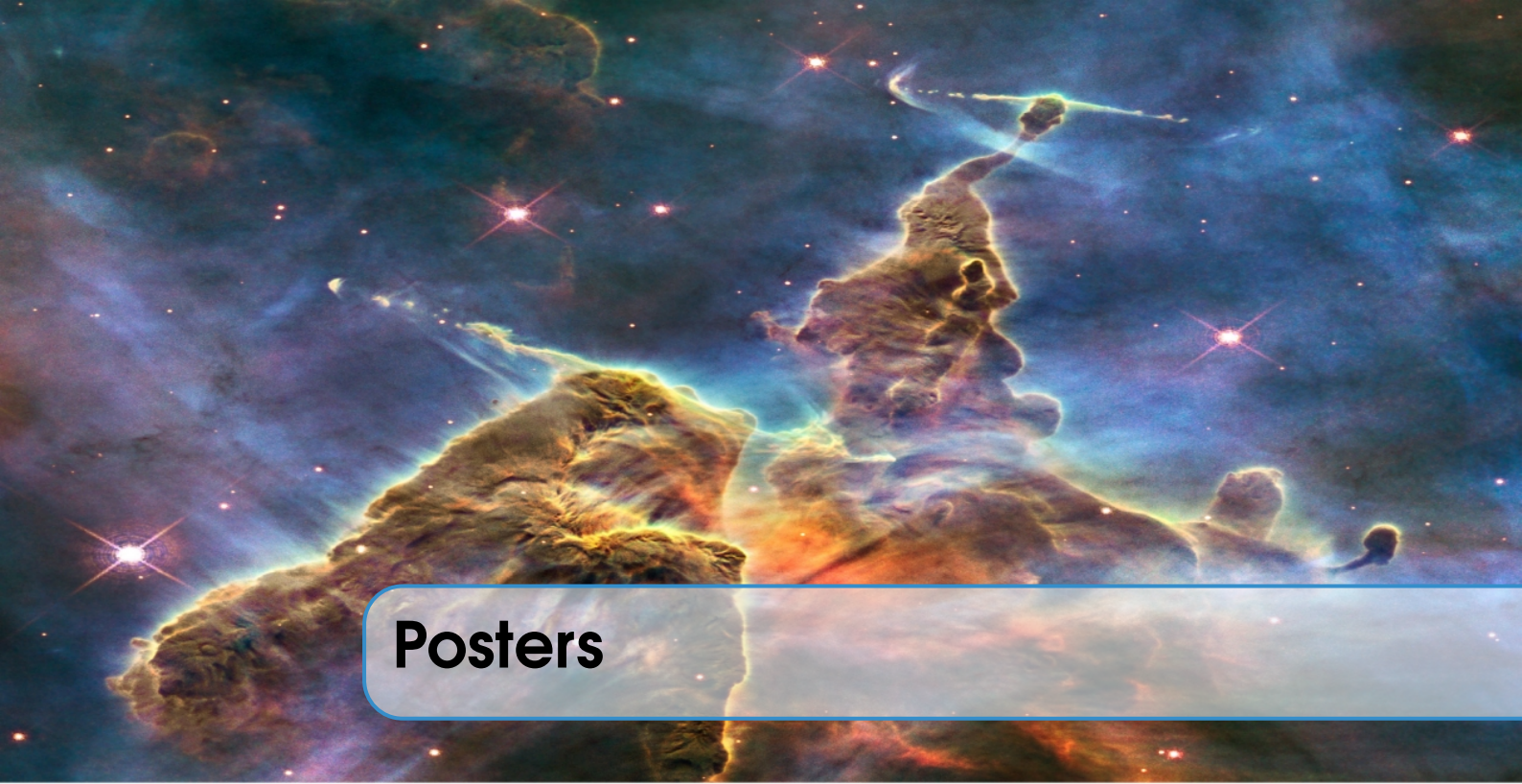
The departure of the water spin temperature from the kinetic temperature of the gas is commonly assumed to be due to the photodesorption of water molecules from cold icy grains [6]. But recent laboratory studies using UV laser photodesorption from cold surfaces (typically 10K) did not produce water with a low OPR [7].

Reanalysis of water line emission (H<sub>2</sub><sup>16</sup>O and H<sub>2</sub><sup>18</sup>O) from the Orion Bar using the Meudon PDR Code [8] will be presented. This model computes the radiative transfer in a stationary plane-parallel slab of gas and takes into account thermal balance and chemistry. It is worth noting that in this model water is formed with an OPR in thermal equilibrium at the local gas temperature. Preliminary results show a good agreement between observed water lines intensity and those predicted by the model, with an OPR always higher than 2.5. Best-fit model parameters (thermal pressure and UV field intensity) are also in agreement with those derived from the analysis of high-J CO lines in the Orion Bar [9].

We will also present the experimental attempts made at LERMA to prepare icy sample from water molecules with a controlled disequilibrium in the water *ortho* and *para* populations in the gas phase in order to study the impact of VUV photodesorption on the water OPR.

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## Posters

**Monday June 25<sup>th</sup> 14:15 : session 1**  
**Tuesday June 26<sup>th</sup> 16:05 : session 2**

## The Local Bubble: a magnetic veil to our Galaxy

Marta I.R. Alves<sup>1,2</sup>, François Boulanger<sup>3,4</sup>, Katia Ferrière<sup>2</sup> and  
Ludovic Montier<sup>2</sup>

<sup>1</sup>*Department of Astrophysics/IMAPP, Radboud University, PO Box 9010, NL-6500  
GL Nijmegen, the Netherlands*

<sup>2</sup>*IRAP, CNRS, Université de Toulouse, CNRS, 9 Avenue du Colonel Roche, BP  
44346, 31028, Toulouse Cedex 4, France*

<sup>3</sup>*IAS, CNRS, Univ. Paris-Sud, Université Paris -Saclay, Bât. 121, 91405 Orsay  
Cedex, France*

<sup>4</sup>*LERMA, CNRS, Observatoire de Paris, 61 Avenue de l'Observatoire, Paris, France*

The magnetic field in the local interstellar medium does not follow the large-scale Galactic magnetic field. The local magnetic field has probably been distorted by the Local Bubble, an interstellar bubble located around the Sun. The Local Bubble is thought to be the result of supernova explosions, which swept out a cavity of hot ionised gas and pushed most of the evacuated matter, together with the frozen-in magnetic field, into a dense shell of cold neutral gas and dust. However, so far no conclusive association between the local magnetic field and the Local Bubble has been established. We developed an analytical model for the magnetic field in the shell of the Local Bubble, which we represent as an inclined spheroid, off-centred from the Sun. We fit the model to Planck dust polarised emission observations within 30deg of the Galactic poles. We find a solution consistent with a highly deformed magnetic field, with significant different directions toward the north and south Galactic poles [1]. This work is a stepping stone towards modelling the 3D structure of the magnetic field in the local interstellar medium, which is a most awaited input for large-scale Galactic magnetic field models.

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## **COPILLOT: C+ Observations of the Interstellar Medium with PILOT**

A. Hughes<sup>1,2</sup> on behalf of the COPILLOT collaboration

<sup>1</sup>*IRAP, 9 Avenue Colonel Roche, BP 44346, F-31028 Toulouse cedex 4 – France*

<sup>2</sup>*Université de Toulouse, UPS-OMP, F-31028 Toulouse cedex 4 – France*

In this poster, we present the COPILLOT (C+ Observations of the ISM with PILOT) concept, a proposed balloon-borne experiment to measure the integrated intensity of 158 $\mu$ m C+ emission line in Galactic star-forming regions, the diffuse ISM of the Milky Way and in Local Group Galaxies. The COPILLOT proposal is to modify the existing PILOT instrument to enable wide-field mapping of the C+ integrated emission with sufficient sensitivity to accurately characterise the faint end of the C+ intensity distribution. In this poster, we present the science goals, planned observing strategy and expected performance of the COPILLOT instrument concept. By observing wide fields in the local Milky Way, COPILLOT will enable a statistically robust estimate of the relative contributions of the atomic gas, the ionised gas and the dense neutral medium to the C+ emission via a correlation analysis with other tracers of ISM phases. This result will be a key reference value for velocity-resolved studies in more complex regions such as the Galactic plane and star-forming regions, and for unresolved observations of the C+ emission in other galaxies. Compared to recent and upcoming heterodyne instruments to observe C+ emission, the low-cost CoPILOT mission occupies a unique niche in terms of sensitivity, resolution and wide-field coverage, enabling important studies of the ISM phase balance, the prevalence of dark gas, star formation and feedback in galaxies. COPILLOT has been proposed to CNES in 2018.

# 100,000 Molecular Clouds Across the Main Sequence: the PHANGS ALMA Large Programme

A. Hughes<sup>1,2</sup>, J. Pety<sup>3,4</sup>, C. N. Herrera<sup>3</sup> et LeReste A.<sup>1,2</sup>  
on behalf of the PHANGS consortium<sup>5</sup>

<sup>1</sup>IRAP, 9 Avenue Colonel Roche, BP 44346, F-31028 Toulouse cedex 4 – France

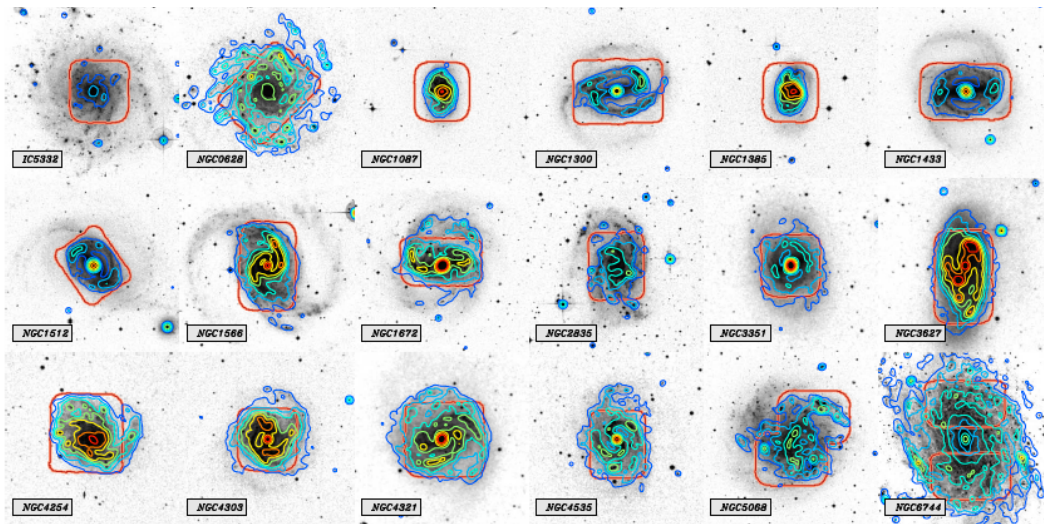
<sup>2</sup>Université de Toulouse, UPS-OMP, F-31028 Toulouse cedex 4 – France

<sup>3</sup>Institut de Radioastronomie Millimétrique, 300 Rue de la Piscine, F-38406 Saint Martin d'Hères – France

<sup>4</sup>Observatoire de Paris, 61 Avenue de l'Observatoire, F-75014 Paris – France

<sup>5</sup><http://www.phangs.org>

For thirty years, our observational understanding of the physical properties and star formation activity of extragalactic giant molecular clouds (GMCs) has been established on poorly resolved extragalactic surveys and on high resolution case studies of individual Local Group galaxies. The Physics at High Angular resolution in Nearby Galaxy Survey (PHANGS) is an ALMA Large Programme that harnesses the survey speed and imaging capabilities of ALMA to move the field of extragalactic star formation into the big survey era. With over 100 hours of awarded main array time, PHANGS-ALMA is imaging the CO(2-1) emission at 1'' resolution across the disks of 80 massive ( $\log M_* > 9.75 M_{\text{sol}}$ ) star-forming galaxies in the local volume ( $d < 17$  Mpc). This will yield measurements for more than 100,000 GMCs spread across a sample of galaxies and interstellar conditions that is truly representative of star formation in the local Universe. In this contribution, we present the science goals, the target galaxy sample and first science results from the PHANGS-ALMA survey.



Digitised sky survey images of 18 PHANGS ALMA targets on a logarithmic stretch. Color contours show 12 $\mu$ m unWISE Band 3 intensities, tracing small dust grains mixed with the ISM. Red rectangles indicate the field of view of the PHANGS ALMA CO (2-1) observations.

# Complex organic molecules in the cold interstellar medium

A. Bacmann<sup>1</sup> & A. Faure<sup>1</sup>

<sup>1</sup> *Univ. Grenoble Alpes, CNRS, IPAG, 38000 Grenoble - France*

Complex organic molecules have been the subject of intensive investigation. Long thought to be characteristic of the hot cores of star forming regions, they are now found in a wide range of regions with various physical conditions, including prestellar dense cores, i.e. at a stage even prior to the formation of protostars. The unexpected detections of terrestrial-like complex organic molecules in these cold ( $\sim 10$  K) sources [1] questioned our understanding of their formation mechanism, since these species were originally thought to result from warm chemistry. In this contribution, recent observational results of complex organic molecules in prestellar cores will be presented, addressing their inventory, spatial distribution and their formation mechanisms. Future progress in this field will in particular depend on efforts combining observations and laboratory experiments and we present opportunities and directions we are planning to follow in the coming years.

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## Sulfur derivatives of interstellar relevance studied in Lille.

Stéphane Bailleux<sup>1</sup>, Roman Motienko<sup>1</sup> and Laurent Margulès<sup>1</sup>, Jose Cernicharo<sup>2</sup>, Arnaud. Belloche<sup>3</sup> and Jean-Claude Guillemin<sup>4</sup>

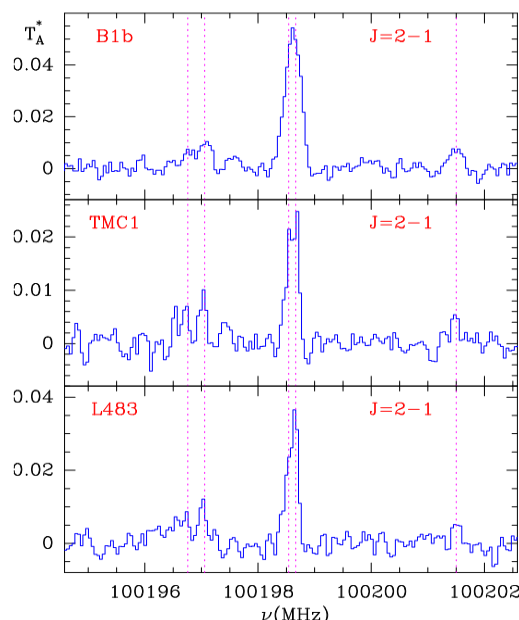
<sup>1</sup> *Laboratoire de Physique des Lasers, Atomes et Molécules, UMR 8523 CNRS – Université de Lille, 59655 Villeneuve d'Ascq Cedex, France*

<sup>2</sup> *Dpt. of Molecular Astrophysics. IFF. CSIC. C/ Serrano 123, E-28006, Madrid, Spain*

<sup>3</sup> *Max-Planck-Institut für Radioastronomie, Auf dem Hügel 69, 53121 Bonn, Germany*

<sup>4</sup> *Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS – ENSCR, Rennes, France*

About 200 molecules have thus far been detected in the interstellar medium. Twenty are sulfur-bearing chemical compounds (and analogues of oxygenated species), making sulfur the tenth most abundant element in the galaxy. We report here the sub-THz spectroscopic observation of two reactive species, thioacetaldehyde ( $\text{CH}_3\text{CHS}$ ) and  $\text{NS}^+$  [1]. This new cation has been firmly detected for the first time (*prior* to laboratory, pointing out the lack of experimental data), towards many interstellar sources (cold molecular clouds, pre-stellar cores and shocks; Fig. 1) using the IRAM-30m radiotelescope. Although a recent study of the chemistry of sulfur in cold dense clouds has been carried out [2], the formation pathways of the title species are not well understood. The rotational spectrum of  $\text{CH}_3\text{CHS}$  was already recorded up to 40 GHz [3]. New spectra were recorded in Lille up to 660 GHz. Spectroscopic analysis, including the internal rotation treatment, and searches for it towards SgrB2 and other sources will be presented.



**Figure 1**  $\text{NS}^+$  detected in various sources.

### Acknowledgement

These results were supported by the Programme National PCMI of CNRS/INSU with INC/INP co-funded by CEA and CNES, the French National Research Agency (ANR-13-BS05-0008 "IMOLABS"), the CaPPA project (ANR-11-LABX-0005-01), the spanish MINECO (grants AYA2012-32032, AYA2016-75066-C2-1-P, CSD2009-00038 and RyC-2014-16277) and the European Research Council (grant ERC-2013-SyG 610256, NANOCOSMOS).

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## Rotational excitation of SiO by collisions with H<sub>2</sub>

Christian Balança<sup>1</sup>, Fabrice Dayou<sup>1</sup>, Alexandre Faure<sup>2</sup>, Laurent Wiesenfeld<sup>2,3</sup> and Nicole Feautrier<sup>1</sup>

<sup>1</sup>*Observatoire de Paris, Université PSL, Sorbonne Université, CNRS, LERMA, F-92195, Meudon, France*

<sup>2</sup>*University Grenoble Alpes, CNRS, IPAG, F-38000 France*

<sup>3</sup>*Laboratoire Aimé-Cotton, Université Paris Saclay and CNRS, Orsay, France*

The SiO molecule is a key species for the study of the interstellar medium as it is used to trace warm shocked gas. A large number of transitions, including high rotational levels, are observed, and the modelling of these emission lines can provide valuable information on the chemical and physical conditions of the observed regions. In these environments where the local thermodynamical equilibrium approximation is not valid, an accurate modelling requires collisional excitation rate coefficients with the most abundant species. We focus on the calculation of rate coefficients of SiO in its ground vibrational state in collision with para- and ortho-H<sub>2</sub> using a new high accurate 4D potential energy surface. Dynamical calculations of pure rotational excitation of SiO were performed for the lowest 21 rotational levels using the close-coupling (CC) approach, while the coupled-state (CS) approximation was used to derive rate coefficients among the first 30 rotational levels. State-to-state rate coefficients were obtained for temperatures ranging from 5 to 300 K in the CC calculations and for temperatures up to 1000 K in the CS approximation. Propensity rules show that rate coefficients for  $\Delta j = 1$  transitions are dominant for both para- and ortho-H<sub>2</sub> colliders. The rotational rate coefficients are compared with recent results obtained for  $j_1 \leq 5$  levels in a full dimensionality approach. These new data will help to model emission lines in warm environments such as shocked layers of molecular outflows in star-forming regions.

## Low-energy water-hydrogen inelastic collisions

Astrid Bergeat<sup>1</sup>, Alexandre Faure<sup>2</sup>, Sébastien B. Morales<sup>1</sup>, Chloé Miossec<sup>1</sup> and Christian Naulin<sup>1</sup>

<sup>1</sup> *ISM, UMR5255 du CNRS / Univ. Bordeaux, Institut des Sciences Moléculaires, 351 cours de la Libération, 33405, Talence Cedex – France ;*

<sup>2</sup> *IPAG, Institut de Planétologie et d'Astrophysique de Grenoble, OSUG-A, 414 rue de la Piscine, Domaine Universitaire, 38400 St-Martin d'Hères– France ;*

The ubiquity of water in the Universe has been demonstrated along the last 40 years through many astronomical observations by ground-based and space-based telescopes [1-3]. In interstellar medium (ISM), water vapour was detected for the first time in 1969 in the Orion nebula [4]. Since then, gaseous water is known to be present in various objects of ISM, such as dense clouds, protostars, star and planet-forming regions, as it has been recently observed by Herschel Space Observatory (see review from [2] and references therein). Water is a key molecule for the understanding of the energy balance and the physical-chemical processes that occur in these environments. Its principal partner of collision is obviously H<sub>2</sub> because of its high abundance in ISM. Therefore, an accurate description of H<sub>2</sub>O-H<sub>2</sub> collision dynamics is requested in order to fully interpret spectral features recorded by astronomers in infrared and submillimeter wavelengths. Populations of each observed rotational levels of gaseous water are determined by the competition between collisional and radiative excitation-relaxation processes. In the context of dense clouds in ISM, gaseous molecules are not in local thermodynamic equilibrium and populations of each state are driven by collision dynamics.

The present study provides the first experimental check of the potential energy surface of Valiron et al. [5] at long-range by measuring scattering cross sections both at the state-to-state level and at very low collision energy (near rotational thresholds) for the inelastic collisions between H<sub>2</sub>O or D<sub>2</sub>O and H<sub>2</sub>.

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# High Temperature Study of the $\text{H}+\text{H}_2(\text{v},\text{j})$ Collisions for Astrophysical Applications.

D. Bossion<sup>1</sup>, Y. Scribano<sup>1</sup>

<sup>1</sup> *LUPM, UMR5299 du CNRS, Université de Montpellier – Campus Triolet, Place Eugène Bataillon – CC 72, 34095 Montpellier, France*

$\text{H}_2$  is the most abundant molecule in the Universe, observed in a large variety of astrophysical environments from the cold Interstellar Medium to the Early Universe. It represents the most efficient coolant and plays an important role in the collapse of the primordial clouds and then in the formation of first stars as well as in the cooling mechanism of the ISM. The main reaction, involving this diatomic, is the collision  $\text{H} + \text{H}_2$  for which a large number of theoretical studies have been performed [1-3] thanks to the small size of this collisional system (it contains only 3 electrons and 3 protons). Due to the numerical cost of the quantum dynamics methods (the state of the art of the collisional dynamics), the rate constants were mainly computed for the low-medium temperature regime. For example, an accurate potential energy surface for  $\text{H}_3$  was developed by Mielke et al [4] from high level electronic structure calculations and used by Lique [5] to determine state-state rate constants; for temperatures less than 5 000 K; using accurate Time Independent Quantum Method (TIQM). However, for some Astrophysical applications, it will be necessary to get those rate constants for a higher temperature range (with high initial ro-vibrational quantum numbers) where TIQM are actually intractable.

I will present our rate constant calculations for a hydrogen atom colliding a hydrogen molecule using a Quasi-Classical Trajectory approach [6] and for temperature growing until 10 000 K. The QCT approach represents a high attractive method to compute those rate constants since it is very less computational demanding than the traditional quantum mechanical approaches. The reliability of the QCT results were benchmarked on the quantum dynamical calculations at lower collisional energy. I will present our results concerning the ortho-para- $\text{H}_2$  conversion process and its evolution with the temperature and also some preliminary results on the cross sections and rate constants for Collision Induced Dissociation of  $\text{H}_2$  by  $\text{H}$  (an important process for the study of molecular clouds behind high-speed shock front in the ISM, and during the collapse of massive clumps into protostellar cores in the primordial Universe).

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## Chemical diversity in massive protostellar envelopes

Laure Bouscasse<sup>1</sup>, Timea Csengeri<sup>1</sup>, Karl M. Menten<sup>1</sup> and the SPARKS Team.

<sup>1</sup> *Max-Planck-Institut für Radioastronomie, Auf dem Hügel 69, 53121 Bonn-Germany*

The physical conditions in massive dense cores (MDCs) leading to high-mass star formation are poorly constrained. Observations are lacking to confront theory. From the 870 micron ATLASGAL survey of the inner Galaxy, in the frame of the SPARKS project (Survey for high-mass Protostars with ALMA Revealed up to Kpc Scales, PI: Csengeri), we performed an ALMA follow-up on the most massive mid-infrared quiet clumps within 5 kpc. In addition to the 8 GHz instantaneous bandwidth at 345 GHz, we obtained a complete spectral survey covering the 1mm atmospheric window with the APEX telescope towards a handful of sources. We determine the chemical composition of the protostellar envelopes, and aim to pin down where different molecules are located within the envelope with a particular focus on the distribution and diversity of complex organic molecules.

## Spatially resolved carbonaceous dust infrared emission in proto-planetary disks around Herbig Ae/Be stars

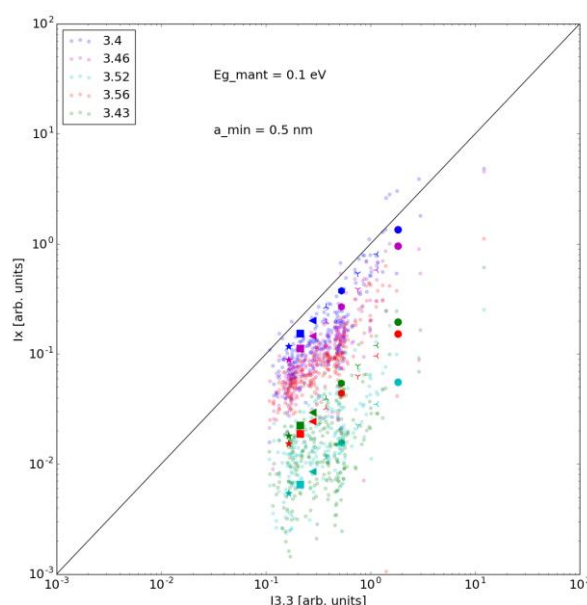
T. Boutéraon<sup>1</sup>, E. Habart<sup>1</sup>, N. Ysard<sup>1</sup> and A. P. Jones<sup>1</sup>

<sup>1</sup> IAS, UMR8617 du CNRS, Institut d'Astrophysique Spatiale, Bat 121, 91405 Orsay

In the ISM, the carbon (nano-)grains are a major component of interstellar dust. This solid phase is more vulnerable to processing/destruction than their silicate counterparts. It exhibits a complex, size-dependent evolution due to photon interactions, which provides a modeling challenge. How these micro-physical processes work under the extreme conditions found in disks (different from the ISM by orders of magnitude in terms of excitation and local gas density)? This study is particularly important since the carbonaceous nano-grains, very well coupled to the gas, are unavoidable in the physics and chemistry of the upper disk layers governed by photons from young stars. In fact, nano-grains could play an essential role in the gas heating, and thus could have a major influence on the disk structure and its evolution. Moreover, due to their large effective surface area, they could play a key role in the formation of molecules. Finally, they are the tracers of the physical conditions (excitation, extinction, geometry).

I will present an analysis of IR ground-based data, obtained with VLT/NACO in the 3-4 micron range (which includes aromatic, olefinic and aliphatic bands), for disks around intermediate mass stars (e.g., HD100546, HD100453, HD169142, HD179218). I will discuss some issues raised by these results: dust composition, evolution and renewal at the disk surface. At last, I will go further in the understanding of the grain properties thanks to

comparison with the THEMIS [1,2] framework.



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# Radical reactivity in interstellar ices studied by EPR spectroscopy

Teddy Butscher<sup>1</sup>, Fabrice Duvernay<sup>1</sup>, Yetsedaw Tsegaw<sup>2</sup>, Fabien Borget<sup>1</sup>, Dirk Grote<sup>2</sup>, Wolfram Sander<sup>2</sup>, Thierry Chiavassa<sup>1</sup>

<sup>1</sup> PIIM, UMR 7345, Aix-Marseille Université, Avenue Escadrille Normandie-Niemen  
13397 Marseille, France

<sup>2</sup> Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum

Astrophysical observations led to the identification of numerous organic molecules in the Interstellar Medium (ISM). Although the main part of these are simple molecules, some have an important number of atoms and are so called Complex Organic Molecules (COMs). COMs are species of interest since they can be incorporated in small bodies of ISM (comets and meteorites) and could have played a role in the emergence of life on Early Earth.

Although COMs characterization is confident, their formation mechanisms are still under investigation. Several formation mechanisms were proposed, either in gas phase or in solid state, each of them dealing with different kinds of reactivity [1].

We focus here on radical reactivity in interstellar ice analogues produced in laboratory and submitted to ISM-like processes-hydrogenation, VUV irradiation, thermal effect- while the chemical composition of the ice analogues are monitored by spectroscopic techniques – IR, MS and, if required, GC-MS [2]. However, radical species produced during these experiments are difficult to study, due to their short lifetime and high reactivity. To overcome this problem, we use cryogenic matrix isolation technique combined with IR and EPR spectroscopies to characterize unstable species and observe their reactivity [3] [4]. Our work focused on formaldehyde (H<sub>2</sub>CO) and methanol (CH<sub>3</sub>OH) precursors submitted to VUV irradiation and heating. During these experiments, we found out that radical species – CH<sub>2</sub>OH, HCO, CH<sub>3</sub>O, CH<sub>3</sub> as well as their recombination products glycolaldehyde, ethylene glycol, and methyl methyl formate - are easily detected by ESR and IR spectroscopies. We showed that radical species can be formed and be stored inside the ice at low temperature before reacting whenever diffusion is triggered by any process. We derived a photochemical branching ratio for methanol photolysis using the ESR spectroscopy. We also showed that radical-radical recombination does not lead mandatorily to an increase in molecular complexity [4].

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## Breakdown curves of C<sub>2</sub>N(+) and C<sub>3</sub>N(+) molecules for astrochemistry

M. Chabot<sup>1</sup>, K. Beroff<sup>2</sup>, T. Mahajan<sup>2</sup>, T. Id Barkach<sup>1</sup>

<sup>1</sup> *Institut de Physique Nucléaire d'Orsay (IPNO), CNRS-IN2P3, Univ. Paris Sud, Université Paris-Saclay, F-91406 Orsay*

<sup>2</sup> *Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS, Univ. Paris Sud, Université Paris-Saclay, F-91405 Orsay*

Correctness of kinetic database such as KIDA [1] is essential for the interpretation of observations. We have studied the fragmentation of neutral and cationic C<sub>n</sub>N molecules (n=1-3). The tool was high velocity collision between C<sub>n</sub>N<sup>+</sup> molecules and He atoms. From these measurements, it was possible to construct semi empirical breakdown curves (BDCs) which are internal energy dependant branching ratios [1]. The BDCs have been used to predict branching ratios of physical and chemical reactions of astrochemical interest.

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

M.CHABOT<sup>1</sup>, K. BEROFF<sup>2</sup>, E. DARTOIS<sup>2</sup>, T. PINO<sup>2</sup>, M. GODARD<sup>3</sup>.

<sup>1</sup> *Institut de Physique Nucléaire d'Orsay (IPNO), CNRS-IN2P3, Univ. Paris Sud, Université Paris-Saclay, F-91406 Orsay*

<sup>2</sup> *Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS, Univ. Paris Sud, Université Paris-Saclay, F-91405 Orsay*

<sup>3</sup> *Centre de Sciences Nucléaires et de Sciences de la Matière (CSNSM), CNRS-IN2P3, Univ. Paris Sud, Université Paris-Saclay, F-91405*

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. Result of calculations for this process will be presented. The IAE model [1] was used for collisional purpose while for fragmentation one, a micro canonical model was used. 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 contains of heavy particles in the impinging CR flux.

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## Thermal desorption of formamide and methylamine from graphite and amorphous water ice surfaces

H. Chaabouni<sup>1</sup>, S. Diana<sup>1</sup>, T. Nguyen<sup>1</sup>, S. Baouche<sup>1</sup>, F. Dulieu<sup>1</sup>

<sup>1</sup>LERMA, Université de Cergy-Pontoise, 5 mail Gay Lussac, 95000 Cergy-Pontoise, France  
Observatoire de Paris, UMR 8112, CNRS, PSL Research University  
Henda.Chaabouni@u-cergy.fr

Formamide ( $\text{NH}_2\text{CHO}$ ) and methylamine ( $\text{CH}_3\text{NH}_2$ ) are known to be the most abundant amine-containing molecules in many astrophysical environments (prestellar objects, hot corinos comets and even in protostellar shocks) [1-3]. The presence of these molecules in the gas phase may result from thermal desorption of interstellar ices.

The aim of the work performed in LERMA laboratory at the University of Cergy-Pontoise is to determine the values of the desorption energies of formamide and methylamine from analogues of interstellar dust grain surfaces and to understand their interaction with water ice [4]. Temperature programmed desorption (TPD) experiments of formamide and methylamine ices were performed in the sub-monolayer and monolayer regimes on graphite (HOPG) and non-porous amorphous solid water (np-ASW) ice surfaces at temperatures 40-240 K. The desorption energy distributions of these two molecules were calculated from TPD measurements using a set of independent Polanyi-Wigner equations. Contrarily to formamide, the desorption profile of methylamine is found to depend strongly on the substrate.

Our results have shown that more than 95 % of solid  $\text{NH}_2\text{CHO}$  diffuses through the np-ASW ice surface towards the graphitic substrate and is released into the gas phase with a desorption energy distribution of (5056–6990 K), which is measured with an arbitrary fixed pre-exponential factor  $A=10^{12} \text{ s}^{-1}$ . The large binding energy distribution of methylamine from graphite surface is found to be (3010–8420 K). A fraction of solid methylamine monolayer of roughly 0.15 diffuses through the water ice surface, and desorbs later with higher binding energies that exceed that of the crystalline water ice (4810 K). Implications of these high binding energies are discussed.

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# Temperature Dependent Infrared Spectroscopy (Experiment and Theory) of PAHs : the case of Pyrene

Shubhadip Chakraborty<sup>1</sup>, Giacomo Mulas<sup>1,2</sup>, Karine Demyk<sup>1</sup> and  
Christine Joblin<sup>1</sup>

<sup>1</sup>IRAP, Université de Toulouse, CNRS, CNES, UPS, 9 Avenue Colonel Roche, 30128,  
Toulouse, Cedex 4, France

<sup>2</sup>Istituto Nazionale di Astrofisica (INAF), Osservatorio Astronomico di Cagliari,  
09047 Selargius (CA), Italy

Polycyclic Aromatic Hydrocarbons (PAHs) are believed to be responsible for the Aromatic Infrared Bands (AIBs) observed in emission in many astronomical environments [1]. The excitation mechanism involves the absorption of an UV photon via an electronic transition and a sequence of radiationless transitions converting most of the absorbed energy to a vibrational excitation in the electronic ground state [2]. The hot molecule then relaxes by emitting IR photons, the resulting spectrum being dominated by a large number of hot bands, all slightly shifted with respect to the corresponding 1-0 fundamentals due to anharmonicity. The resulting bands are very broad and their interpretation complex.

In order to progress on the analysis of the IR spectra of hot PAHs we studied the case of pyrene (C<sub>16</sub>H<sub>10</sub>) from an experimental and theoretical perspective. We recorded the infrared spectrum of solid pyrene in KBr pellets from 14K to 723K. With increasing temperature a gradual red shift of the band positions and increase of the bandwidth are observed. We also studied the variation of the band intensities at different temperatures. For some of the bands the absolute intensity decreased with temperature while in some cases a reverse trend has been found. From the computational side we calculated the variable temperature infrared spectrum of pyrene using generalised second order perturbation theory in Van Vleck framework as presented in Ref 3. We computed the anharmonic infrared spectrum of pyrene up to 600K. The results of these calculations are compared to our experimental and available gas phase data [4].

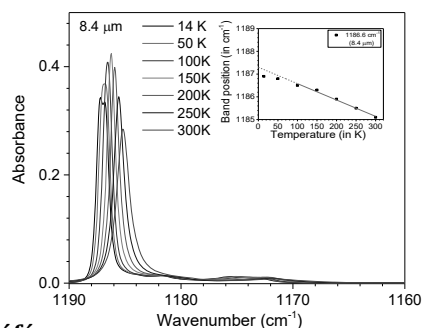


Fig. 1. Evolution of the 8.4  $\mu\text{m}$  band of pyrene with temperature. Variation of the band position with temperature is shown in the inset

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## Caractérisation de la structure de PAH par dissociation par collisions dans le dispositif AROMA

Mickaël Carlos<sup>1,2</sup>, Hassan Sabbah<sup>1,2</sup> et Christine Joblin<sup>1,2</sup>

<sup>1</sup> Université de Toulouse, UPS-OMP, Institut de Recherche en Astrophysique et Planétologie, 9 avenue du Colonel Roche, 31028 Toulouse Cedex 4 (France)

<sup>2</sup> CNRS, IRAP, 9 avenue du Colonel Roche, 31028 Toulouse Cedex 4 (France)

E-mail: [mickael.carlos@irap.omp.eu](mailto:mickael.carlos@irap.omp.eu)

AROMA (*Astrochemistry Research of Organics with Molecular Analyser*) est un analyseur moléculaire qui est développé dans le cadre du projet de synergie ERC Nanocosmos afin de caractériser le contenu moléculaire d'analogues de poussière cosmique. Ce dispositif est composé de trois parties : une source d'ions couplée à un piège à ion quadrupolaire linéaire (LQIT) et à un spectromètre de masse à temps de vol orthogonal (oTOF). L'information obtenue est donc un spectre de masse. Afin de progresser dans l'analyse structurale des espèces moléculaires, nous utilisons la capacité de piégeage du LQIT pour mener des expériences de dissociation induite par collisions (CID) ou par absorption de photons.

Ce travail présente une étude sur le cation du pyrène, un ion polycyclique aromatique hydrogéné (PAH) majoritaire dans la météorite de Murchison comme l'a montré une étude récente avec le dispositif AROMA [1]. Cet ion est produit par désorption/ionisation à deux étapes à partir d'un dépôt de pyrène  $C_{16}H_{10}$  sur un support métallique suivi d'une étape de refroidissement et d'isolation de l'espèce isotopique  $^{12}C_{16}H_{10}^+$ . Cette dernière est soumise à des collisions avec des atomes d'argon sous excitation dipolaire afin d'activer la CID. Ces conditions d'excitation sont optimisées pour observer la dissociation au seuil (perte de H dans le cas du pyrène). Des simulations utilisant le logiciel SIMION sont menées afin de quantifier les caractéristiques des collisions (énergies mises en jeu, nombres de collisions). Ceci nous permet de montrer qu'il s'agit d'un régime de chauffage doux et de mieux caractériser, en lien avec les résultats expérimentaux le transfert d'énergie mis en jeu dans les collisions.

### Acknowledgments

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## Revealing the ISM properties of star-forming dwarf galaxies

Diane Cormier<sup>1</sup>, Suzanne Madden<sup>1</sup>, Nick Abel<sup>2</sup>, Vianney Lebouteiller<sup>1</sup>, Sacha Hony<sup>3</sup>, Frédéric Galliano<sup>1</sup>, et al.

<sup>1</sup> *Laboratoire AIM, CEA/DSM - CNRS - Université Paris Diderot, Irfu/Service d'Astrophysique, CEA Saclay, 91191, Gif-sur-Yvette, France*

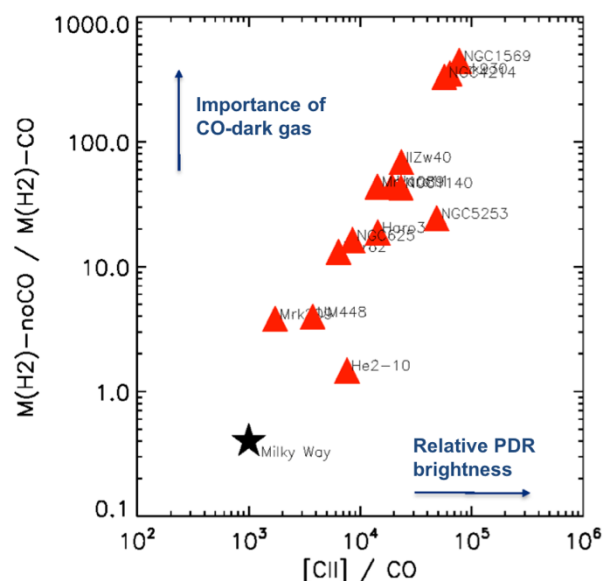
<sup>2</sup> *University of Cincinnati, Clermont College, Batavia, OH, 45103, USA*

<sup>3</sup> *ITA, ZAH, University of Heidelberg, Albert-Ueberle Str. 2, D-69120 Heidelberg, Germany*

To understand how star formation depends on the environmental properties of galaxies, and especially on fundamental parameters of galaxy evolution such as metallicity and star formation activity, a better characterization of their interstellar medium is needed. Thanks to Spitzer, Herschel, and now SOFIA, ALMA, we have detected for the first time in low-metallicity galaxies important cooling lines that provide great insight on the structure and physical conditions of the ISM closely related to star formation. I will talk about our on-going efforts to understand the emission from those cooling lines in the galaxies of the Herschel Dwarf Galaxy Survey ([1]) and model their multi-phase ISM with the spectral synthesis code Cloudy ([2,3,4,5]). We find that the low-metallicity ISM differs dramatically from that of more metal-rich objects. It is characterized by harder radiation fields and a porous structure. While the C+ emission arises mostly from photodissociation regions (PDRs), those PDRs have lower covering factors and moderate UV fields. We also find that most of the molecular gas mass in those galaxies resides in PDRs not traced by CO ([6,7, figure]). This highlights the necessity to take PDR tracers into account for a full picture of star formation at low metallicity.

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# Selection of Spitzer YSO candidates using Deep learning classifiers

D. Cornu and J. Montillaud

Institut UTINAM, CNRS UMR 6213, Univ. de Bourgogne Franche-Comté

The robust identification of Young Stellar Objects (YSOs) is an important step for characterizing star forming regions, e.g. by their star formation efficiency (SFE) and history. YSOs are typically observed in the infrared (IR) domain. Since multiple types of sources like external galaxies or AGB stars are also detected in IR surveys, it is necessary to classify all kinds of objects and extract the good YSO candidates as well as their evolution stage (Class 0, I, II).

Such classification is commonly performed using straight cuts in color-color and color-magnitude diagrams (CMD)[1]. Most of the time these studies are done in a well-known and nearby star forming region where YSO identification is less difficult. These days, several IR surveys are available and cover large sky areas, providing the astrophysics community with large data sets of various characteristics (set of photometric bands, sensitivity, resolution, ...). However, since the various kinds of objects show substantial overlaps in CMDs, straight-cut methods are intrinsically limited. Machine learning solve this problem with adaptive and non linear separations in any number of dimensions. Several corresponding methods have already been employed to produce YSO catalogs, like Support Vector Machine (SVM)[2]... However, most of them have bad-performance scaling with the number of data and input dimensions.

As most machine learning methods, deep learning methods belong to the supervised learning approach which means that they learn from a pre-selected training set. These methods have the ability to manage large datasets in reasonable computation time, which guarantees that each defined class can be sufficiently represented in the training sample. They are based on deep Artificial Neural Network and can perform classification by correlating input data to given classes.

Our objective is to make a census of YSOs in the full Spitzer/IRAC mid-IR maps using several deep learning classifiers. It is motivated by Spitzer's performances which remain superior to comparable surveys in terms of sensitivity and resolution. The training set is build from well known regions where usual classification is used with enough confidence[3][4]. We will present our preliminary results of classifications using deep neural networks on large datasets build from such regions and explain our expectations for the full Spitzer catalogue. We will show the performance and the classification efficiency for multiple methods, and will compare the associate SFE with other studies in different star formation regions.

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

Vincent Deguin,<sup>1</sup> Joëlle Mascetti,<sup>1</sup> Aude Simon,<sup>2</sup> Nadia Ben Amor,<sup>2</sup>  
Christian Aupetit,<sup>1</sup> and Jennifer Anna Noble.<sup>1,3</sup>

<sup>1</sup> ISM, UMR5255, Université de Bordeaux and CNRS, 33405 Talence, France

<sup>2</sup> LCPQ-IRSAMC, UMR5626, CNRS and Université Paul Sabatier, 31062 Toulouse, France.

<sup>3</sup> PhLAM, UMR8523, Université Lille 1 and CNRS, 59655 Villeneuve D'Asq, France.

The interstellar medium 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. On the one hand, we observed the formation of adducts of iron monomers and dimers with water molecules in the MIR and UV-visible spectral domains. On the other hand, upon irradiation with a UV radiation source, the iron species were inserted into the water molecules to form HFeOH and HFe<sub>2</sub>OH, leading in some cases to the formation of FeO possibly accompanied by the production of H<sub>2</sub>. DFT and multireference wavefunction calculations (SO CASPT2 and SO-MS-CASPT2) confirmed our attributions. 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 [1, 2]. The study presented here confirms that neutral iron is highly reactive with water at cryogenic temperatures [3-6]. This suggests that such reactions could potentially occur in dense astrophysical regions irradiated by UV. The identification of spectral bands in the mid-IR and UV-visible regions may also help with the identification of iron-bearing species in such interstellar environments. These results, combined with our previous work on PAH: H<sub>2</sub>O [7-8], represent a strong benchmark for further experimentation on ternary systems including Fe, PAH and H<sub>2</sub>O.

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## **Enveloppe of early stages of protostellar phase objects in three Hobys regions.**

Didelon, P. <sup>1</sup>, Motte, F. <sup>2</sup>

<sup>1</sup> *CEA/DAP-AIM, 91191 Gif sur Yvette Cedex – France*

<sup>2</sup> *IPAG, Université Grenoble Alpes 38058 Grenoble Cédex 9 – France*

The characteristics of the density envelopes of early protostellar objects revealed by Herschel in three Hobys regions (M16, Vela C and Mon R2) enable us to define a mean general value of some interesting primary parameter (mean density, sizes and density gradient), which can be compared to theoretical values and the ones obtained in simulations.

Moreover it allows us to determine in most cases infall ages, generalizing the Shu and Larson inside-out infall concept.

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## Theoretical characterization of amorphous carbonaceous clusters of astrophysical interest.

Clément DUBOSQ<sup>1</sup>, Aude SIMON<sup>1</sup>, Michael HERNANDEZ<sup>1</sup> et Mathias RAPACIOLI<sup>1</sup>

<sup>1</sup> *Laboratoire de Chimie et Physique Quantiques (LCPQ) – IRSAMC UMR 5626 CNRS, 118 route de Narbonne, 31062, Toulouse Cedex 09, France*

A large variety of carbon-based species have been identified [1] in the interstellar medium (ISM) through their spectra ranging from radio to ultraviolet. It has been established that a rich carbon-based chemistry takes place in the ISM [2 – 4]. Thanks to observations and a large set of data, astronomers are able to propose advanced scenario to explain the formation of these molecular species and their abundances. In particular, a set of mid-infrared emission bands is observed in many regions of the ISM. Bands are referred to aromatic infrareds bands (AIBs). These have been assumed to be carried by a population of polycyclic aromatic hydrocarbons (PAHs) molecules. However, a specific molecule has not been identified despite many experimental and theoretical studies, and exact nature of the carriers of AIBs remains an open question. In this project, we explore the possibility for the AIBs to originate not only from PAH molecules but from more disordered structures.

In the framework of the PACHYNO project (Probing the diversity of Astrophysically relevant Carbon and HYdrogen NanOparticles) based on the close collaboration between experimentalists and theoreticians, we computationally explore a variety of structures of carbon-based molecules and nanoparticles. The final goal is to identify families of structures based on their spectroscopic responses (IR or UV).

In this poster, I will present the first results issued from Self-Consistent Charge Density Functional based Tight binding (SCC-DFTB) calculations for carbon clusters. The calculation were achieved under the deMonNano code [5]. Local optimizations were performed using a variety of isomers resulting from parallel tempering molecular dynamics (PTMD) calculations by Falvo et al. [6, 7] using the AIREBO[8] potential (~ 45000 geometries). The SCC-DFTB potential is benchmarked on DFT(B3LYP)/pc-1 calculations for a few representative structures. Some spectroscopic signatures can be assigned to some vibrational modes of specific families. These observations will help us in the interpretation of results for larger structures.

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## Segregation effect and N<sub>2</sub> binding energy reduction in CO-N<sub>2</sub> systems adsorbed on water ice substrates

T. Nguyen<sup>1</sup>, S. Baouche<sup>1</sup>, E. Congiu<sup>1</sup>, S. Diana<sup>1</sup>, L. Pagani<sup>1\*</sup>, E. Dulieu<sup>1</sup>,

<sup>1</sup> *LERMA, Sorbonne Université, Observatoire de Paris, PSL University, CNRS, Université de Cergy-Pontoise, F-95000, Cergy-Pontoise*

<sup>1\*</sup> *LERMA, F-75014, Paris*

CO and N<sub>2</sub> are two abundant species in molecular clouds. CO molecules are heavily depleted from the gas phase towards the centre of prestellar cores, whereas N<sub>2</sub> maintains a high gas phase abundance. For example, in the molecular cloud L183, CO is depleted by a factor of  $\approx 400$  in its centre with respect to the outer regions of the cloud, whereas N<sub>2</sub> is only depleted by a factor of  $\approx 20$  (Pagani et al 2012). The reason for this difference is not clear yet, because CO and N<sub>2</sub> have identical masses, similar sticking properties, and a relatively close energy of adsorption.

We present a study of the CO-N<sub>2</sub> system in submonolayer regimes, with the aim to measure, analyse and elucidate how the adsorption energy of the two species varies with coverage, with much attention to the case where CO is more abundant than N<sub>2</sub>.

Experiments were carried out using the ultra-high vacuum (UHV) set-up called VENUS. Submonolayers of pure and mixed <sup>13</sup>CO and <sup>15</sup>N<sub>2</sub> molecules were deposited on three different types of water ice substrates (compact amorphous solid water, porous amorphous solid water, and crystalline ice). Temperature-programmed desorption experiments, monitored by mass spectrometry, are used to analyse the distributions of binding energies of <sup>13</sup>CO and <sup>15</sup>N<sub>2</sub> when adsorbed together in different proportions.

The distribution of binding energies of pure species varies from 990 K to 1630 K for <sup>13</sup>CO, and from 890 K to 1430 K for <sup>15</sup>N<sub>2</sub>. When a CO-N<sub>2</sub> mixture is deposited, the <sup>15</sup>N<sub>2</sub> binding energy distribution is strongly affected by the presence of <sup>13</sup>CO, whereas the adsorption energy of CO is unaltered.

Whatever types of water ice substrate we used, the N<sub>2</sub> effective binding energy was significantly lowered by the presence of CO molecules. We discuss the possible impact of this finding in the context of prestellar cores.

# Experimental study of the chemical network of $\text{CH}_3\text{NC}$ on interstellar dust grains

F.Dulieu<sup>1</sup>, T.Nguyen<sup>1</sup>, E.Congiu<sup>1</sup>, S.Baouche<sup>1</sup>, and J.C.Guillemain<sup>2</sup>

<sup>1</sup> *Universite de Cergy Pontoise, Sorbonne Universite, Observatoire de Paris, PSL Universite, CNRS, LERMA, F-95000, Cergy Pontoise, France*

<sup>2</sup> *Institut des Science Chimiques de Rennes, CNRS, ENSCR, 35708 Rennes, France*

Methyl Isocyanide ( $\text{CH}_3\text{NC}$ ) and Acetonitrile ( $\text{CH}_3\text{CN}$ ) are two complex organic molecules (COMs) which are detected in the interstellar medium and in comets [1, 2, 3]. They are nodes of the very entangled chemical network leading to the molecular complexity. We aim at exploring the solid-state chemistry which may lead to COMs.

We developed a new experimental set-up named VENUS, in which we can deposit different reactants together on the cold surface (10K-40K).  $\text{CH}_3\text{NC}$  or  $\text{CH}_3\text{CN}$  and H/D atoms were co-deposited at different temperatures in presence or absence of water. Thanks to Infrared spectroscopy and mass spectrometry, we detected products and remnants after completing the depositions.

We obtained the following observations and measurements:

- i) Methyl Isocyanide ( $\text{CH}_3\text{NC}$ ) reacts with H, but Acetonitrile ( $\text{CH}_3\text{CN}$ ) is unreacted.
- ii)  $\text{CH}_3\text{NC}$  reacts with H atoms via quantum tunneling at low temperatures.
- iii) Ratio of products is changing with the surface temperature. It indicates the presence of barriers.
- iv) Hydrogenations, isomerization, and fragmentations are competitive mechanisms.
- v) The presence of  $\text{H}_2\text{O}$  enhances the hydrogenation efficiency.

We will present the experimental results and discuss the chemical network in details, unveiling the presence of activation barriers and (very likely) the role of the quantum tunneling in the formation of COMs on grains.

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# Interaction between water and coronene on graphite

A-S.MOHAMED-IBRAHIM, S.BAUCHE et F.DULIEU

LERMA Université de Cergy Pontoise, Sorbonne Université, Observatoire de Paris, PSL Université, CNRS, LERMA  
F-95000, Cergy Pontoise, France

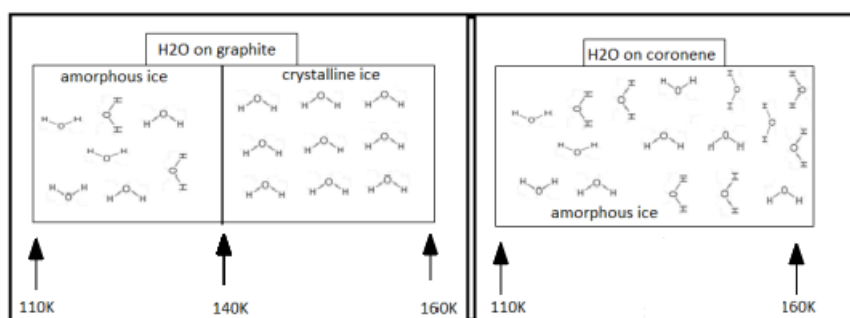
*Abstract for poster*

Polycyclic aromatic hydrocarbons (PAHs) and water are two molecules that are probably omnipresent in the universe. PAHs constituting a family of molecules composed of at least two aromatic rings are linked to hydrogen atoms and astrophysical interest.

Solid water ice is the most abundant condensed component in the cosmos and especially on the icy mantle of dust grains in dense molecular clouds. It is also the most abundant species in icy mantles that cover the dust grains [1] [2] in the interstellar medium (ISM). In this context of abundance of two molecules in the ISM, we studied the interaction of the molecule water and coronene on graphite. As part of these experiments, we used the FORMOLISM device [3]. We have two sets of experiments using the temperature programmed desorption method, the first experiment set is to deposit a variable amount of water on the graphite surface at 110K. The second experiment was the deposition of water from a coronene film.

We obtained the following observations and measurements:

- (i) For the graphite water experiment, the structure of the ice depends on the temperature at which it is formed, therefore the temperature of the surface. At low temperatures, the water will condense immediately without internal rearrangements, the ice will be amorphous. At higher temperatures ( $> 140$  K), the condensation will be slower, the ice will be crystalline
- (ii) For the coronene water experiment, we did not observe the transition from the amorphous phase to the crystalline phase. This could be an indication that the water ice remains amorphous and finds it difficult to crystallize.



(iii) We also found that the coronene delays the desorption of water on graphite

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## X-ray photodesorption from interstellar ice analogs

R. Dupuy<sup>1</sup>, M. Bertin<sup>1</sup>, G. Féraud<sup>1</sup>, M. Hassenfratz<sup>1</sup>, X. Michaut<sup>1</sup>, T. Putaud<sup>1</sup>, L. Philippe<sup>1</sup>, P. Jeseck<sup>1</sup>, M. Angelucci<sup>4</sup>, R. Cimino<sup>4</sup>, V Baglin<sup>3</sup>, C. Romanzin<sup>2</sup> and JH Fillion<sup>1</sup>

<sup>1</sup>*Sorbonne Université, Observatoire de Paris, Université PSL, CNRS, LERMA, F-75005, Paris, France*

<sup>2</sup>*Laboratoire de Chimie Physique, Université Paris Sud 11, CNRS UMR 8000, 91405 Orsay, France*

<sup>3</sup>*CERN, CH-1211 Geneva 23, Switzerland*

<sup>4</sup>*Laboratori Nazionali di Frascati, LNF-INFN I-00044 Frascati*

The icy mantles of interstellar dust grains are exposed to a variety of processes, including cosmic ray bombardment, collisions and irradiation by photons, 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 modelling. The interaction of UV photons with ice analogs, for example, has been studied in detail in laboratory studies [1]. Many experimental works in recent years have been dedicated to the understanding of UV photodesorption [2], i.e. the ejection of molecules back to the gas phase by UV irradiation, and as a result the process is well implemented in astrochemical models and contributes to the understanding of the physico-chemistry of cold regions of the ISM [3]. X-ray irradiation of interstellar ice analogs, and in particular the photodesorption of neutral molecules, on the other hand, has almost not been explored so far.

Using our upgraded SPICES 2 set-up at the SEXTANTS beamline of the SOLEIL synchrotron, we studied X-ray photodesorption from H<sub>2</sub>O and CO ices around the O 1s resonance (500 – 600 eV). The set-up allows a complete characterization of the desorbed species: I will report the measurement and quantification of the photodesorption of neutral species, positive and negative ions, and the electron yield. Photodesorption spectra of the different species and electron yield spectra give us insights on the physical mechanisms behind dissociation and desorption, as well as on the X-ray induced chemistry in the ice.

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## Nitrile versus Isonitrile adsorption on interstellar grains: a first step towards the formation of amines

Y. Ellinger<sup>1</sup>, I. Fourré<sup>1</sup>, O. Matz<sup>1</sup>, V. Utard<sup>1</sup>, M. Doronin<sup>1,2</sup>, M. Bertin<sup>2</sup>,  
J.-H. Fillion<sup>2</sup>, F. Dulieu<sup>2</sup>, T. Nguyen<sup>2</sup>, E. Congiu<sup>2</sup>, A. Markovits<sup>1</sup>, F. Pauzat<sup>1</sup>,  
and J.-C. Guillemin<sup>3</sup>

<sup>1</sup> Sorbonne Université, CNRS, Laboratoire de Chimie Théorique, LCT,  
F. 75005 Paris, France

<sup>2</sup> Sorbonne Université, CNRS, Observatoire de Paris, LERMA, F. 75005 Paris, France

<sup>3</sup> Institut des Sciences Chimiques de Rennes, UMR - CNRS 6226, ENSCR, F-35700 Rennes,  
France.

Among the ~200 different species detected in the ISM, about 20% present a carbon atom linked to a nitrogen atom by a triple bond in the form of R-CN (nitrile) or R-NC (isonitrile). When R is a saturated hydrocarbon group, the number of detected isomers is limited to CH<sub>3</sub>CN, CH<sub>3</sub>CH<sub>2</sub>CN, *n*-C<sub>3</sub>H<sub>7</sub>CN, and *i*-C<sub>3</sub>H<sub>7</sub>CN for nitriles and to one, CH<sub>3</sub>NC, for isonitriles. How these species behave in presence of the grain surfaces and how they behave with respect to hydrogenation are still open questions. Answering these questions might explain their observed relative abundances and the fact that no single amine, after CH<sub>3</sub>NH<sub>2</sub>, has ever been observed since 1974 [1]. H<sub>2</sub>NCN and H<sub>2</sub>NCH<sub>2</sub>CN are not considered here.

These problems have been addressed with concerted experimental/theoretical approaches of CH<sub>3</sub>CN and CH<sub>3</sub>NC on three surfaces of astrophysical interest, looking for possible adsorption selectivity on water ice, hydroxylated silica and aromatic carbonaceous supports [2]. The reactivity aspect has been thoroughly investigated on water ice [3]. The experiments were carried out under Ultra-High Vacuum using infrared spectroscopy and mass spectrometry to identify the chemical and the thermal evolution of the condensed molecules. The theoretical approach consisted in “First principle” simulations based on periodic DFT including correction for dispersion effects to describe molecule-solid long-range interactions [2] and use ab initio MP2/CCSD(T) methods for the reactivity part.

First, we found that adsorption energies of both CH<sub>3</sub>CN and CH<sub>3</sub>NC are extremely similar regardless of their supporting substrate. The energies are lower onto quartz and defective graphite surface, and much higher when the molecules are condensed onto the water-ice surface, with energies similar to the cohesion energy of the water ice itself. It is true for both experiments and numerical simulations and the quantitative agreement is excellent.

Another point is that experimentally, the addition of H atoms to CH<sub>3</sub>CN on the ice substrate is found ineffective, which is consistent with the calculated high activation barrier.

The addition of H atoms to CH<sub>3</sub>NC appeared to be a faster process leading in the end to CH<sub>3</sub>NHCH<sub>3</sub>; in the course of that process we were able to identify an intermediate species, CH<sub>3</sub>NCH<sub>2</sub>, corresponding to the lowest energy structure. The calculations show much smaller activations barriers allowing efficient tunneling, in total agreement with the experiments using D in place of H.

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## Photodesorption of an intact organic molecule and of its fragments: Formaldehyde (H<sub>2</sub>CO)

G. Féraud<sup>1</sup>, M. Bertin<sup>1</sup>, C. Romanzin<sup>2</sup>, R. Dupuy<sup>1</sup>, F. Le Petit<sup>1</sup>, L. Philippe<sup>1</sup>, X. Michaut<sup>1</sup>, P. Jeseck<sup>1</sup>, H. Linnartz<sup>3</sup> & J.-H. Fillion<sup>1</sup>

<sup>1</sup>*Sorbonne Université, Observatoire de Paris, Université PSL, CNRS, LERMA, F-75005, Paris, France*

<sup>2</sup>*Laboratoire de Chimie Physique, Université Paris Sud 11, CNRS UMR 8000, 91405 Orsay, France*

<sup>3</sup>*Sackler Laboratory for Astrophysics, Leiden Observatory, Leiden University, P.O. Box 9513, 2300 RA Leiden, The Netherlands*

In cold and dense regions of the interstellar medium (ISM), molecules are found either in gas phase or accreted at the surface of dust grains. The interplay between gas and ice is expected to play an important role in the observed molecular abundances. In this context, the role of non-thermal desorption from grains in the origin of the gaseous organic molecules observed in these regions is still an open question. Formaldehyde (H<sub>2</sub>CO), the simplest of organic molecules, has been detected in gas phase in several environments such as protoplanetary disks (e.g. [1]) and low UV-flux Photon-Dominated Regions (PDR) [2], and it is a likely identified species in solid phase (e.g. [3]). UV photodesorption from icy grains has been invoked as a non-thermal mechanism that participate to the observed gas phase H<sub>2</sub>CO abundance in these cold regions [2].

We studied the photon-induced desorption of H<sub>2</sub>CO ices in the VUV range at the SOLEIL synchrotron (DESIRS beamline, 7-14 eV), and we detected the gas phase release of intact H<sub>2</sub>CO and of CO and H<sub>2</sub> fragments as a function of the photon energy. The photodesorption of intact H<sub>2</sub>CO from pure H<sub>2</sub>CO ice is found relatively efficient in the VUV: H<sub>2</sub>CO average photodesorption yield is higher than CH<sub>3</sub>OH average photodesorption yield from pure CH<sub>3</sub>OH ice [4]. This shows the ability of UV photons to desorb a small organic molecule such as H<sub>2</sub>CO.

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## Rotational excitation of CO by H<sub>2</sub>O collisions

Alexandre Faure<sup>1</sup>, Jérôme Loreau<sup>2, 3</sup>, François Lique<sup>2</sup>,  
Yulia Kalugina<sup>4</sup>, Ad van der Avoird<sup>5</sup>, Kyle Walker<sup>2</sup>

<sup>1</sup> Univ Grenoble Alpes, CNRS, IPAG, F-38000 Grenoble, France

<sup>2</sup> LOMC - UMR 6294, Normandie Université, Université du Havre and CNRS, 25  
rue Philippe Lebon, BP 1123 - 76 063 Le Havre Cedex, France

<sup>3</sup> Service de Chimie Quantique et Photophysique, Université libre de Bruxelles (ULB) CP  
160/09, B-1050 Brussels, Belgium

<sup>4</sup> Department of Optics and Spectroscopy, Tomsk State University, 36 Lenin av., Tomsk  
634050, Russia

<sup>5</sup> Institute for Molecules and Materials, Radboud niversity, Heyendaalseweg 135, 6525  
AJ Nijmegen, The Netherlands

Collisions between H<sub>2</sub>O and CO play a crucial role in the gaseous component of comets and protoplanetary disks. We have recently computed a five-dimensional potential energy surface (PES) for the H<sub>2</sub>O–CO collisional complex [1]. *Ab initio* calculations were carried out using the explicitly-correlated closed-shell single- and double-excitation coupled cluster approach with non-iterative perturbative treatment of triple excitations [CCSD(T)-F12a] method with the augmented correlation-consistent aug-cc-pVTZ basis sets. The most stable configuration of the complex, where the carbon atom of CO is pointing towards the OH bond of water, has a binding energy  $De = 646.1 \text{ cm}^{-1}$ . The end-over-end rotational constant of the H<sub>2</sub>O–CO complex was extracted from bound state calculations and it was found to be  $B_0 = 0.0916 \text{ cm}^{-1}$ , in excellent agreement with experimental measurements. Cross sections for the rotational excitation of CO by H<sub>2</sub>O were also computed for *s*-wave ( $J = 0$ ) scattering at the full close-coupling level of theory. Owing to the heavy computational cost of these calculations, alternative scattering methods have been investigated. We will present preliminary and encouraging results based on the statistical [2] and quasi-classical approaches [3].

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## Rotational excitation of $C_4H^-$ by collision with para- $H_2$ .

N. Feautrier<sup>1</sup>, F. Dumouchel<sup>2</sup>, F. Dayou<sup>1</sup>, and M.-L. Senent<sup>3</sup>

<sup>1</sup>*Sorbonne Université, Observatoire de Paris, Université PSL, CNRS, LERMA, F-92195 Meudon, France ;*

<sup>2</sup>*LOMC - UMR 6294, CNRS-Université du Havre, 25 rue Philippe Lebon, BP 1123, 76 063 Le Havre cedex, France ;*

<sup>3</sup>*Departamento de Química y Física Teóricas, IEM-CSIC, Serrano 121, Madrid 28006, Spain*

Anions are very reactive species that can play important roles in the chemical evolution of the interstellar medium. Their presence has important consequences on the free electron density that affects star formation rates.

Following the detection of  $C_6H^-$  carbon chains, investigations on detectable anions started, leading to the discovery of five new anions :  $C_4H^-$ ,  $C_8H^-$ ,  $CN^-$ ,  $C_3N^-$ ,  $C_5N^-$ .  $C_4H^-$  was first observed in the circumstellar envelope of IRC+10216 and in TMC-1 by Cernicharo et al. (2007) [1]. In these cool and low-density regions, an accurate modeling of the chemical and physical conditions of the observed spectra through radiative transfer calculations, requires the knowledge of both radiative and collisional rates.

We present here inelastic rate coefficients for  $C_4H^-$  in collision with para- $H_2$ . Full quantum scattering calculations are carried out on a new calculated ab initio potential energy surface. The close-coupling (CC) method is used to compute cross-sections for the first 21 rotational levels of  $C_4H^-$  and for collisional energies up to 500  $cm^{-1}$ . Rate coefficients are obtained for the temperature range of 5-100 K. The cross sections and rate coefficients are compared with the previous calculated ones for  $C_2H^-$  [2] and  $C_6H^-$  [3].

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# New templates for the analysis of Aromatic Infrared Bands in the JWST era

S. Foschino<sup>1\*</sup>, O. Berné<sup>1</sup>, P. Pilleri<sup>1</sup> and C. Joblin<sup>1</sup>

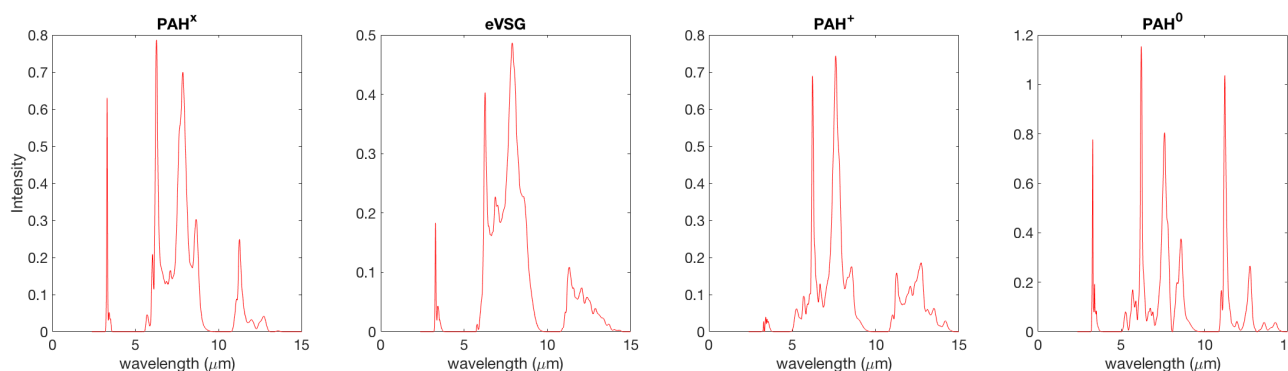
<sup>1</sup>*Institut de Recherche en Astrophysique et Planétologie, Université de Toulouse, CNRS, CNES, UPS,*

*9 avenue du Colonel Roche, 31028 Toulouse Cedex 4 (France)*

*\*Corresponding author e-mail address: [sacha.foschino@irap.omp.eu](mailto:sacha.foschino@irap.omp.eu)*

Observations of the mid-infrared (mid-IR, 3-15  $\mu\text{m}$ ) spectra of photo-dissociation regions (PDRs) reveal ubiquitous and intense emission (the Aromatic Infrared Bands), attributed to polycyclic aromatic hydrocarbons (PAHs) [1]. Using “Non-negative Matrix Factorization” (NMF) [2], earlier studies extracted, from Spitzer IRS observations, three spectra in reflection nebulae (RNe), which were attributed to cationic and neutral PAHs (PAH<sup>+</sup> and PAH<sup>0</sup>) and evaporating very small grains (eVSG) [3]. A fourth spectrum, attributed to large ionized PAHs (named PAH<sup>x</sup>) was invoked based on the analysis of the spectra of planetary nebulae (PNe) [4]. These spectra have been used by the community to interpret Spitzer observations of various sources with the help of a dedicated tool i.e. PAHTAT [5].

The James Webb Space Telescope (JWST), with an unprecedented sensitivity, will provide IR spectra over the 0.6-28  $\mu\text{m}$  range with an increased level of detail including better spectral resolution than previous missions. In preparation for the arrival of JWST data, we conducted an analysis using archival ISO-SWS data which were obtained at higher spectral resolution ( $R=260$  instead of  $R=70$  for Spitzer) and over larger spectral coverage (2.8 - 15  $\mu\text{m}$  vs 5-15  $\mu\text{m}$  for Spitzer). The ISO data consisted of a catalog of 31 spectra from a variety of sources (HII regions, RNe, PNe, Post AGB, HAeBe stars). Using a sparse fitting algorithm, we first removed the noise, gas lines and continuum from this catalog. NMF was applied to the obtained noiseless catalog. We initialized NMF with a geometrical method [6] to reduce variability of the results caused by random initialization [2]. Using this approach, we extracted four noiseless template spectra of PAH<sup>0</sup>, PAH<sup>+</sup>, eVSG and PAH<sup>x</sup>.



**Acknowledgments:** This work was supported by the European Research Council (project ERC-2013-SyG NANOCOSMOS).

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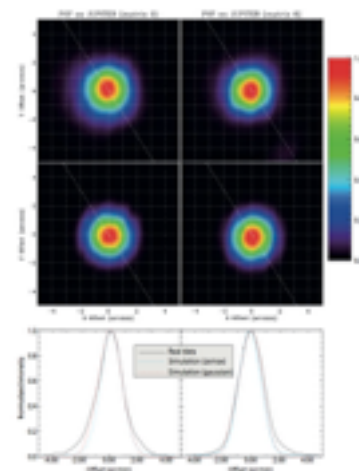
## In-FLight performance and first results of the PILOT balloon-borne experiment

G. Foënard<sup>1</sup>, J.-Ph. Bernard<sup>1</sup>, on behalf of the PILOT collaboration<sup>2</sup>.

<sup>1</sup> IRAP, UMR5277 du CNRS, 9 Avenue du colonel Roche, 31028, Toulouse France

<sup>2</sup> <http://pilot.irap.omp.eu>

Measuring precisely the faint polarization of the Far-Infrared and sub-millimetre sky is one of the next observational challenges of modern astronomy and cosmology. We will describe the concept and science goals of the PILOT balloon-borne instrument, dedicated to measure the linear polarization of the faint interstellar diffuse dust emission in the Far-Infrared in our Galaxy and nearby galaxies. We will present the two successful flights of PILOT from Timmins, Canada in September 2015 and from Alice Springs, Australia in April 2017 ([1]). We will discuss the in-flight performance of the instrument. The accuracy of the measurements was limited during flight#1 due to a deteriorating front baffle during day-time observations. However, the main characteristics of the instrument such as the quality of the optics, pointing reconstruction, residual atmospheric emission subtraction are fully satisfactory during flight#2. In particular, we accurately measure the variations of the detector response using the residual atmospheric emission and the noise properties are consistent with expectation and stable in time. These performance lead to expected in-flight sensitivity sufficient to reach our most ambitious science goals.



Right: The PILOT experiment ready for flight in Alice Springs, Australia. Left: Observed Point spread Function the PILOT instrument as measured on Jupiter at 240 microns, compared to predictions.

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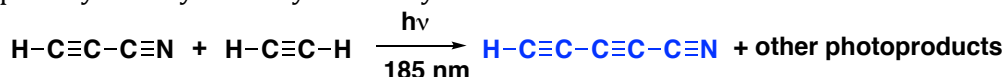
# The Complex Question of the Formation of Cyanopolyynes in the Interstellar Medium.

Jean-Claude Guillemin, Yann Trolez.

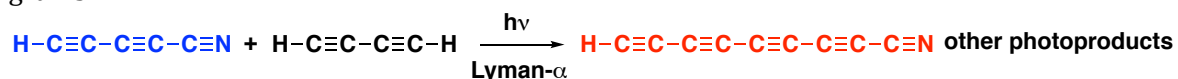
*Univ Rennes, Ecole Nationale Supérieure de Chimie de Rennes, CNRS, ISCR –  
UMR6226, F-35000 Rennes, France*

Cyanopolyynes ( $\text{H}(\text{C}\equiv\text{C})_n\text{CN}$  with  $n=1-4$ ) and the corresponding methylated derivatives ( $\text{Me}(\text{C}\equiv\text{C})_n\text{CN}$  with  $n=1,2$ ) are considered as a particular family among the compounds detected in the interstellar medium (ISM) by their number and the ubiquitous character of the simplest ones. The smallest cyanopolyynes are often proposed as the precursors of higher homologs and many studies have been done starting from cyanoacetylene ( $\text{HC}\equiv\text{C-CN}$ ).

In the lab, although an effective preparation of cyanoacetylene has been described at the beginning of the 20<sup>th</sup> century,[1] it was only in 2005 that the following element, cyanobutadiyne, was isolated in pure form.[2] This made it possible to highlight its formation in the photolysis of cyanoacetylene-acetylene mixtures.



Similarly, photolyses of the propyne-cyanoacetylene mixture led to the formation of cyano-2,4-pentadiyne ( $\text{MeC}_5\text{N}$ ),[3] another compound detected in the ISM. To be feasible, however, these gas phase studies have used pressures and temperatures far too high to simulate the conditions of the ISM satisfactorily. Other approaches used the photolysis of matrix at 10K and, thanks to phosphorescence, cyanopolyynes ( $\text{H}(\text{C}\equiv\text{C})_n\text{CN}$  with  $n=2-4$ ) and ( $\text{Me}(\text{C}\equiv\text{C})_n\text{CN}$  with  $n=2,3$ ) have been observed in photoproducts.[4,5] Nevertheless, these reactions, which fairly satisfactorily simulate the chemistry of such systems on interstellar grains, must take into account the non-observation to date of the  $\nu_{\text{CN}}$  infrared band on these grains.



Very recently, on the basis of the proportion of isotopomers detected for  $\text{HC}_5\text{N}$  and  $\text{HC}_7\text{N}$  in TMC-1, it has been proposed that these cyanopolyynes could rather be formed by reaction of atomic nitrogen with hydrocarbon ions.[6] It should be noted that these reactive ions or primary products have not been detected to date in the ISM.

All these studies show the difficulty of understanding the chemistry of the ISM including for abundant compounds. The fact of forming a compound under conditions more or less simulating the ISM is not sufficient to prove its formation pathway in this medium which can also vary from one interstellar cloud to another if the physicochemical parameters are different. This presentation will review the possible syntheses of cyanopolyynes in the ISM.

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# A Dust Spectral Energy Distribution Model with Hierarchical Bayesian Inference and Its Application to the Nearby Universe

Frédéric Galliano<sup>1,2</sup>

<sup>1</sup> IRFU, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France

<sup>2</sup> Université Paris-Diderot, AIM, Sorbonne Paris Cité, CEA, CNRS, F-91191

The properties of interstellar dust (chemical composition, size distribution, *etc.*) depend on the local environmental conditions, and on the elemental enrichment history of the galaxy (*e.g.* Galliano *et al.*, 2018). However, the individual processes controlling this evolution (dust production by stars, dust growth in the ISM, dust destruction by shocks, *etc.*) are not known accurately enough to unambiguously model the evolution of galaxies. One of the ways to refine our knowledge of these evolutionary processes consists in studying the variations of local observed dust properties, measured via their spectral energy distribution (SED), as a function of the local physical conditions (gas density, temperature, metallicity, *etc.*). These trends between dust properties and physical conditions are valuable constraints on the nature and efficiency of the grain evolutionary processes.

This leaves us with the task of properly deriving dust parameters and their uncertainties from broadband infrared (IR) and submillimeter (submm) observations. This task is known to present several intricate degeneracies and noise-induced false correlations (*e.g.* Shetty *et al.*, 2009). We have recently applied the refined statistical approach of hierarchical Bayesian inference to fitting a full dust model, including realistic laboratory optical properties, stochastic heating, mixing of stellar heating along the sightline and instrumental effects (Galliano, 2018), in order to solve these methodological issues.

I will first present the principle of this model, in a didactic way, and will demonstrate its power and its limits, on several examples. I will then discuss the application of this model to the SEDs of the DustPedia sample (Davies *et al.*, 2017), which is a reference sample of 3000 nearby galaxies.

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## Rotation of Class 0/I protostellar envelopes from the CALYPSO survey

M. Gaudel<sup>1</sup>, A. Maury<sup>1</sup>, A. Belloche<sup>2</sup>, Ph. André<sup>1</sup> and S. Maret<sup>3</sup>.

<sup>1</sup>AIM, CEA/DRF-CNRS-Université Paris Diderot, IRFU/Département d'Astrophysique, CEA Saclay, 91191 Gif-sur-Yvette - France

<sup>2</sup>Max-Planck-Institut fuer Radioastronomie, Auf dem Huegel 69, D-53121 Bonn - Germany

<sup>3</sup>UJF-Grenoble/CNRS-INSU, Institut de Planétologie et d'Astrophysique de Grenoble, UMR 5274, 38041 Grenoble - France

One of the main challenges to the formation of solar-like stars is the “angular momentum problem”: if the angular momentum of the gas contained in a typical star-forming core is transferred to the star during the accretion phase, the gravitational force can not counter the centrifugal force and the star breaks up before it reaches the main sequence. Studying the kinematics of protostellar cores and understanding the distribution of the angular momentum during the main accretion phase is of uttermost importance to test possible solution to this problem. In order to tackle this issue, the CALYPSO (Continuum and Lines in Young Protostellar Objects, PI: Ph. André) IRAM large program provides Plateau de Bure Interferometer (PdBI) and the 30m telescope observations of the dust continuum emission and a dozen of molecular lines from a sample of 16 Class 0 protostars. We used the  $C^{18}O(2-1)$  and  $N_2H^+(1-0)$  molecular lines to trace kinematic of the envelopes combining PdBI and 30m datasets to probe scales down to 50 au in the envelope ( $0.5''$ ) and provide a high dynamic range allowing to reach the outer envelope scales (5000 au). I will present the method used to create radial profiles of rotation motions along the plane perpendicular to the outflows in a sample of prototypical Class 0 objects. This analysis allows us to establish radial distribution of specific angular momentum, therefore shedding light a possible evolution of angular momentum during solar type star formation.

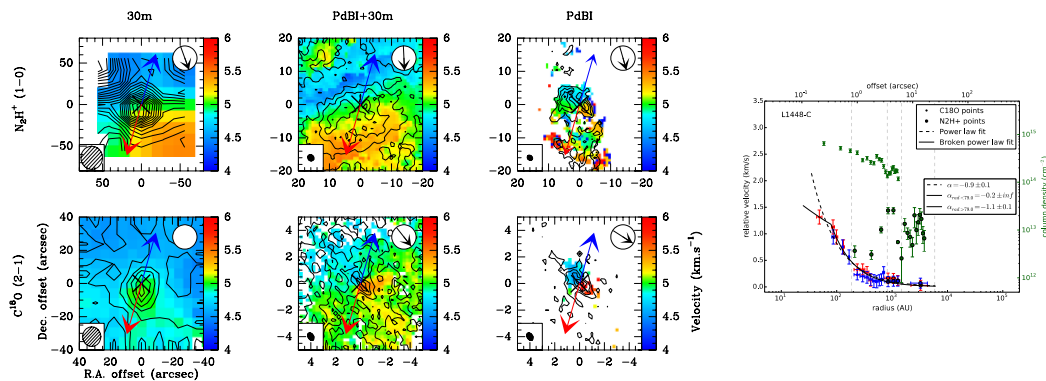


Figure: Left: Velocity maps with integrated intensity overlaid on for L1448-C. Blue and red solid arrows represent the outflow directions. Black arrows show the orientations of velocity gradient obtained by performing a fit of a linear velocity gradient. Right: Position-velocity profile for L1448-C. Blue and red marks show the data points measured at blue- and red-shifted velocities along the equatorial plane.

## Model of irradiated shocks : new classes of stationary solutions

Benjamin Godard<sup>1</sup>, Guillaume Pineau des Forêts<sup>1,2</sup>, Pierre Lesaffre<sup>1</sup>,  
Edith Falgarone<sup>1</sup> and Antoine Gusdorf<sup>1</sup>

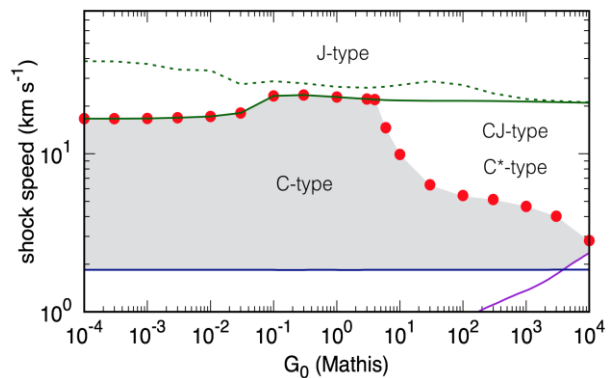
<sup>1</sup> Sorbonne Université, Observatoire de Paris, Université PSL, École normale supérieure, CNRS, LERMA, F-75005, Paris, France

<sup>2</sup> Institut d'Astrophysique Spatiale, CNRS UMR 8617, Université Paris-Sud, 91405 Orsay, France

The recent discovery of CH<sup>+</sup> in absorption and emission in submillimeter bright galaxies at the peak of the star formation history [1] has challenged our understanding of the interplay between the accretion and ejection processes and the surrounding material. In absorption, CH<sup>+</sup> traces large halos of diffuse and turbulent media which act as reservoirs of mass extending the starburst phase. Conversely, the broad line profiles seen in emission ( $\sim 1000 \text{ km s}^{-1}$ ) likely trace a turbulent gas bred in the wake of galactic outflows. All these observations therefore motivated the development of irradiated shock models, i.e. models capable of following turbulent dissipation in environments illuminated by strong UV fields.

External UV photons strongly modify the chemistry and the dynamics of interstellar shocks. For  $G_0/nH > 0.03$  we find that pure C-type shocks, i.e. supersonic shocks where the ions and neutrals are fully decoupled, cease to exist. Indeed, such conditions trigger the emergence of another category of stationary solutions [2,3], which we call C\* and CJ. Those solutions, which are unique for a given set of physical conditions, correspond to dissipative structures where the gas is heated up to temperatures comprised between those found in pure J-type (shocks without ion-neutral decoupling) and pure C-type shocks. Such high temperatures favor the production of molecular species even in environments with low molecular fraction (below 1%), hence leading to specific spectroscopic tracers which can be observed using ALMA and the JWST.

Figure label : Sound (magenta), Alfvén (blue), magnetosonic (green), and critical (red points) velocities as function of the UV radiation field intensity  $G_0$ . The grey shaded area indicates the domain of parameters where pure C-type shocks can exist. Above this limit, only J-, C\*- or CJ-type shocks develop.



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# Characterising the physical properties of the ISM from molecular emission

P. Gratier<sup>1</sup>, E. Bron<sup>2</sup>, J. Pety<sup>3,4</sup>, M. Gerin<sup>4</sup>, F. Le Petit<sup>4</sup>, J. Orkisz<sup>3,4</sup>

<sup>1</sup> *Laboratoire d'Astrophysique de Bordeaux*

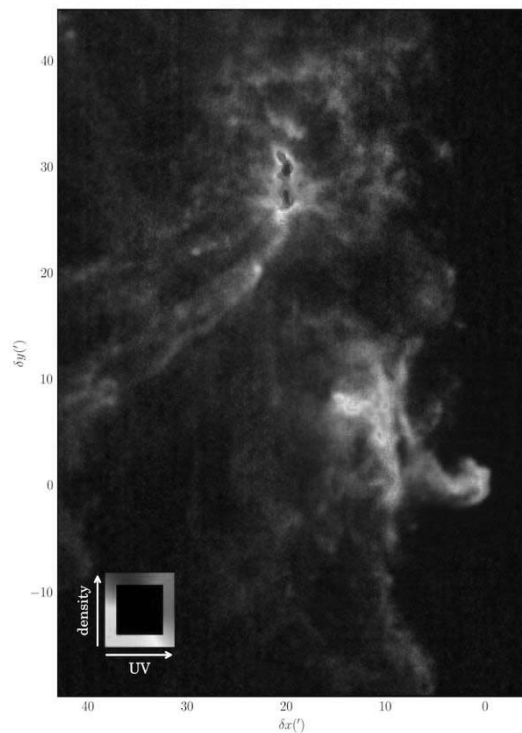
<sup>2</sup> *Instituto de Ciencia de Materiales de Madrid*

<sup>3</sup> *Institut de Radioastronomie Millimetrique, Grenoble*

<sup>4</sup> *Laboratoire d'Etude du Rayonnement et de la Matière en Astrophysique, Paris*

New receivers and spectrometers installed at millimeter and submillimeter telescopes now have very large bandwidths spanning tens of gigahertz with very high resolutions ( $\sim 50\text{-}200\text{kHz}$ ) yielding spectra comprising of hundred thousand channels. These observing modes are now standard, which means that spectral surveys are the observations obtained by default. With these instruments, large, several square degree, maps of the ISM are starting to be observed yielding massive hyperspectral datasets combining the emission of tens of species.

The observed line intensities are function of both the ISM chemical composition and physical condition, using these molecular datasets it is possible to extract these ISM properties. In the framework of the ORIONB IRAM 30m large program we have developed statistical methods to infer the physical conditions of the ISM solely from the observed molecular emission. I will present in particular:



i) the application of a Principal Component Analysis to decompose the maps into regions of low/high density and low/high UV illumination [1] (see Figure)

ii) the application of the MeanShift clustering algorithm to segment the molecular cloud into physically/chemically similar regions [2]

iii) and preliminary results on the application of supervised machine learning to infer the column density maps from the molecular emission

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## The gamma-ray view on dust evolution in nearby clouds

Grenier I. A.<sup>1</sup> and Remy Q.<sup>2</sup>

<sup>1</sup> *Laboratoire AIM, CEA-IRFU/CNRS/Université Paris Diderot, Département d'Astrophysique, CEA Saclay, F-91191 Gif sur Yvette – France*

<sup>2</sup> *Laboratoire Univers et Particules de Montpellier, Université de Montpellier, CNRS/IN2P3, Montpellier– France*

In order to follow the evolution of dust grains across the gas phases of nearby clouds in the Chamaeleon and anticentre regions, we have compared the 0.4-100 GeV gamma-ray intensity recorded by the Fermi Large Area Telescope, the  $E(B - V)$  stellar reddening inferred from Pan-STARRS and 2MASS photometry, and the optical depth of the dust thermal emission derived at 353 GHz from Planck and IRAS observations. We have modelled the gamma-ray and dust data as a combination of HI-bright, CO-bright, dark-neutral, and ionised gas components in order to retrieve the gas column densities in the different phases as well as the total column density along the lines of sight.

We have quantified the variations of the dust properties per gas nucleon through the structure of the clouds, from the diffuse atomic envelopes to the CO-bright cores, down to parsec scales [1,2]. We will show how the emission cross section and the specific reddening of the grains evolve across the gas phases and with the colour temperature and spectral index of the thermal emission. We will compare these trends with recent models of dust evolution.

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## Chameleon's Dark Neutral Medium

Grenier I. A.<sup>1</sup>, Gérin M.<sup>2</sup>, and Liszt H.<sup>3</sup>

<sup>1</sup> *Laboratoire AIM, CEA-IRFU/CNRS/Université Paris Diderot, Département d'Astrophysique, CEA Saclay, F-91191 Gif sur Yvette – France*

<sup>2</sup> *LERMA, Observatoire de Paris, PSL Research University, CNRS, Sorbonne Universités, UPMC Univ. Paris 06, Ecole Normale Supérieure, F-75005 Paris – France*

<sup>3</sup> *National Radio Astronomy Observatory, 520 Edgemont Road, Charlottesville, VA, USA 22903*

Observations of the interstellar gamma-ray emission and of the dust thermal emission in the nearby Chamaeleon complex have jointly revealed that there is more gas at the atomic-molecular interface than traced by HI and CO emission [1]. This dark neutral medium (DNM) is likely composed of diffuse H<sub>2</sub> with too low a CO abundance to produce significant CO emission, but cold optically-thick HI could also be abundant. Using Alma, we have searched for HCO<sup>+</sup> and C<sub>2</sub>H absorption lines against 13 background quasars sampling directions around the CO clouds of the Chamaeleon. We will discuss the results which show that diffuse H<sub>2</sub> can fully account for the measured DNM column densities in the directions where they exceed a few 10<sup>20</sup> cm<sup>-2</sup>.

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## Impact of grain-grain coagulation on the MHD properties of dense cores in gravitational collapse

V. Guillet<sup>1,2</sup>, A. Marcowith<sup>2</sup>, P. Hennebelle<sup>3,4</sup>, G. Pineau des Forêts<sup>4,1</sup>,  
B. Commerçon<sup>5</sup>, P. Lesaffre<sup>6</sup>

<sup>1</sup> IAS, Institut d'Astrophysique Spatiale, Bât 121, Université Paris-Sud, 91405 Orsay Cedex

<sup>2</sup> Laboratoire Univers et particules de Montpellier, Université de Montpellier, CNRS/IN2P3, CC 72, Place Eugène Bataillon, 34095 Montpellier Cedex 5, France

<sup>3</sup> Laboratoire AIM, Paris-Saclay, CEA/IRFU/SaP – CNRS – Université Paris Diderot, 91191 Gif-sur-Yvette Cedex

<sup>4</sup> LERMA (UMR CNRS 8112), École Normale Supérieure, 75231 Paris Cedex

<sup>5</sup> École normale supérieure de Lyon, CRAL, UMR CNRS 5574, Université de Lyon, F-69364 Lyon Cedex 07, France

<sup>6</sup> Laboratoire de Radioastronomie Millimétrique, UMR 8112 du CNRS, École Normale Supérieure et Observatoire de Paris, 24 rue Lhomond, 75231 Paris Cedex 05, France

Interstellar dust grains play a major role in the physical properties of dense cores. They participate to the ionization equilibrium of the gas, as well as to the dynamical coupling between the gas and the magnetic field. To proceed, MHD simulations of collapsing cores bear on hypotheses about the size distribution of dust grains, which are still not well constrained from observations in these dense phases of the interstellar medium (ISM). Zhao et al. (2016) have demonstrated that a high abundance of very small grains ( $\sim 5$  nm) during the core collapse can prevent the formation of a proto-stellar disk. This abundance is controlled by the efficiency of grain coagulation and fragmentation in grain-grain collisions, during the core collapse, and eventually by the grain dynamics.

Marchand et al. (2016) have studied how the Ohmic, Hall, and ambipolar diffusion resistivities evolve in the collapsing core when the size distribution of grains is fixed to that characteristic of the diffuse ISM (Mathis, Rumpl & Nordsieck 1977). In current works, grain coagulation is on the way to be integrated into the study of the MHD evolution of collapsing cores. In this talk, I will present our approach of this problem using a version of the Paris-Durham shock code dedicated to the coagulation and fragmentation of dust grains (Guillet et al 2017). I will detail the evolution of the size distribution of grains during the isothermal phase of a collapsing core ( $n_H < 10^{12} \text{ cm}^{-3}$ ), and the feedback of this evolution on the MHD properties of the core. I will conclude by commenting on the modeling of grain dynamics in the dense phase of the ISM.

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## Collisional excitation of CH<sub>3</sub>CHCH<sub>2</sub>O by He

Majdi Hochlaf<sup>1</sup>, François Lique<sup>2</sup>, and Alexandre Faure<sup>3</sup>

<sup>1</sup>*Laboratoire Modélisation et Simulation Multi Echelle, UMR 8208 CNRS, 5 Bd Descartes Champs sur Marne, Université Paris Est Marne la Vallée, France*

<sup>2</sup>*LOMC—UMR 6294, Normandie Université, Université du Havre and CNRS, 25 rue Philippe Lebon, BP 1123-76 063 Le Havre cedex, France*

<sup>3</sup>*Université Grenoble Alpes, CNRS, IPAG, 38000 Grenoble, France*

In this poster, we present the first study of the collisional excitation of the chiral molecule CH<sub>3</sub>CHCH<sub>2</sub>O by He. CH<sub>3</sub>CHCH<sub>2</sub>O was recently detected in the ISM [1] and accurate modelling of its abundance requires non-local thermodynamic equilibrium (LTE) analysis. Thus, solving the radiative transfer requires the availability of collisional rate coefficients. The computation of such data is highly challenging because of the size of the CH<sub>3</sub>CHCH<sub>2</sub>O molecule that prevent the use of standard techniques usually applied.

Hence, we have taken advantage of the new explicitly correlated coupled clusters approach to compute an accurate potential energy surface (PES) for the CH<sub>3</sub>CHCH<sub>2</sub>O-He colliding system. The new PES is found to be highly anisotropic with respect to the rotation of the molecule. The PES was incorporated in the molscat scattering code and collisional excitation cross sections were obtained using a quantum approach. These data are the first one published for a chiral interstellar molecule.

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## Rotational Spectroscopy and Conformational Study of Nitrile Species

Brian Hays<sup>1,2</sup>, Deepali Mehta-Hurt<sup>1</sup>, Khadija Jawad<sup>1</sup>, Alicia Hernandez-Castillo<sup>1</sup>, Chamara Abeysekara<sup>1</sup>, Di Zhang<sup>1</sup>, and Tim Zwiér<sup>1</sup>

<sup>1</sup> *Department of Chemistry, Purdue University, 560 Oval Dr., West Lafayette, IN 47907, USA*

<sup>2</sup> *Institut de Physique de Rennes, Département Physique Moléculaire, UMR 6251 du CNRS - Université de Rennes 1, Bat. 11c, Campus de Beaulieu, 263 Avenue du Général Leclerc, 35042 Rennes Cedex, France*

The microwave spectra of 4-pentynenitrile, 4-pentenitrile, and glutaronitrile were acquired using chirped pulse Fourier transform microwave spectroscopy. These molecules are predicted to form from radical-radical recombination reactions in astrophysical and planetary environments. The cyanomethyl radical, which has been detected in several sources in the interstellar medium, is expected to be instrumental in producing these molecules. 4-pentynenitrile is also a structural isomer of the prebiotically relevant pyridine, which has yet to be detected in space. The jet cooled microwave spectroscopy of these molecules revealed complicated spectra with a wide range of conformers available. These spectra were assigned and the conformer populations were determined. These results will be discussed in the context of astrophysical and planetary environments.

# Electron Spin Resonance Studies of Novel Radical Species of Astrochemical Interest

Thomas S. Hearne<sup>1,2</sup>

<sup>1</sup> *Institut de Physique de Rennes, Département Physique Moléculaire, UMR 6251 du CNRS - Université de Rennes 1, Bat. 11c, Campus de Beaulieu, 263 Avenue du Général Leclerc, 35042 RENNES CEDEX, France*

<sup>2</sup> *School of Molecular Sciences, M310 Faculty of Science, The University of Western Australia, 35 Stirling Highway, Crawley WA, 6009, Australia*

Unpaired electrons in a magnetic field occupy discrete energy levels based on the direction of their spin. Electron Spin Resonance (ESR) spectroscopy combines a changing magnetic field with a fixed frequency microwave source to probe the transitions between the energy levels of unpaired electrons. The experimental setup at the University of Western Australia (UWA), School of Molecular Sciences (SMS) uses ESR spectroscopy to study novel radical species trapped in matrix isolation at 4.5 K. The radicals are primarily generated through the reaction of a particular gas with the plume of a laser ablated metal. Radicals studied in this manner give a set of magnetic parameters particular to the species, which are compared against theoretical results. This research has been primarily centred on the identification of radical species of astrochemical relevance that have little or no previously published information.

Magnesium is the 9<sup>th</sup> most abundant element in the universe, and there are a few magnesium containing molecules confirmed to be present in circumstellar shells. In this experiment, two novel magnesium radical molecules, MgN<sup>1</sup> and MgCH, were successfully synthesised and identified in matrix isolation. The complete set of magnetic parameters for the molecules in matrix isolation as determined, including g, zero-field splitting and hyperfine splitting factors. These were compared to theoretical calculations, and a PES of several of the low lying states of each molecule as a function of the magnesium bond length was produced. It is hoped that this work will lead to the eventual detection of these species in circumstellar or interstellar space.

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## Exploring the brightest, most massive molecular cloud in the nearby spiral galaxy M74 with ALMA

Herrera, Cinthya N.<sup>1</sup>, Pety, J.<sup>1,2</sup> et Hughes, A.<sup>3,4</sup>, and PHANGS consortium<sup>5</sup>.

<sup>1</sup> *Institut de Radioastronomie Millimétrique, 300 Rue de la Piscine, F-38406 Saint Martin d'Hères – France*

<sup>2</sup> *Observatoire de Paris, 61 Avenue de l'Observatoire, F-75014 Paris – France*

<sup>3</sup> *IRAP, 9 Avenue Colonel Roche, BP 44346, F-31028 Toulouse cedex 4 – France*

<sup>4</sup> *Université de Toulouse, UPS-OMP, IRAP, F-31028 Toulouse cedex 4 – France*

<sup>5</sup> <https://sites.google.com/view/phangs/team-members>

Giant molecular clouds (GMCs) are the sites of star formation in galaxies. They are the link between the large-scale galactic dynamics and small-scales where star formation takes place. Both the environment within their host galaxy and the star formation process shape the GMC structure and determine their evolution and lifetime. However, the details on how these processes occur are still poorly understood. In the ALMA/NOEMA era, the CO emission in nearby galaxies can at last be resolved in individual GMCs, providing promising new avenues. The PHANGS consortium aims to image 74 nearby galaxies at a linear resolution of  $\sim 100$  pc. This will deliver a unique catalog of 100.000 GMCs in the local universe. A first catalog is available for 19 galaxies observed in prototype studies. I will present the properties of an extreme GMC in this preliminary sample, the brightest cloud of the grand-design spiral M74 (NGC 628). It has a molecular mass of  $10^7$  Msun, 100 more than a typical molecular cloud in this galaxy. Excitation studies of the CO low-J lines, HCO<sup>+</sup> and HNC(1-0) lines allow us to constrain its temperature and density. Complementary MUSE data are used to trace recent massive star formation and its accompanying stellar feedback mechanisms. This cloud is located in a region where the flows of gas are minimal (co-rotation between the spiral pattern and disk material). This favors a positive scenario where the galaxy gas accumulates in this GMC. We discuss the possibility that this GMC will give birth to a stellar cluster.

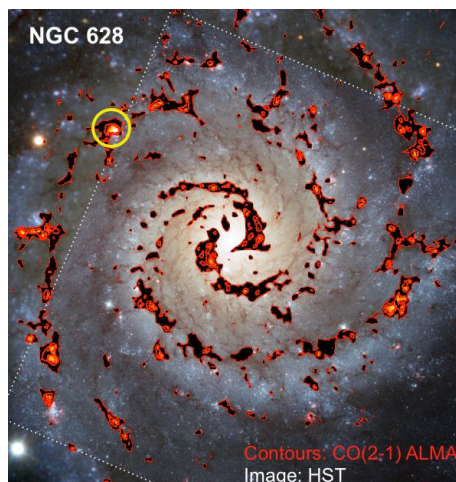


Fig.: NGC 628 seen by the HST with CO contours overplotted in red. The brightest cloud is highlighted in a yellow circle.

## Identification of the fragment of the 1-methylpyrene cation by mid-IR spectroscopy

Pavol Jusko<sup>1,2</sup>, Aude Simon<sup>3</sup>, Gabi Wenzel<sup>1</sup>, Sandra Brünken<sup>2,4</sup>,  
Stephan Schlemmer<sup>2</sup>, Christine Joblin<sup>1</sup>.

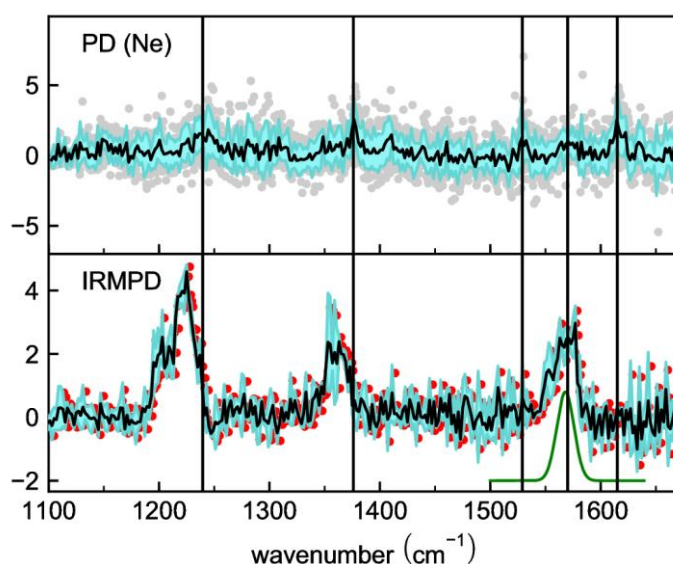
<sup>1</sup> *Institut de Recherche en Astrophysique et Planétologie (IRAP), Université de Toulouse (UPS), CNRS, CNES, 9 Av. du Colonel Roche, 31028 Toulouse Cedex 4, France*

<sup>2</sup> *I. Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77, Köln, Germany*

<sup>3</sup> *Laboratoire de Chimie et Physique Quantiques LCPQ/IRSAMC, Université de Toulouse (UPS) and CNRS, 118 Route de Narbonne, 31062 Toulouse, France*

<sup>4</sup> *Radboud University, Institute for Molecules and Materials, FELIX Laboratory, Toernooiveld 7c, 6525 ED Nijmegen, The Netherlands*

The fragment of the 1-methylpyrene cation,  $C_{17}H_{11}^+$ , is expected to exist in two isomeric forms, 1-pyrenemethylium  $PyrCH_2^+$  and the tropylium containing species  $PyrC_7^+$  [1]. We measured the infrared (IR) action spectrum of cold  $C_{17}H_{11}^+$  tagged with Ne using a cryogenic ion trap instrument coupled with the FELIX laser, as well as a Multi-Photon Dissociation spectrum, following the  $C_2H_2$  loss channel (cf. Figure). We discuss the differences between the two spectra,



in particular the bands that are missing in the IRMPD spectrum in comparison to the one-photon photodissociation (PD) spectrum. Molecular dynamics simulations were used to support an interpretation in which the dissociation involves complex isomerisation pathways with several intermediates as well as anharmonicity effects [2]. The spectral signatures of tropylium ( $Tr^+$ ) and benzylium ( $Bz^+$ ) are best studied on derivatives of the one-ring  $C_7H_7^+$  ion. We will report on our current studies of the one-photon predissociation spectrum of weakly bound  $He/Ne.C_7H_7^+$  species, in order to assign the IR spectra of  $Tr^+$  and  $Bz^+$ .

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## **Energetic and non-Energetic Processing of Interstellar ice Analogs: Chemo-selective reduction of $C\equiv C$ and $C=C$ bonds over $C=O$ functional group.**

Mindaugas Jonusas<sup>1</sup>, Jean-Claude Guillemin<sup>2</sup> and Lahouari Krim<sup>1</sup>

<sup>1</sup> *MONARIS, UMR 8233, Sorbonne Universités, 4 Place Jussieu, 75252 Paris Cedex 05, France.*

<sup>2</sup> *ISCR, UMR 6226, Institut des Sciences Chimiques de Rennes, École Nationale Supérieure de Chimie de Rennes, 11 Allée de Beaulieu, CS 50837, 35708 Rennes Cedex 7, France.*

The hydrogenation of the simplest aldehyde  $H_2CO$  to form  $CH_3OH$  would not justify the existence of links between other aldehydes species and their corresponding alcohols in icy mantles on the interstellar grains. Propynal, propenal and propanal have been observed in the ISM where the H addition reactions are predominant while neither propargyl or propanol alcohols have been detected. In this context, we have investigated the hydrogenation process of alcohols and aldehydes involving triple, double and single CC bonds under ISM conditions for a better understanding of their chemistry. Pure aldehyde and alcohol ices formed at 10 K have been bombarded by H-atoms and the yield of the reactions have been measured in situ in solid phase by infrared spectroscopy. We show through this laboratory study that unsaturated alcohols can be reduced to fully or partially saturated alcohols while unsaturated aldehydes such as propynal and propenal are exclusively reduced to fully saturated aldehyde, propanal. We also show that there is no link between large aldehydes and their corresponding reduced alcohols via successive H-addition occurring in solid phase at cryogenic temperatures. Consequently the presence of aldehydes and saturated alcohols, very often not in the same interstellar regions, does not imply that alcohols species are necessarily produced on icy grains via aldehydes + H surface reactions. Thus, rather than H thermal reactions, we show that other energetic reactions should be taken into account to explain the formation pathways of large alcohol species detected in hot cores.

## Collisions of ISM-relevant molecules with electrons

V. Laporta<sup>1,2</sup>, J. Zs. Mezei<sup>1,3</sup>, A. Abdoulanziz<sup>1,2</sup>, K. Chakrabarti<sup>4</sup>,  
N. Pop<sup>5</sup>, F. Iacob<sup>6</sup>, D. Talbi<sup>7</sup>, E. Roueff<sup>8</sup>, J. Tennyson<sup>2</sup> and I. F. Schneider<sup>1,9</sup>

<sup>1</sup>Laboratoire Ondes et Milieux Complexes, UMR6294 CNRS, Université du Havre, France

<sup>2</sup>Dept. of Physics and Astronomy, University College London, London WC1E 6BT, UK

<sup>3</sup>Inst. of Nuclear Research of the Hungarian Academy of Sciences, Debrecen, Hungary

<sup>4</sup>Department of Mathematics, Scottish Church College, 700 006 Kolkata, India

<sup>5</sup>Fundamental of Physics for Engineers Dept., Politehnica University Timisoara, Romania

<sup>6</sup>Department of Physics, West University of Timisoara, Romania

<sup>7</sup>Laboratoire Univers et Particules de Montpellier, UMR5299 CNRS, Montpellier, France

<sup>8</sup>LERMA, Observatoire de Paris, UPMC Univ. Paris 06, F-92190 Meudon, France

<sup>9</sup>Laboratoire Aimé Cotton, UMR9188 CNRS, ENS Cachan, Univ. Paris-Sud, Orsay, France

Theoretically determined rate coefficients for electron-impact dissociative recombination and vibrational excitation of  $\text{SH}^+$  [1] and  $\text{ArH}^+$  – Figure 1 – recently discovered in the ISM, will be presented and discussed. The recombination of the very first molecular cation detected in this environment,  $\text{CH}^+$ , not well understood so far, is re-visited, and carefully analysed with respect to vibrational, rotational and core-excited Rydberg states effects [2].

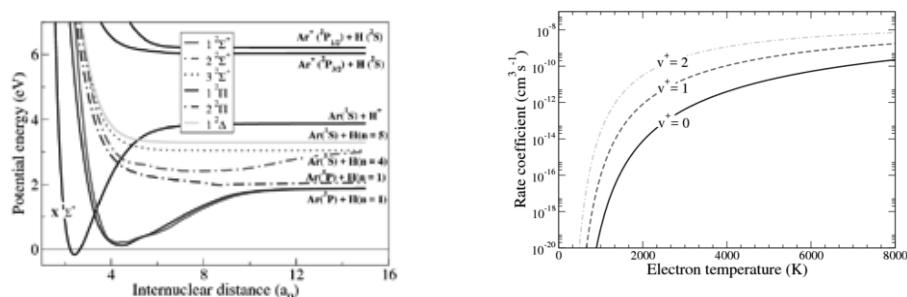


Figure 1: Potential energy curves and rate coefficients for  $\text{ArH}^+$  dissociative recombination.

Whereas the Multichannel Quantum Defect Theory [1] and the R-Matrix method [3] has been employed for the above-invoked processes, the latter technique and the Configuration Interaction method has been successfully employed in the production of rate coefficients for the dissociative attachment and excitation of CO [4, 5],  $\text{O}_2$  [6] and  $\text{CO}_2$ .

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# Radiative electron attachment and photo-detachment: A single center expansion approach.

Miguel Lara-Moreno<sup>1</sup>, Philippe Halvick<sup>1</sup>, Jean Cristophe Loison<sup>1</sup>,  
Thierry Stoecklin<sup>1</sup>

<sup>1</sup> *Universite de Bordeaux, ISM, CNRS UMR 5255, 33405, Talence.*

The discovery of molecular anions in the interstellar medium (ISM)<sup>1-3</sup> has recently brought to discussion their possible mechanisms of destruction and formation, as for example photo-detachment and radiative electron attachment. Photodetachment is the main source of destruction of this anions in ISM sources with a high photons density. On the other hand radiative electron attachment is thought to be the main mechanism of formation for this anions. Over the years, photodetachment have been both experimentally<sup>4,5</sup> and theoretically<sup>6,7</sup> employed for studying the structure and dynamics of molecular anions. However, only a few theoretical determination of radiative electron attachment rates exist<sup>6,7</sup>. In the present work a single center expansion approach is applied to the study of both photo-detachment and radiative electron attachment. Benchmark studies for  $O_2^-$ ,  $CN^-$ ,  $C_2H^-$ ,  $OH^-$ ,  $C_3N^-$ ,  $NO_2^-$  shows a good agreement between experiments and the calculated values. The effect of the different contributions of the interaction potential to the resulting rates have been also analyzed.

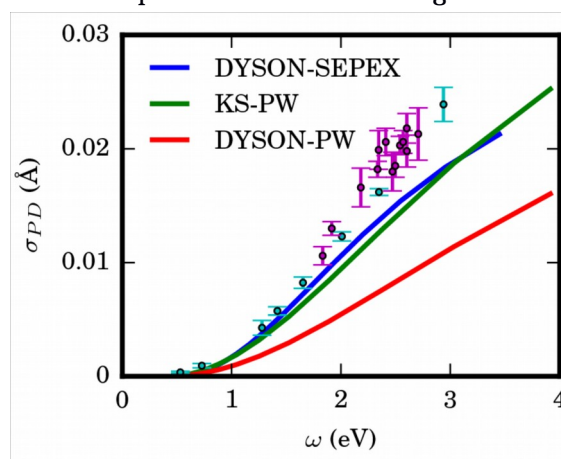


Figure: Photo-detachment cross-section for  $O_2^-$  as a function of the photon energy. The calculated data is represented with solid lines. The cyan and purple points correspond to experimental data.

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# How molecular ortho-to-para ratios probe our Universe

Romane Le Gal<sup>1</sup>

<sup>1</sup> *Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, USA*

Multi-hydrogenated species can be found with different spin configurations, and thus exist as different spin symmetry isomers, labeled as para and ortho for two-hydrogen molecules. Although distinct, these isomers present the specificity of sharing very similar formation pathways. Therefore, the study of their abundance ratios can provide valuable information and constraints on their chemistry and on the physical and chemical conditions of their environment. For instance, ortho-to-para ratios (OPRs) were commonly believed to reflect a “formation temperature” [1], since in thermal equilibrium OPRs are only functions of the temperature.

Numerous new measurements of OPRs were recently performed with the new era of telescopes, reviving the interest for nuclear-spin astrochemistry. These measurements include those of  $\text{H}_3^+$ ,  $\text{H}_2\text{O}$ ,  $\text{NH}_3$ ,  $\text{NH}_2$  [2],  $\text{C}_2\text{H}_2$  [3],  $\text{H}_2\text{CO}$  [4], and also the newly detected ions  $\text{H}_2\text{O}^+$  and  $\text{H}_2\text{Cl}^+$  [5]. In particular, some of these OPRs were found to differ from their thermal equilibrium values, such as those of  $\text{NH}_3$  [6] and  $\text{NH}_2$  [2,7]. Moreover, an OPR of 3:1 for a two-hydrogen molecule can refer to either a high-temperature thermal equilibrium limit or a statistical result [5]. It is thus crucial to well determine how these OPRs are obtained in order to properly constrain the information such new probes provide. This requires a comprehensive analysis of the processes governing nuclear-spin astrochemistry including the formation and possible conversions of the different spin symmetries both in the gas and solid phases. In this context, I will present how the recent observations of non-thermal equilibrium values for the OPRs of  $\text{NH}_3$  and  $\text{NH}_2$  toward several high-mass star-forming regions [6,1], and a 3:1 value measured for the  $\text{H}_2\text{Cl}^+$  OPR toward diffuse and denser gas [5], led us to develop detailed studies of the mechanisms involved in obtaining such OPRs with the aid of quasi-classical trajectory calculations [6,7,5]. I will also discuss some newest results of non-equilibrium OPRs measured in more complex environments such as hot core regions [3] and protoplanetary disks [4]. More generally, I will highlight how my research combines radioastronomical observations and astrochemical modeling fed by theoretical and experimental studies to better understand our chemical Universe and its history from extragalactic gas [5] and protostar envelopes [2,6,7] to protoplanetary disks [4].

In a nutshell, I will demonstrate how the study of nuclear-spin astrochemistry, while still in its infancy, promises a florescence of new probes for the Universe comprehension.

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# Is all CO emission in nearby galaxies Giant Molecular Cloud like?

A. Le Reste<sup>1 2</sup>, A. Hughes<sup>2</sup>, J. Pety<sup>3</sup>, C. Herrera<sup>3</sup>, on behalf of the PHANGS consortium

<sup>1</sup> *Université Toulouse III – Paul Sabatier, 118 route de Narbonne, 31062, Toulouse cedex 9 – France*

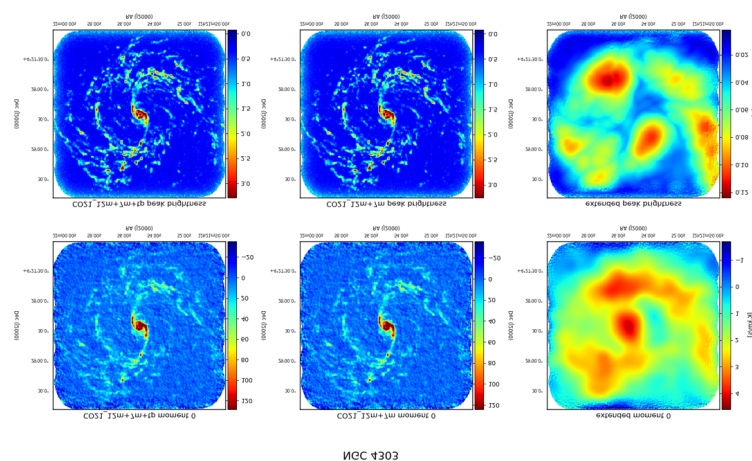
<sup>2</sup> *IRAP, 9 Avenue du Colonel Roche, 31028, Toulouse cedex 4 – France*

<sup>3</sup> *IRAM, 300 rue de la Piscine, 38406 Saint Martin d'Hères – France*

Molecular gas in galaxies has long been thought to be found only in the large cold and dense complexes called Giant Molecular Clouds. However, recent studies have been challenging this view of the interstellar medium by providing evidence for the existence of a diffuse and extended disk of molecular gas in several nearby galaxies [1] [2].

Previous studies of the CO emission in nearby galaxies brought us valuable insights on the distribution of the different phases of the interstellar medium and their link to star formation. But due to poor spatial resolution or to limited galaxy samples they were unable to link the molecular emission to galaxy properties in a statistically rigorous way.

The PHANGS ALMA Large Programme will solve this problem by providing CO emission data for 74 nearby galaxies at cloud-scale resolution. Using data from the cycle 3 pilot study, we studied the diffuse component of the molecular emission in 12 nearby galaxies. In this contribution, we present the properties of the diffuse, extended component of the molecular gas in PHANGS galaxies, and the relationship between this component and host galaxy properties. The implications for galactic-scale theories of star formation and the application of simple scaling relations for interpreting high-redshift surveys will also be discussed.



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# Realistic dust properties for grain growth in dense cores

C. Lefèvre<sup>1</sup>, L. Pagani<sup>2</sup>, M. Min<sup>3</sup>, H. Hirashita<sup>4</sup>

<sup>1</sup> IRAM, 300 rue de la piscine, 38400 Saint Martin d'Hères

<sup>2</sup> LERMA & UMR 8112 du CNRS, Observatoire de Paris, 61 Av. de l'Observatoire,  
75014, Paris, France

<sup>3</sup> Sterrenkundig Instituut Anton Pannekoek, University of Amsterdam, Science Park  
904, 1098 XH Amsterdam, The Netherlands

<sup>4</sup> ASIAA, P.O. Box 23-141, Taipei 10617, Taiwan

Grain growth is expected from far infrared observations but the emission process implies a degeneracy between dust properties and temperatures. On the contrary, the scattering phenomenon does not depend on temperature but relies on dust geometry (size and shape). Nowadays, no dust grain model is able to reproduce consistently the multi-wavelength observations of dense cores including both scattering and emission. Recent laboratory works show the impact of dust composition on emissivities [1]. Dust grain models from the literature suffer from a lack of flexibility: either the dust composition is fixed and too constraining for dense cores (with a magnesium over iron ratio too low [2]) or the dust size distribution is set for given density, porosity, and coagulation time [3,4], that likely differ from one core to the other.

Based on methods used to derive aggregate properties for protoplanetary disks [2,5], I calculate dust properties for dense cores that take into account dust composition, size distribution and shape (porosity and irregularity). I will present a fast method used to derive realistic dust properties for dense cores in a short computation time. In particular, I will illustrate the impact of porosity on scattering efficiency and dust emissivity. I will also review the consequences on dust amount, and show that grain growth requests cold dust in starless cores. Finally, I will discuss the coagulation time needed to build large dust aggregates [3,6].

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# Origin of the Stellar IMF in the W43-MM1 hyper-massive cloud, and first results of the ALMA-IMF Large programme

Louvet<sup>1</sup>, Motte<sup>2</sup>, Nony<sup>2</sup>, Bontemps<sup>3</sup>, Ginsburg<sup>4</sup>, Sanhueza<sup>5</sup> et al.

<sup>1</sup> *Universidad de Chile, 1515 Camino el Observatorio, Santiago, Chile*

<sup>2</sup> *Université Grenoble Alpes, CNRS, Institut de Planétologie et d'Astrophysique de Grenoble, F-38000 Grenoble, France*

<sup>3</sup> *OASU/Laboratoire d'Astrophysique de Bordeaux, Univ. de Bordeaux – CNRS/INSU, BP 89, F-33271 Floirac Cedex, France*

<sup>4</sup> *National Radio Astronomy Observatory, Socorro, NM 87801 USA*

<sup>5</sup> *National Astronomical Observatory of Japan, National Institutes of Natural Sciences, 2-21-1 Osawa, Mitaka, Tokyo 181-8588*

Understanding the processes that determine the stellar Initial Mass Function (IMF) is a critical unsolved problem, with profound implications for many areas of astrophysics [1]. In molecular clouds, stars are formed in cores, gas condensations which are sufficiently dense that gravitational collapse converts most of their mass into a star or small clutch of stars. In nearby star-formation regions, the core mass function (CMF) is strikingly similar to the IMF, suggesting that the shape of the IMF may simply be inherited from the CMF [2,3,4,5].

Studying extreme protoclusters is necessary to test if the IMF origin can be independent of cloud local characteristics. The W43-MM1 ridge, being extreme in terms of cloud concentration and star formation activity, is a case-study to confront models up to their limits. In Cycle 2, ALMA performed a deep, large mosaic of the 5 pc<sup>2</sup> ridge. The 1mm image reveals an exquisite hub of spiraling filaments and a rich cluster of about 300 cores with 2000 AU sizes. A temperature model was built from the spectral energy distribution fit of Herschel, APEX, NOEMA, and ALMA images with the bayesian PPMAP procedure () and the knowledge of the hot cores identified with ALMA. The resulting core mass function (CMF) is 'top-heavy', for both the low- and high-mass regimes. For the first time, one can question the origin of stellar masses for solar-type to O-type (1-100 Msun) stars in a single cloud. I will present various interpretations for this 'top-heavy' CMF in the framework of mini-starburst events. This result motivated the setting up the ALMA-IMF Large Program, project, which was accepted for Cycle 5 and whose first results will be presented.

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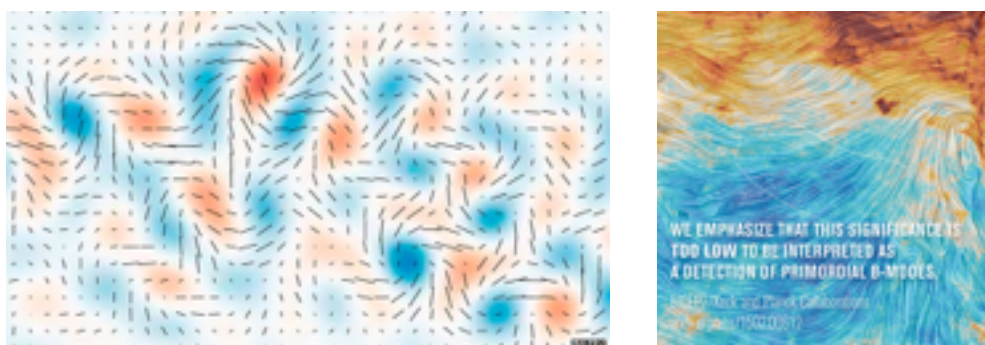
# Constraining CMB polarization foregrounds with PILOT

A. Mangilli<sup>1</sup>, on behalf of the PILOT collaboration<sup>2</sup>.

<sup>1</sup> IRAP, UMR5277 du CNRS, 9 Avenue du colonel Roche, 31028, Toulouse France

<sup>2</sup> <http://pilot.irap.omp.eu>

Measuring precisely the faint polarization of the Far-Infrared and sub-millimetre sky is one of the next observational challenges of modern cosmology. In particular detection of the CMB polarization B-modes, which are uniquely produced by primordial gravitational waves generated during inflation, is hampered by polarized thermal dust emission from our own Galaxy. This has clearly been illustrated by the BICEP2 claim of a B-mode detection, that actually turned out to be a dust polarization detection ([1]). In this context, being able to very accurately extrapolate dust polarized emission in frequency in the most diffuse regions of the sky is critical. The PILOT balloon-borne experiment has recently obtained data on the BICEP2 field at 240 microns, during its second flight from Alice Springs, Australia in April 2017. According to the in-flight performance of the instrument ([2]), the data obtained, once averaged over the whole BICEP2 field, will have sufficient sensitivity to measure the dust polarization fraction in this very diffuse field with SNR on the polarization fraction of 16. In this poster, we will show preliminary results of the demanding data processing to reach this goal.



Right: BICEP2 measurement of dust B-mode polarization in the BICEP2 field. Left: A view of the Planck polarization in the BICEP2 field at 353 GHz.

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## Extracting the multi-phase and multi-scale structure of the neutral interstellar medium using the 21 cm line.

A. Marchal<sup>1,2</sup>, M.A. Miville-Deschênes<sup>2</sup>, A. Revault-d'Allonnes (LIASD),  
N. Gac (L2S), M-J. Lesot (LIP6), F. Orieux (L2S), Q. Salomé (IRyA)  
and C. Soussen (L2S)

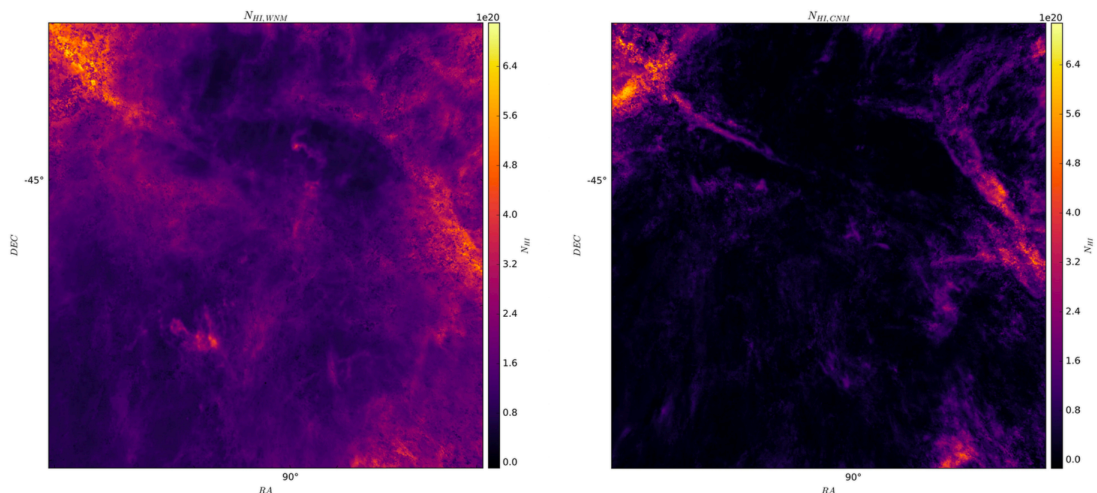
<sup>1</sup> *Institut d'Astrophysique Spatiale, CNRS UMR 8617, Université Paris-Sud 11,  
Orsay, France*

<sup>2</sup> *Laboratoire AIM, Paris-Saclay, CEA/IRFU/Sap - CNRS - Université Paris  
Diderot, 91191, Gif-sur-Yvette Cedex, France.*

Our understanding of the star formation in galaxies is highly constraint by our knowledge of the physical processes which govern the interstellar gas. Stars forms in very dense and cold molecular clouds whose formation is strongly constraint by the structure of the cold clouds of neutral hydrogen (CNM). Understand the formation of these structures appears to be important in the global view of the processes which rule the galaxies.

Several previous work used magneto-hydrodynamical simulation to study the condensation of the warm diffuse gas (WNM) into CNM considering the turbulence coupled with the thermal instability. Observational studies (and comparison with numerical simulations) of this multi-phase medium are key to understand this transition. Nevertheless, even if the two phases are seen in emission, it is difficult to separate them due to the fact that both are mixed in the hyper-spectral observation of the 21 cm line (HI).

I will present an original method to extract several informations about the multiphase structure of HI based on a new optimisation algorithm using regularisation of the parameter space. The result of this work provides a powerful tool to decompose and to segment any 3D data (HI, CO etc) into coherent structures whether observationally or by the use of numerical simulations. The statistical properties of the extracted clumps will then be an essential tool to understand turbulence and thermal instability and more generally the star formation in galaxies.



Estimated column density  $\tilde{N}_{HI,WNM}$  and  $\tilde{N}_{HI,CNM}$  of the Warm Neutral Medium (left) and the cold neutral medium (right) for a large south galactic field (HI4PI).

# Properties of disks in Class 0 protostars: results from the IRAM CALYPSO survey

Anaëlle J. Maury<sup>1,2</sup> and the CALYPSO collaboration<sup>3</sup>

<sup>1</sup> CEA Saclay, Département d'Astrophysique, AIM, Université Paris-Saclay, France

<sup>2</sup> Harvard-Smithsonian Center for Astrophysics, Cambridge, USA

<sup>3</sup> see [http://irfu.cea.fr/Projets/Calypso/About\\_CALYPSO.html](http://irfu.cea.fr/Projets/Calypso/About_CALYPSO.html)

At the simplest level, the formation of circumstellar disks is a natural consequence of the conservation of angular momentum during the collapse of rotating protostellar envelopes. Hydrodynamic simulations show that rotationally-supported disks form and grow quickly to reach large radii  $> 100$  au, only a few thousand years after the beginning of the Class 0 phase. On the other hand, magneto-hydrodynamics (MHD) numerical simulations describing the protostellar collapse of magnetized envelopes tend to form much smaller rotationally-supported disks at scales  $r \sim 10$ -30 au, due to strong magnetic braking.

High-resolution studies of Class 0 protostars are the key to constrain theoretical models for the formation of protostellar disks. Imaging deeply embedded disks requires long-wavelength observations to peer through dense protostellar envelopes, sub-arcsecond resolution to match the disk sizes at the typical distances of nearby star-forming clouds and high sensitivity to detect the weak fluxes of the youngest disks. Until recently, the small number of Class 0 protostars in nearby clouds, and their relatively weak emission on small scales, have restricted the millimeter interferometric studies needed to reach sub-arcsecond ( $< 100$  au) resolution to the most extreme objects.

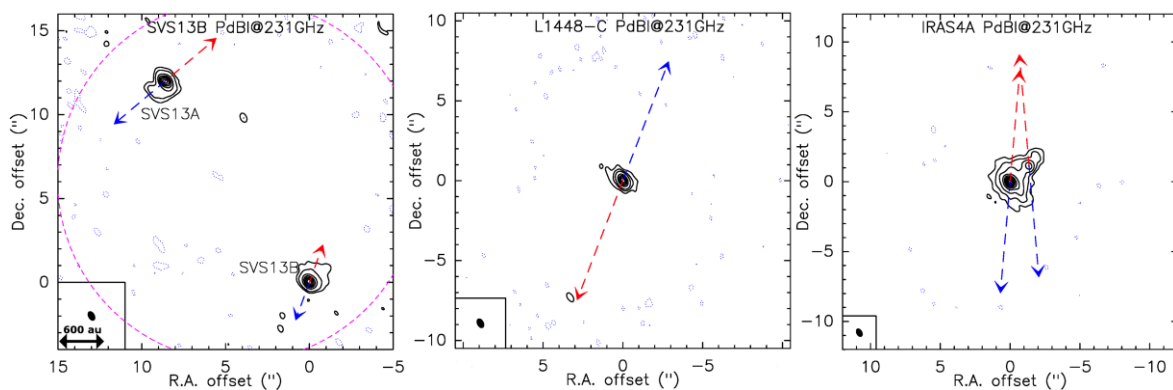


Figure 1: Examples of dust continuum emission maps obtained with the PdBI in the CALYPSO sample (Maury et al. 2018).

I will present the results of our CALYPSO survey of 16 Class 0 protostars, carried out with the IRAM PdBI. I will show our analysis of the continuum visibilities and argue that the bulk of the Class 0 disks reside at much smaller scales than previously predicted. I will compare the constraints on early disk sizes these data provide with different theoretical models of low-mass star formation, and discuss the implications these finding might have on our understanding of both star and planet formation.

## Molecular complexity in the star forming region W43-MM1.

J. Molet<sup>1</sup>, N. Brouillet<sup>1</sup>, D. Despois<sup>1</sup>, F. Motte<sup>2,3</sup>, T. Nony<sup>2</sup>,  
S. Bontemps<sup>1</sup>, F. Herpin<sup>1</sup>

<sup>1</sup> *Laboratoire d'astrophysique de Bordeaux, Univ. Bordeaux, CNRS, B18N, allée  
Geoffroy Saint-Hilaire, 33615 Pessac, France.*

<sup>2</sup> *University Grenoble Alpes, CNRS, Institut de Planétologie et d'Astrophysique de  
Grenoble, F-38000 Grenoble, France.*

<sup>3</sup> *Laboratoire AIM, CEA/IRFU – CNRS/INSU – Université Paris Diderot, CEA-  
Saclay, 91191 Gif-sur-Yvette Cedex, France.*

The study of the distribution of molecules in star forming regions helps to constrain the chemical models. The "mini-starburst" region associated to W43-MM1, located at a distance of 5.5 kpc, includes a number of massive cores from  $\sim 1M_{\odot}$  to  $\sim 100M_{\odot}$  with pre-stellar and proto-stellar cores candidates (e.g. Motte et al., submitted to Nature Astronomy and Nony et al. in preparation). Hence, it is an important sample of molecular cores at various evolutionary stages and moreover, it may contain the most massive cold core known in the whole Galaxy.

In this talk I will present the current state of our comparison of the molecular composition of the cores in W43-MM1. We used high spectral and spatial resolution data from ALMA Cycle 2 and Cycle 3 at 230 GHz, covering a total bandwidth of 4 GHz with a 0.5'' ( $\sim 2400$  AU) spatial resolution. In addition we had a spectral survey obtained at the IRAM 30m telescope covering a total of 153 GHz at 1, 2 and 3mm. I will introduce the technique I developed to subtract automatically the continuum in order to study weak emission lines, similar to the one presented by Jørgensen et al. (2016) [1] and better adapted to large regions of molecular emission. Finally I will present the molecular content and the physical parameters of the different continuum sources identified in Motte et al.

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## The optical response of carbonaceous nanoparticles

J. Montillaud<sup>1</sup>, S. Picaud<sup>1</sup>, M. Devel<sup>2</sup>, and C. Garcia-Fernandez<sup>1,3</sup>

<sup>1</sup> *Institut UTINAM, CNRS UMR 6213, Univ de Bourgogne Franche-Comté*

<sup>2</sup> *FEMTO-ST institute, Univ de Bourgogne Franche-Comté, CNRS*

<sup>3</sup> *Donostia International Physics Center, Donostia-San Sebastian, Spain*

Carbonaceous nanoparticles play a key role in the physics and chemistry of both planetary atmospheres (including the Earth) and the interstellar medium (ISM). Their exact contribution to the formation and structure of atmospheric particles, especially those including soot, remains controversial [1]. Their optical response impacts the atmosphere radiative transfer, and therefore its global energetic balance and climate models [2]. In the ISM, the exact nature of carbonaceous macromolecules and very small grains is also controversial. The knowledge of their optical response is key to characterize their contribution to (i) the ISM extinction curve, (ii) the energetic balance of interstellar gas through the photoelectric effect, and (iii) to decipher their nature and their evolutionary paths [3].

Although polycyclic aromatic hydrocarbons (PAHs) and their clusters have been extensively studied as good candidates and/or analogues of atmospheric and interstellar carbonaceous particles, their visible-UV response is accurately characterized only for a few species. To extend this knowledge to the wide range of possible structures, we have used the Point Dipole Interaction method (PDI) [4,5], an atomistic variant of the Discrete Dipole Approximation (DDA). The numerical efficiency of our approach makes it possible to compute the visible-UV response of a large amount of nanoparticles with sizes up to several thousands of atoms. These results will enable us to seek for variations in the optical response between families of structures of as a function of parameters like the size or the H/C ratio of the structures.

As a first step, we applied the PDI method to the several hundreds hydrocarbons whose structures and theoretical spectra are available in the NASA Aims PAH database. Feeding an interstellar-PAH evolutionary model [6] with these data, we computed the time evolution of the charge and hydrogenation state of these species as a function of the intensity of the interstellar UV radiation field. We will show the variations in the optical response between the various families of molecules, and discuss their probable fate in astrophysical conditions typical of the diffuse ISM and of photodissociation regions.

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## Galactic environment in three-dimensions

J.Montillaud<sup>1</sup>, D.Marshall<sup>2</sup>, L.Cambr sy<sup>3</sup>, H.Arab<sup>3</sup> and D.Cornu<sup>1</sup>

<sup>1</sup> *Institut UTINAM, CNRS UMR 6213, Univ de Bourgogne Franche-Comt *

<sup>2</sup> *Laboratoire AIM, IRFU/Service d'Astrophysique, CEA/DSM, CNRS – Universit  Paris Diderot*

<sup>3</sup> *Observatoire astronomique de Strasbourg*

A key question in the understanding of Galactic evolution is the effect of Galactic environment on star formation. Studying such effects in the Milky Way (MW) is essential since no other Galaxy can be observed with such a level of details. However, our location in the disk of the Galaxy prevents us from getting a clear view of its 3D structure. Our goal is to produce 3D maps of the distribution and properties of the interstellar matter which could be used to characterise the environment of star forming regions.

The Besan on Galaxy Model (BGM) [1] is a reference tool to model the statistical distribution of MW stars in 3D. Marshall et al. [2] have developed a method, based on the comparison of star counts from BGM predictions and large sky surveys (e.g. 2MASS), which produced the most cited 3D extinction map so far. RedLine, an update of this method, has enabled us to produce a new 3D extinction map of the Galactic disk which extends beyond the Galactic centre, an unprecedented reach for such maps [3]. In an effort to include as many data as available and in particular SDSS and Gaia data, the complementary method MACHETTE (MArkov CHain Extinction in Three dimEnsions) has been developed which enables us to probe regions of lower extinction and nearby molecular complexes [4].

In parallel, we developed a forward modelling approach to investigate the consistency between the dust distribution predicted from extinction methods and the dust emission observed in the mid- to far- IR observations (especially Spitzer, IRAS, and Planck). In GOLEM (Galactic mODEL of stellar and dust Emission, [5]), the stellar fluxes predicted by the BGM are combined with the dust distribution derived from extinction methods like RedLine using a 3D radiative transfer code to estimate the spectrum of the interstellar radiation field (ISRF) at each position in the Galaxy. The dust emission is then computed with the model DustEM [6] and synthetic sky maps are produced for comparison with observations.

We will present our latest 3D extinction maps and discuss their consistency with dust emission.

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## Colliding filaments in the Mon OB1 molecular complex

J. Montillaud<sup>1</sup>, M. Juvela<sup>2</sup>, I. Ristorcelli<sup>3</sup>, D. Cornu<sup>1</sup>  
and the *Galactic cold cores* collaboration

<sup>1</sup> *Institut UTINAM, CNRS UMR 6213, Univ de Bourgogne Franche-Comté*

<sup>2</sup> *University of Helsinki, Department of Physics, Finland*

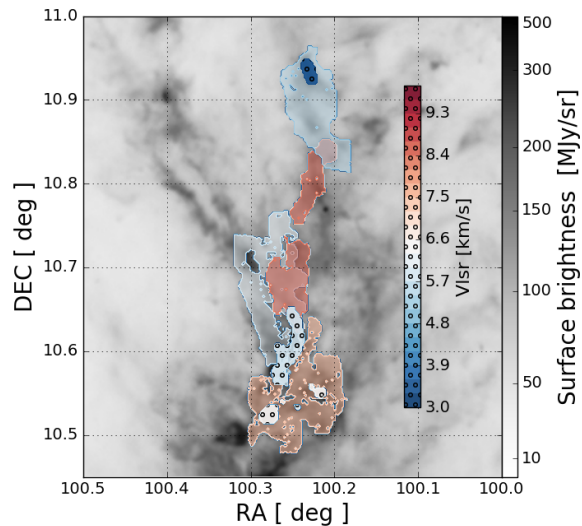
<sup>3</sup> *IRAP, Université de Toulouse, CNRS, UPS, CNES, Toulouse, France*

An important question in star formation addressed by the *Galactic cold cores* programme [2] (GCC, see abstract by I. Ristorcelli et al.) is the dynamical interplay between cores, filaments, and their parent cloud. The molecular complex of the Mon OB1 association ( $d=760$  pc) is a high-mass ( $3.7 \times 10^4 M_{\text{sun}}$ ) and relatively evolved (3 Myr) star formation region. It hosts the open cluster NGC 2264 where star-formation is still very active [1]. G202, a peripheral structure north to NGC 2264, was mapped by Herschel as part of the GCC revealing a ramified structure converging toward NGC 2264. We characterised the embedded compact sources [3], and showed the presence of a gradient in star-formation activity which peaks in NGC 2264 and systematically decreases towards G202 (Montillaud et al. in prep.).

We mapped a  $\sim 8$  pc long piece of G202 with the IRAM 30m telescope in  $^{13}\text{CO}$  ( $J=1-0$ ),  $\text{C}^{18}\text{O}$  ( $J=1-0$ ),  $\text{N}_2\text{H}^+$  ( $J=1-0$ ) and CS ( $J=2-1$ ). These molecular data enabled us to constrain the volume density along the filament, which is found to correlate with the gradient in star-formation activity, and to identify an outflow from the densest part of G202. The complex dynamics of the cloud was characterised using a friends-of-friends algorithm. The velocity coherent structures in the  $^{13}\text{CO}$  position-position-velocity cubes suggest that the structure is made of two colliding filaments, the enhanced star formation activity corresponding to the region of on-going collision. We will put these results in perspective with the morphology of magnetic field lines and predictions of numerical simulations modelling global collapse of star-formation regions [4].

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Thermal emission of dust in G202 at  $250\mu\text{m}$  (Herschel/SPIRE). Coloured regions show the velocity coherent structures identified from a friends-of-friends algorithm applied to IRAM data for  $^{13}\text{CO}$   $J=1-0$  (no symbol) and  $\text{N}_2\text{H}^+$   $J=1-0$  (with circles). The colour scale shows the average radial velocity of each structure.

## PAH Reactivity : hydrogenation, oxygenation

S. Morisset ,N. Rougeau, D. Teillet-Billy

*Institut des Sciences Moléculaires d'Orsay, CNRS, Université Paris-Sud, Université Paris Saclay, F-91405 Orsay, France.*

H<sub>2</sub> is one of the most abundant molecules in the Universe and it is implied in many reactions in InterStellar Medium (ISM), consequently its formation reaction is an important step in astrochemistry. The H<sub>2</sub> formation can be catalyzed by Polycyclic Aromatic Hydrocarbons (PAH) molecules [1]. In the ISM, neutral PAHs are present either as gas phase species [2] or as condensed species on interstellar dust grains [3]. The Aromatic Infrared Bands (AIBs) [4] in the ISM are commonly attributed to PAH molecules either in neutral or cationic forms [5]. Corresponding stable superhydrogenated species could be promising models with IR spectra showing mixed aromatic and aliphatic CH infrared bands.

Our purpose is to present our recent theoretical studies on the hydrogenation of a PAH cation in the gas phase [6], on the comparison between hydrogenation of a neutral PAH in the gas phase and deposited on a graphenic surface [7], and on the oxygenation reaction (with O <sup>3</sup>P) of PAH and hydrogenated HPAH [8]. Theoretical and experimental studies will be discussed. In our studies, the coronene is chosen as a prototypical PAH molecule.

The main results of the super hydrogenation of coronene cations [6] show the existence of magic numbers in the sequential hydrogenation process. The quantum chemistry calculations demonstrate that the hydrogenation follows a site-specific sequence leading to the accumulation of cations having 5, 11, or 17 hydrogen atoms attached, in agreement with the magic numbers found in the experiments. Furthermore, these calculations also put forward a sequence leading to a complete hydrogenation.

In parallel, a theoretical study [7] has been performed on the first steps of the hydrogenation of neutral PAH deposited on a graphene surface using Density Functional Theory including van der Waals functional. The role of the surface is highlighted by comparing hydrogenation reactions in the gas phase and on the surface. The main results are that the radical hydrogenated species are stabilized on the surface with respect to closed-shell hydrogenated species. The resulting formation energies are respectively greater and smaller with respect to the gas phase values.

The reaction of O (<sup>3</sup>P) with PAHs and/or hydrogenated PAHs [8] reveals formation of oxygenated species, as well as OH formation or fragmentations. These later reactions could lead to the formation of interstellar molecule such as HCCO.

In conclusion, the hydrogenation or oxygenation reactions of PAHs are involved in the formation processes of molecules such as H<sub>2</sub>, OH, H<sub>2</sub>O and contribute to their abundance in the ISM.

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## The CH + CO<sub>2</sub> Reaction. An Atypical Example of Quantum Mechanical Tunneling at Low Temperature

Dianailys Nuñez Reyes, Kevin M. Hickson and Jean-Christophe Loison

*ISM, Institut des Sciences Moléculaires, 351 Cours de la Libération, 33405, Talence cedex-France*

In recent years, quantum-mechanical tunneling (QMT) has been highlighted as the most likely mechanism to explain the abrupt reactivity increases observed in certain gas-phase reactions characterized by barriers at low temperatures. To date, several neutral-neutral<sup>1-3</sup> reactions have been shown to exhibit negative temperature dependences with an increase of several orders of magnitude in the rate constant at low temperature. In these studies, the experimental results were validated by calculations concluding that the most probable reaction pathways involved H-atom transfer via QMT to form products. Direct product branching ratio measurements for the reactions of C(<sup>3</sup>P) with H<sub>2</sub>O/D<sub>2</sub>O have recently confirmed the role of H/D QMT through the barrier rather than complex stabilization<sup>1</sup>.

Regardless of the numerous experimental studies of the role of light atoms in QMT at low temperature in the interstellar medium, there is little or no experimental evidence regarding the importance of tunneling for higher mass species. In this presentation, I will report the results of our experimental and theoretical investigation of the reactivity of CH and CD radicals with CO<sub>2</sub>; processes that are characterized by small activation barriers. While the CH radical is an important intermediate in the production and destruction of organic molecules in the interstellar medium, CO<sub>2</sub> has not been detected due to its lack of permanent dipole moment, however recent studies<sup>5</sup> report the detection of the protonated carbon dioxide ion (HOCO<sup>+</sup>) and predict an abundance of CO<sub>2</sub> of 2x10<sup>-7</sup> relative to H<sub>2</sub>.

Measurements were performed in a continuous supersonic flow reactor over the temperature range 50-296 K, employing pulsed laser photolysis to produce CH radicals coupled with a chemiluminescent tracer method to follow their decay in the presence of CO<sub>2</sub>. While the rate constants for both processes increase significantly at low temperatures due to QMT, quantum chemical calculations show that this effect is not due to H-atom transfer. Indeed, the measured rate constant for the CD + CO<sub>2</sub> reaction is considerably larger than the CH + CO<sub>2</sub> one at the lowest temperature; clear evidence for a mechanism other than H/D transfer. Statistical calculations using the MESMER (Master Equation Solver for Multi Energy-well Reactions) software were performed to validate the experimental findings and to help our understanding of the overall reaction mechanism.

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## Gas Phase Reaction Kinetics of Complex Organic Molecules Investigated by the CRESU Technique between 21 and 107K

A. J. Ocaña<sup>1</sup>, S. Blázquez<sup>1</sup>, M. Antiñolo<sup>2</sup>, B. Ballesteros<sup>1,2</sup>, A. Canosa<sup>3</sup>,  
J. Albaladejo<sup>1,2</sup> and E. Jiménez<sup>1,2</sup>.

<sup>1</sup> *Departamento de Química Física, Facultad de Ciencias y Tecnologías Químicas, Universidad de Castilla-La Mancha, Avda. Camilo José Cela, 1B. 13071 Ciudad Real, Spain*

<sup>2</sup> *Instituto de Combustión y Contaminación Atmosférica (ICCA), Universidad de Castilla-La Mancha, Camino Moledores s/n. 13071 Ciudad Real, Spain*

<sup>3</sup> *Département de Physique Moléculaire, Institut de Physique de Rennes, UMR CNRS-UR1 6251, Université de Rennes 1, Campus de Beaulieu, 263 Av. du Général Leclerc, 35042 Rennes Cedex, France*

Complex Organic Molecules (COMs) have been found in many interstellar objects. Interestingly, for quite a long time, COMs have been observed in "lukewarm" regions such as hot cores and hot corinos. Grain surface chemistry was claimed to be the source for the synthesis of COMs during the warm-up of grains at temperatures > 30 K. These were subsequently expected to desorb to the gas phase at temperatures > 100 K. In contrast, only a few observations of COMs were available in the cold gas environments until recently. In objects like the dense core B1-b or prestellar cores ( $T \sim 10$  K) the previous mentioned formation process on grains does not hold to explain the presence of COMs. Gas phase reactions, which were left apart at first sight, were reconsidered as a possible route to the formation of COMs in these environments.

In a joint collaboration between the University of Castilla-La Mancha (Spain) and the University of Rennes 1 (France), the reactivity of OH radicals with a series of COMs has been explored recently using the CRESU method (*Cinétique de Réaction en Ecoulement Supersonique Uniforme*, standing for *Reaction Kinetics in a Uniform Supersonic Expansion*), associated to the PLP-LIF technique (Pulsed Laser Photolysis – Laser Induced Fluorescence) [1-4]. The present contribution will focus on reactants such as ethanol and methanol whose reactivity was studied in the temperature range 21 – 107 K. Although these reactions present an Arrhenius behavior at temperatures around 300 K and higher, the experimental rate constants were found to dramatically increase at very low temperatures. These temperature evolutions of the rate constants will be presented and potential effects of the environmental pressure discussed. The apparatus available in Ciudad Real was recently improved in order to lower the temperature. Uniform supersonic flows at 18 and 12 K are now available and the most recent results will be presented as well.

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## **The first Hot Corino detected towards an Isolated Intermediate-Mass protostar CepE-mm.**

**Juan Ospina-Zamudio<sup>1</sup>, Bertrand Lefloch<sup>1</sup>**

<sup>1</sup>*Univ. Grenoble Alpes, CNRS, IPAG, 38000 Grenoble, France*

Complex organic molecules (COMs) and carbon-chains have been detected towards the early stages of solar-like protostars. They have revealed two different chemical pathways in these regions: the hot corino rich in COMs (homologue of the hot core in high-mass protostars), and the WCCC rich in carbon-chains. Intermediate-mass (IM) protostars can provide the link between the solar-like and high-mass chemical complexity, but this is still to be constrained. We report here a systematic study of a template isolated IM protostar CepE-mm carried out with the IRAM 30m antenna and Plateau de Bure Interferometer.

CepE-mm is an IM Class 0 protostar located in the Cepheus OB3 association. We report the binarity of the source, which was previously suggested by multiple outflows morphology. We detected a strong chemical differentiation between the two protostars. The brighter continuum protostar harbours a rich content in COMs such as methanol, dimethyl ether, methyl formate and formamide among others, resulting on a hot corino activity. On the other hand, the fainter continuum source seems to be devoid of molecular emission. We report a rich content in carbon-chains towards the cold outer envelope of CepE-mm, similar to WCCC sources.

The COMs and carbon-chains column densities will be analysed to discuss the effects of the chemistry associated with IM protostars, and will be compared to solar-like and high-mass protostars. We will also discuss about the emerging binary chemical differentiation also observed towards low-mass protostars.

## Controversial determination of a key parameter to astrochemistry: the adsorption energy

F. Pauzat<sup>1</sup>, A. Markovits<sup>1</sup>, Y. Ellinger<sup>1</sup>, F. Fuster<sup>1</sup>

O.Ozgurel<sup>1</sup>, M. Doronin<sup>1</sup>, G. Marloie<sup>1</sup>, M. Lattelais<sup>1</sup>

<sup>1</sup> Sorbonne Université, UMR – CNRS 7616, Laboratoire de Chimie Théorique, 75252, Paris, France

A top priority of astrochemistry is to investigate the role of interstellar surfaces in the release of molecules from grains, depending on the environment. Gas phase chemistry alone cannot account for the abundances of complex molecules (COM) observed in the ISM. Solid-gas reactions and chemical processes involving adsorbed partners have to be considered, making adsorption energies a key factor for the determination of abundances in the gas phase. In spite of the strong demand, too little quantitative data are available.

Grain models have been proposed such as ices, refractory minerals and carbonaceous dust particles. Though the two last cases, often designed by the generic name of “bare” surfaces, only begin to be taken into consideration, water ices which constitute a major part of the condensed matter of the ISM are preferentially aimed at. Most of these ices are believed to be in amorphous phase, but crystalline ices have also been detected in warmer regions.

The adsorption energies can be determined experimentally by TPD techniques [1], theoretically by quantum chemistry computations [2]. Both are sensitive procedures, not at all straightforward [3]. Some parametrized procedures have also been tentatively suggested.

We propose here a review of the difficulties and possibilities for the theoretical determination of such energies. The adsorption energy  $E_{ads}$  is obtained as:

$$E_{ads} = E(\text{surface+molecule}) - [E(\text{surface}) + E(\text{molecule})]$$

where the energy of each system is calculated by quantum chemistry methods.

Two ways of describing the solid surface coexist, the cluster model and the solid state periodic model. Representing a grain as a cluster seems a natural approach, but in this model, the surface is that of a molecular aggregate of limited dimension constrained by the number of molecules participating, which generates several drawbacks that we will discuss. In the periodic representation there is no limitation to the surface size that is treated as the frontier of a solid of infinite dimensions. Contrary to what is generally thought, not only crystalline representation is possible, and we will show that other types of ices can be modelled.

Anyway, both approaches have to deal with the difficulty of representing weak interactions and with the problem of the multiplicity of the possible adsorption sites on the surface [4].

Such methods can give reliable adsorption energies but have a real cost in human and computer time. So, tentative parametrized methods [5] have been proposed to obtain quickly, at least orders of magnitude of those quantities. This should be especially interesting for large molecules but most of them exhibit bi-dentate attachments, making too simplified models inadequate. A reasonable balance between efficiency and reliability has yet to be found.

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# Optical properties of dust from single particle scattering measurement in ion trap

J. Pedregosa<sup>1</sup>, S. Barbosat<sup>2</sup>, L. Couëdel<sup>1,3</sup>, P. Theulé<sup>1</sup>

<sup>1</sup> *Laboratoire de Physique des Interactions Ioniques et Moléculaires (PIIM, 7345)*

*Aix-Marseille Université, Campus de l'Etoile, Marseille*

<sup>2</sup> *Institut Universitaire des Systèmes Thermiques Industriels (IUSTI, UMR 7343)*

*Aix-Marseille Université, Campus de l'Etoile, Marseille*

<sup>3</sup> *Physics & Engineering Physics, University of Saskatchewan, Saskatoon, Canada*

Dust is ubiquitous in space and plays an important role in various astrophysical regions. In particular it absorbs, scatters, polarizes and emits electromagnetic radiation. The combined effect of absorption and scattering is responsible of the extinction of light by dust particles[1]. Analyzing the effect of extinction on the spectral energy distribution of objects relies on the knowledge of dust particles optical constants[2]. The constants depend on the size, shape, and chemical composition of the dust and the direction at which the light is scattered[3].

We designed a novel experimental apparatus to isolate single dust particles of defined chemical composition size and shape to measure their optical constants at different wavelengths and angles. Micrometric size particles are trapped into a quadrupole ion trap operating at 50 Hz. The scattering light of a diode laser light by a single dust particle is imaged at different angles. The scattering spectrum is inverted to retrieve optical constant of the isolated dust particle. Single particle optical constants can differ from those obtained from thin film measurements and can improve the modeling of galaxies, and stars spectral energy distribution.

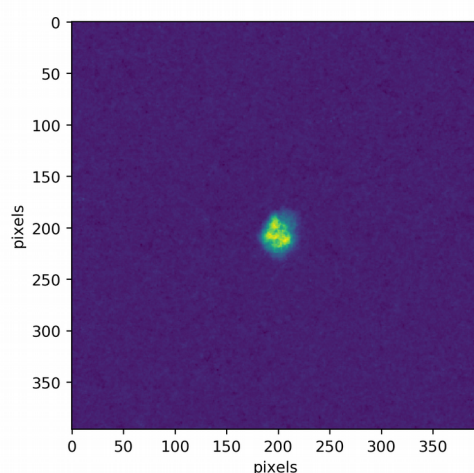


Figure 1: Diffusion at 90° of a single *Lycopodium Clavatum* spore particle

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## Outstanding Radio-Imaging of Orion-B: Characterizing the different environments of a GMC

J. Pety<sup>1,2</sup>, M. Gerin<sup>2</sup>, J. Orkisz<sup>1,2,3</sup>, S. Bardeau, E. Bron, J. R. Goicoechea, P. Gratier, V. V. Guzman, A. Hughes, D. Languignon, F. Le Petit, F. Levrier, H. S. Liszt, K. Oberg, N. Peretto, E. Roueff, A. Sievers, and P. Tremblin

<sup>1</sup> IRAM, <sup>2</sup> Sorbonne Université, <sup>3</sup> Université Grenoble Alpes

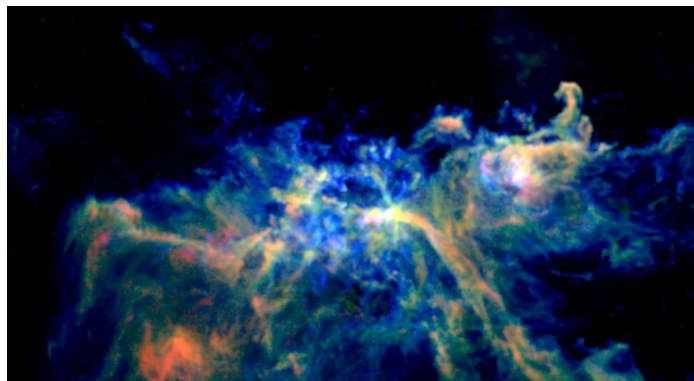
Giant molecular clouds (GMC) are known to exhibit a complex structure, shaped by turbulence, gravity and magnetic fields. From the most diffuse envelope to the densest cores, GMCs harbour large gas density variations, strong temperature gradients and dramatically different chemical environments. To better understand the transition from one environment to another, and eventually the path that leads to star formation, the different environments present in a GMC must be precisely identified and characterized. The ORION-B project (Outstanding Radio-Imaging of Orion B) currently uses the IRAM-30m/EMIR 3mm receiver to image a field of 5 square degrees, located near the southern edge of the Orion B molecular cloud. A total frequency bandwidth of 40 GHz is being observed with a spectral resolution of 195 kHz (0.6 km/s), a typical spatial resolution of 27'' (i.e., 50 mpc or  $10^4$  AU at 400 pc – the distance of Orion B), and a typical sensitivity of 0.1 K. We succeeded to image the J=1-0 line of the isotopologues of CO as well as the 3mm lines of HCO<sup>+</sup>, HCN, HNC, CN, CCH, C<sub>3</sub>H<sub>2</sub>, CS, SO, N<sub>2</sub>H<sup>+</sup>, SiO, H<sub>2</sub>CO, CH<sub>3</sub>OH, DCO<sup>+</sup> and many other weaker features.

This poster summarizes the team results. First, we show how tracers of different optical depth like the CO isotopologues allow us to fully trace the molecular medium, from the diffuse envelope to the dense cores, while various chemical tracers can be used to reveal different environments. A clustering algorithm applied to the intensities of selected molecular lines reveals spatially continuous regions characterized e.g. by their mean extinction, density or UV illumination. A global Principal Component Analysis of the line integrated brightnesses reveals which are the combinations of lines sensitive to the column density, the density, and the UV field. We also characterized the ratio of compressive vs. solenoidal motions in the turbulent flow, and we relate this to the star formation efficiency in various regions of Orion B. The dynamics of the filamentary network in the Orion B cloud also bear information on the filaments' origin, and show several possible mechanisms of dense core formation in filaments.

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Composite image of the emission of <sup>12</sup>CO(1-0) in blue, <sup>13</sup>CO(1-0) in green, and C<sup>18</sup>O(1-0) in red.



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

R Ramachandran<sup>1</sup>, F Lique<sup>1</sup>

<sup>1</sup>*Laboratoire Ondes et Milieux Complexes (LOMC), Université du Havre, 25 Rue Philippe Lebon, BP 540, 76 058 Le Havre Cedex, France .*

Right from the discovery of Ammonia in the interstellar medium in 1968, the study of nitrogen chemistry has been in the limelight. It is now well established that the NH molecule plays a crucial role as it acts as an intermediate during the formation of the ubiquitous ammonia. Abundance of this species is a crucial probe of the nitrogen chemistry. With the advancements in the observational techniques, highly resolved transitions of these molecules in the ISM have been observed. However, the observed abundance ratios of nitrogen hydrides (NH: NH<sub>2</sub>: NH<sub>3</sub>) do not match with astrochemical models. Accurate determination of the abundance is still hampered by the lack of NH molecular data. In particular, modelling of NH abundance relies on collisional rate coefficients. In this work, we present fine and hyperfine resolved rate coefficients for the excitation of NH due to collisions with He and H<sub>2</sub> that should allow accurate determination of the NH abundance from the observational spectra.

For calculating collisional rate coefficients, the first step is to define the potential energy surface (PES) of the colliding system. So, we perform highly correlated ab initio calculations to determine PESs of the NH-He and NH-H<sub>2</sub> van der waals complexes. The accuracy of our new PESs has been assessed by comparing the energies of the bound states supported by both PESs to the available spectroscopic studies. The very good agreement between theoretical results obtained from the new PESs and experimental results<sup>1</sup> demonstrates the high accuracy our new PESs.

Then, using the new PES, calculations of the collisional excitation cross sections of the fine-structure levels of NH by He were performed for energies up to 3500 cm<sup>-1</sup>, which yield, after thermal average, rate coefficients up to 350 K. 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 is a significant difference between the present and the previous<sup>2</sup> rate coefficients, which is attributed essentially to the inclusion of vibrational effect in the new calculations. We also observe a good agreement with the experiments<sup>3</sup> confirming that inclusion of NH vibration is needed to accurately model the energy transfer in the NH-He collisional system. We also present the first cross section calculations for NH-H<sub>2</sub>. These results would be of particular interest because H<sub>2</sub> is the dominant collisional partner in molecular clouds. As the He and H<sub>2</sub> rate coefficients differ significantly, both the NH-He and NH-H<sub>2</sub> sets of collisional data should be used to revise the NH abundance in space.

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## Modelling dust evolution in the Horsehead Nebula

Schirmer Thiébaut-Antoine<sup>1</sup>, Abergel Alain<sup>1</sup>, Verstraete Alain<sup>1</sup>, Ysard Nathalie<sup>1</sup>, Habart Émilie<sup>1</sup> and Jones Anthony<sup>1</sup>.

<sup>1</sup> IAS, UMR8617 du CNRS, Institut d'Astrophysique Spatiale d'Orsay, Bât 120 – 121, Université Paris-Sud, 91405, Orsay Cedex – France

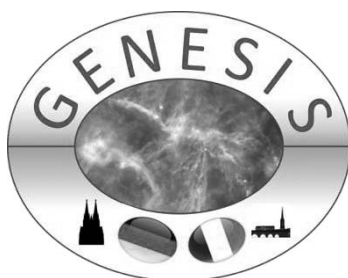
Dust plays an important role in numerous physical and chemical processes in the interstellar medium (ISM). The large disparity of the physical conditions in the ISM (i.e. particle density and radiation field) triggers an evolution of the dust properties (i.e optical properties, abundances, size distribution,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

We propose to study dust evolution, through its emission, in regions where the physical conditions are strongly contrasted and can be spatially resolved. Photodissociated regions (PDRs) gather these characteristics. Observations from the Herschel Space Telescope together with those from the Spitzer Space Telescope provide us a wealth of spatial and spectral information of dust and gas emission in the Horsehead Nebula from the mid-IR to the submillimeter spectral ranges. To model the dust emission across this PDR, we use the THEMIS dust model [1], included in the dust physics modelling tool DustEM [2]. A radiative transfer code is then used to assess dust emission at different positions inside the PDR. The observations are compared with the outputs of our model using grains properties from the diffuse medium [1], then with dust whose optical properties vary with the local density, which is possible with the THEMIS model because it includes the effects of dust evolution in denser regions of the ISM [3] [4].

We will discuss dust evolution as constrained from the comparison of our model with the available data and the perspectives expected with the JWST, which will observe with a sensitivity and a spatial resolution better than one to two orders of magnitude than Spitzer. The observations with the JWST will, for the first time, spatially resolve the individual IR dust signatures from the sub-regions present within a PDR. It should offer an unprecedented look at the evolution of the interstellar matter.

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## The GENESIS project

N. Schneider<sup>1</sup>, R. Simon<sup>1</sup>, V. Ossenkopf<sup>1</sup>,  
S. Bontemps<sup>2</sup>, A. Roy<sup>2</sup>, L. Bonne<sup>2</sup>, H. Yahia<sup>3</sup>, and the GENESIS team

<sup>1</sup>*I. Physik. Institut, University of Cologne, Germany*

<sup>2</sup>*LAB, Bordeaux, Université, de Bordeaux, <sup>3</sup>INRIA Bordeaux, GeoStat, France*

The formation of stars is intimately linked to the structure and evolution of molecular clouds in the interstellar medium. The ANR/DFG project **GENESIS (GEneration and Evolution of Structures in the ISm)**, <http://www.astro.uni-koeln.de/GENESIS>, explores this link with a new approach: by combining far-infrared data of dust (*Herschel*), observations of major ISM cooling lines (CII, CI, CO, OI with *SOFIA*), and molecular line maps from ground-based telescopes.

Dedicated analysis tools such as N-PDFs [1], power spectra [2,3], Delta-variance [4, 5], the wavelet-based cross-correlation (WWCC, [6]), and anisotropic wavelets [7] are used to characterise molecular cloud structure, and to investigate the importance of turbulence for generating structure. Particularly, we explore the role of filamentary structures in building-up dense cores. With these tools, we also intend to trace the HI/H<sub>2</sub> transition and to quantify the spatial scales on which turbulence couples with heating and cooling processes.

We here present a study employing power-spectra, Delta-variance, and N-PDFs on dust continuum maps of ISM regions covering a large parameter space in density and temperature. Special attention is given to identify characteristic scales such as filament widths in these maps. First results are presented and the problems associated with these methods are discussed.

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## Theoretical studies of PAHs' energetic processing: isomerisation and dissociation

A. Simon<sup>1</sup> and M. Rapacioli<sup>1</sup>

<sup>1</sup> *Laboratoire de Chimie et Physique Quantiques (LCPQ), UMR5626 CNRS-Université de Toulouse [UPS], IRSAMC, Bât 3R1b4, 118 route de Narbonne, 31062, Toulouse Cedex 09 – France*

The study of the energetic processing, *i.e.* formation, destruction and reactivity of interstellar polycyclic aromatic hydrocarbons (PAHs) is a current extensive research area [1]. Key questions that are addressed concern in particular the role of PAH in the formation of small molecules such as H<sub>2</sub> and the potential link between PAH and the formation of neutral or cationic fullerenes, that have been detected in the ISM [2]. Indeed, although astrophysical PAHs can be seen as mostly remaining at very low energy in their ground electronic and vibrational state, they may very rarely receive a large amount of energy: they can be submitted to photon irradiation coming from stars or collide with hot gas, energetic/ionized particles depending on the local environment. Improving the understanding of these processes requires the synergy of experimental, astrophysical and chemical modelling, and we will focus on the latter.

Given the size of the systems, an explicit description of the electronic structure requires the use of methods based on Density Functional Theory (DFT).

A common approach consists in determining DFT static reaction paths to get insights into isomerisation and dissociation mechanisms. Such an approach is often used to complement UV-photodissociation experiments. We will mention the particular the recent example of the dissociation of the dibenzopyrene cationic isomers [3]. However, many isomerisation reactions (H-shifts, ring openings, Stone-Wales isomers...[4]) are likely to occur and an exhaustive study with such an approach becomes out-of-reach.

An interesting alternative is to run extensive molecular dynamics (MD) simulations, with the electronic structure computed on-the-fly using the Self-Consistent Charge Density Functional based Tight Binding method (SCC-DFTB), an approximate DFT scheme [5]. Such simulations, achieved at several energies, allow to get insights into isomerisation and dissociation mechanism, and to determine kinetic rates and branching ratios. We will give some examples of MD/SCC-DFTB studies of PAHs<sup>+</sup> [6]. We will discuss the limits of the approach and to which extent they can be used to interpret experimental results.

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## Molecular level investigation of PAHs adsorption on interstellar ice

*E. Michoulier<sup>1,2</sup>, A. Simon<sup>2</sup>, C. Toubin<sup>1</sup>, J. Noble<sup>1</sup>, J. Mascetti<sup>3</sup>*

<sup>1</sup> *Laboratoire PhLAM, UMR CNRS 8523, Université de Lille, 59655, Villeneuve d'Ascq Cedex-France*

<sup>2</sup> *Laboratoire LCPQ, Université Paul Sabatier 31062 Toulouse Cedex 09, France*

<sup>3</sup> *Institut des Sciences Moléculaires (ISM), UMR CNRS 5255, Université de Bordeaux, 33405 Talence cedex*

Polycyclic Aromatic Hydrocarbons (PAHs) are a family of molecules which represent the best candidates to explain the observation of one set of features in the Interstellar Medium (ISM): the Aromatic Interstellar Bands (AIBs). They could also contribute to the Diffuse Interstellar Bands (DIBs). In dense molecular clouds, PAHs may condense onto interstellar grains, contributing to the complex chemistry occurring in their icy mantles, composed essentially of water.

In connection with IR spectroscopy experiments [1] carried out at the Institut des Sciences Moléculaires (Université de Bordeaux), the adsorption of various aromatic molecules, from benzene to ovalene, on different ices - both amorphous and crystalline- is investigated by means of classical molecular dynamics simulations with a benchmarked force field.

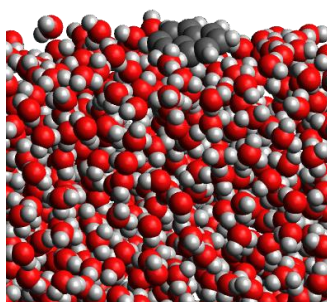
Binding energy maps constructed for each PAH-ice pair give valuable insight into adsorption site densities and barriers to surface diffusion. A direct correlation between the location of energetically favorable adsorption sites and the presence of dangling H-bonds is also demonstrated using these maps, showing that PAHs adsorb preferentially on sites offering dangling H-bonds. The present work represents a complete description of PAH-ice interaction in the ground electronic state and at low temperature [2], providing binding energies and barrier heights necessary to the ongoing improvement of astrochemical models.

In addition, the configurations sampled here are further exploited using electronic structure calculations to characterize the influence of the icy environment on the ionization potential [3] and the IR spectra of the PAH and the ice.

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## Unveiling the 3D structure of the ISM

Valdivia, V.<sup>1</sup>, Godard, B.<sup>2</sup>, Bellomi, E.<sup>2</sup>, Hennebelle, P.<sup>1</sup>, Gerin, M.<sup>2</sup> et Lesaffre, P.<sup>2</sup>

<sup>1</sup> *Laboratoire AIM, Paris-Saclay, CEA/IRFU/DAP – CNRS – Université Paris Diderot, 9119 Gif-sur-Yvette Cedex, France*

<sup>2</sup> *Laboratoire de Radioastronomie, LERMA, Observatoire de Paris, École Normale Supérieure (UMR 8112 CNRS), 24 rue Lhomond, 75231 Paris Cedex, 05, France*

The star formation is a multi-scale and multi-physics process that covers several orders of magnitude in spatial and temporal scales. The complex interplay between coupled physical processes involving turbulence, magnetic fields, and thermochemical processes create an interwoven mixture of gas with very different local properties. Our understanding of the gas distribution relies on the modelisation of observations of chemical tracers, which provide integrated properties and are thus affected by optical-depth effects and line confusion. Therefore understanding the actual gas distribution is far from straightforward.

Using high-resolution numerical magnetohydrodynamics simulations, that include the formation of H<sub>2</sub>, we compute the abundances of several chemical species to unveil the actual 3D distributions.

## VUV photoprocessing of large PAH cations: ionization versus fragmentation processes

Gabi Wenzel<sup>1</sup>, Ming-Chao Ji<sup>1</sup>, Sarah Rodriguez Castillo<sup>1,2</sup>, Giacomo Mulas<sup>1,3</sup>, Hassan Sabbah<sup>1,4</sup>, Alexandre Giuliani<sup>5,6</sup>, Laurent Nahon<sup>5</sup>, and Christine Joblin<sup>1</sup>

<sup>1</sup> IRAP, Université de Toulouse (UPS), UMR5277 du CNRS, CNES, 9 Avenue du Colonel Roche, 31028 Toulouse Cedex 4 – France

<sup>2</sup> LCPQ/IRSAMC, Université de Toulouse (UPS), CNRS, 118 Route de Narbonne, 31062 Toulouse – France

<sup>3</sup> Istituto Nazionale di Astrofisica – Osservatorio Astronomico di Cagliari, Via della Scienza 5, 09047 Selargius (CA) – Italy

<sup>4</sup> LCAR, Université de Toulouse (UPS), IRSAMC, CNRS, 118 Route de Narbonne, 31062 Toulouse – France

<sup>5</sup> Synchrotron SOLEIL, L'Orme des Merisiers, Saint Aubin, 91192 Gif-sur-Yvette – France

<sup>6</sup> INRA, UAR1008, CEPIA, 44316 Nantes – France

Interstellar polycyclic aromatic hydrocarbons (PAHs) are processed by the interaction with vacuum ultraviolet (VUV) photons emitted by young stars [1]. After absorption of a VUV photon, an isolated PAH can undergo different relaxation processes: ionization, dissociation and radiative cooling, including infrared (IR) fluorescence which results in the aromatic infrared bands (AIBs) observed in many astronomical objects [2].

In this study, we investigate the competition between the photofragmentation and the photoionization processes induced by VUV photons in the range of 8 – 20 eV for large PAH cations. We employed action spectroscopy performed in the LTQ linear ion trap setup available at the DESIRS beamline at the SOLEIL synchrotron, following an earlier study on smaller PAHs [3]. For our molecules ranging in size from 30 to 48 carbon atoms, the photoionization process is found to strongly dominate the competition, with the photoionization yield increasing with increasing number of carbon atoms. The experimental results are compared to the theoretical photoabsorption cross sections which have been computed using the real time, real space implementation of time dependent density functional theory (TD-DFT) from the OCTOPUS code [4].

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## Photo-ionisation dissociative du formaldéhyde: aperçu sur les différents mécanismes et fragments produits

A. Zanchet<sup>1</sup>, S. Marggi-Poullain<sup>2</sup>, G. García<sup>3</sup>, L. Nahon<sup>3</sup> et L. Bañares<sup>1</sup>

<sup>1</sup> *Universidad Complutense de Madrid, Dpto. de Química Física I, Facultad de Química, Avda. Complutense s/n, Madrid – Espagne;*

<sup>2</sup> *Universidad Autonoma de Madrid, Dpto. de Química, Facultad de Ciencias, Ciudad Universitaria de Cantoblanco, 28049 Madrid.*

<sup>3</sup> *Synchrotron SOLEIL, L'Orme des Merisiers, Saint Aubin BP 48, F-91192 Gif sur Yvette Cedex, France*

Le formaldéhyde est la plus simple molécule (non radical) organique contenant les atomes C, O et H et est considéré comme un des précurseur de molécules organiques plus complexes dans le milieu interstellaire, et en particulier des molécules d'intérêt astrobiologique comme les sucres[1]. Outre les mécanismes de formation, il est donc utile de s'intéresser aux différents mécanismes de destructions de cette molécule. Outre la dégradation par réactions bimoléculaires[2,3], le formaldéhyde peut également être détruit par l'absorption de photons qui peuvent provoquer sa photodissociation[4] ou sa photo-ionisation[5]. Cependant, si l'énergie du photon est suffisante, il est également possible d'ioniser le formaldéhyde dans un état électronique excité du cation qui pourra à son tour se fragmenter, donnant lieu à de nouveaux produits.

Dans ce contexte, et pour améliorer la compréhension de ce type de processus, la photo-ionisation dissociative du formaldéhyde a été étudiée par spectroscopie en coïncidence photo-ion/photo-électron (PEPICO) au Synchrotron SOLEIL (DELICIOUS III). Ces résultats seront exposés, et en les combinant à une étude théorique sur le cation  $\text{H}_2\text{CO}^+$  et ses états excités, de nouvelles conclusions pourront être tirées sur les différents mécanismes de fragmentation en compétition et sur les différents fragments produits.

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## List of participants

Allys  
Alves  
André  
Assadourian  
Bacmann  
Bailleux  
Balança  
Bellomi  
Berard  
Bergeat  
Bernard  
Berné  
Biennier  
Bontemps  
Borget  
Bossion  
Boulanger  
Bouscasse  
Boutéraon  
Brechignac  
Bron  
Cabrit  
Cambresy  
Carlos  
Caux  
Chaabouni  
Chabot  
Chakraborty  
Chapillon  
Chastenet  
Chiavassa  
Cimino

Erwan  
Marta  
Philippe  
Céline  
Aurore  
Stephane  
Christian  
Elena  
Rémi  
Astrid  
Jean-Philippe  
Olivier  
Ludovic  
Sylvain  
Fabien  
Duncan  
François  
Laure  
Thomas  
Philippe  
Emeric  
Sylvie  
Laurent  
Mickaël  
Emmanuel  
Henda  
Marin  
Shubhadip  
Edwige  
Jeremy  
Thierry  
Roberto

erwan.allys@ens.fr  
m.alves@astro.ru.nl  
pandre@cea.fr  
celine.assadourian@etu.univ-amu.fr  
aurore.bacmann@univ-grenoble-alpes.fr  
stephane.bailleux@univ-lille1.fr  
Christian.Balanca@obspm.fr  
bellomi.elena@gmail.com  
rberard@irap.omp.eu  
astrid.bergeat@u-bordeaux.fr  
Jean-Philippe.Bernard@irap.omp.eu  
olivier.berne@irap.omp.eu  
ludovic.biennier@univ-rennes1.fr  
sylvain.bontemps@u-bordeaux.fr  
Fabien.Borget@univ-amu.fr  
duncan.bossion@umontpellier.fr  
Francois.boulanger@ias.u-psud.fr  
lbouscasse@mpifr-bonn.mpg.de  
thomas.bouteraon@ias.u-psud.fr  
philippe.brechignac@u-psud.fr  
emeric.bron@obspm.fr  
sylvie.cabrit@obspm.fr  
laurent.cambresy@astro.unistra.fr  
mickael.carlos@irap.omp.eu  
emmanuel.caux@irap.omp.eu  
henda.chaabouni@u-cergy.fr  
chabot@ipno.in2p3.fr  
shubhadip.chakraborty@irap.omp.eu  
chapillon@iram.fr  
jchastenet@ucsd.edu  
thierry.chiavassa@univ-amu.fr  
roberto.cimino@lnf.infn.it

Commerçon	Benoît	benoit.commercon@ens-lyon.fr
Cormier	Diane	diane.cormier@cea.fr
Cornu	David	david.cornu@utinam.cnrs.fr
Couturier	Isabelle	isabelle.couturier@univ-amu.fr
Cox	Nick	nick.cox@acri-st.fr
Danger	Grégoire	gregoire.danger@univ-amu.fr
Dartois	Emmanuel	emmanuel.dartois@u-psud.fr
Demyk	Karine	karine.demyk@irap.omp.eu
Didelon	Pierre	pddidelon@cea.fr
Dimarcq	Noel	noel.dimarcq@obspm.fr
Dubosq	Clément	clement_dubosq@hotmail.fr
Dulieu	Francois	francois.dulieu@obspm.fr
Dupuy	Rémi	remi.dupuy@obspm.fr
Duvernay	Fabrice	fabrice.duvernay@univ-amu.fr
Ellinger	Yves	ellinger@lct.jussieu.fr
Faure	Alexandre	alexandre.faure@univ-grenoble-alpes.fr
Feautrier	Nicole	Nicole.Feautrier@obspm.fr
Féraud	Géraldine	geraldine.feraud@upmc.fr
Fillion	Jean-Hugues	jean-hugues.fillion@upmc.fr
Foschino	Sacha	sfoschino@irap.omp.eu
Galametz	Maud	maud.galametz@cea.fr
Galliano	Frédéric	frederic.galliano@cea.fr
Gaudel	Mathilde	mathilde.gaudel@cea.fr
Georges	Robert	robert.georges@univ-rennes1.fr
Gérin	Maryvonne	maryvonne.gerin@ira.ens.fr
Ghesquiere	Pierre	pierre.ghesquiere@u-bourgogne.fr
Godard	Benjamin	benjamin.godard@obspm.fr
Gratier	Pierre	pierre.gratier@u-bordeaux.fr
Grenier	Isabelle	isabelle.grenier@cea.fr
Gry	Cecile	cecile.gry@lam.fr
Guillard	Pierre	guillard@iap.fr
Guillemin	Jean-Claude	jean-claude.guillemin@ensc-rennes.fr
Guillet	Vincent	vincent.guillet@ias.u-psud.fr
Hays	Brian	brian.hays@univ-rennes1.fr
Hearne	Thomas	thomas.hearne@univ-rennes1.fr
Herrera	Cinthya	herrera@iram.fr
Hily-Blant	Pierre	pierre.hily-blant@univ-grenoble-alpes.fr
Joblin	Christine	christine.joblin@irap.omp.eu
Josselin	Eric	eric.josselin@obs-mip.fr
Jusko	Pavol	pavol.jusko@irap.omp.eu
Kleiner	Isabelle	isabelle.kleiner@lisa.u-pec.fr
Krim	Lahouari	lahouari.krim@upmc.fr
Lacinbala	Ozan	ozan.lacinbala@u-psud.fr
Lagache	Guilaine	guilaine.lagache@lam.fr
Laibe	Guillaume	guillaume.laibe@ens-lyon.fr
Laporta	Vincenzo	vincenzo.laporta@univ-lehavre.fr
Lara Moreno	Miguel Del Jesus	miguel-del-jesus.lara-moreno@u-bordeaux.fr
Le Gal	Romane	romane.le_gal@cfa.harvard.edu
Le Petit	Franck	Franck.LePetit@obspm.fr
Le Reste	Alexandra	lerestea@gmail.com

Le Sergeant D Hendecourt	Louis	<a href="mailto:louis.hendecourt@gmail.com">louis.hendecourt@gmail.com</a>
Lebouteiller	Vianney	<a href="mailto:vianney.lebouteiller@cea.fr">vianney.lebouteiller@cea.fr</a>
Lefèvre	Charlène	<a href="mailto:lefevre@iram.fr">lefevre@iram.fr</a>
Lehmann	Andrew	<a href="mailto:andrew.lehmann@ens.fr">andrew.lehmann@ens.fr</a>
Lique	François	<a href="mailto:francois.lique@univ-lehavre.fr">francois.lique@univ-lehavre.fr</a>
Lopez	Sepulcre Ana	<a href="mailto:lopez@iram.fr">lopez@iram.fr</a>
Loreau	Jerome	<a href="mailto:jlureau@ulb.ac.be">jlureau@ulb.ac.be</a>
Louvet	Fabien	<a href="mailto:fabien.louvet@cea.fr">fabien.louvet@cea.fr</a>
Mangilli	Anna	<a href="mailto:anna.mangilli@irap.omp.eu">anna.mangilli@irap.omp.eu</a>
Markovits	Alexis	<a href="mailto:alexis.markovits@upmc.fr">alexis.markovits@upmc.fr</a>
Martin-Drumel	Marie-Aline	<a href="mailto:marie-aline.martin@u-psud.fr">marie-aline.martin@u-psud.fr</a>
Mascetti	Joëlle	<a href="mailto:joelle.mascetti@u-bordeaux.fr">joelle.mascetti@u-bordeaux.fr</a>
Maury	Anaëlle	<a href="mailto:anaelle.maury@cea.fr">anaelle.maury@cea.fr</a>
Mccoustra	Martin	<a href="mailto:m.r.s.mccoustra@hw.ac.uk">m.r.s.mccoustra@hw.ac.uk</a>
Michaut	Xavier	<a href="mailto:xavier.michaut@upmc.fr">xavier.michaut@upmc.fr</a>
Michoulier	Eric	<a href="mailto:eric.michoulier@irsamc.ups-tlse.fr">eric.michoulier@irsamc.ups-tlse.fr</a>
Minissale	Marco	<a href="mailto:marco.minissale@univ-amu.fr">marco.minissale@univ-amu.fr</a>
Molet	Jordan	<a href="mailto:jordan.molet@u-bordeaux.fr">jordan.molet@u-bordeaux.fr</a>
Montillaud	Julien	<a href="mailto:julien.montillaud@univ-fcomte.fr">julien.montillaud@univ-fcomte.fr</a>
Morisset	Sabine	<a href="mailto:sabine.morisset@u-psud.fr">sabine.morisset@u-psud.fr</a>
Mouzay	Julie	<a href="mailto:julie.mouzay@univ-amu.fr">julie.mouzay@univ-amu.fr</a>
Núñez Reyes	Dianailys	<a href="mailto:dianailys.nunez-reyes@u-bordeaux.fr">dianailys.nunez-reyes@u-bordeaux.fr</a>
Ospina	Juan	<a href="mailto:Juan-David.Ospina-Zamudio@univ-grenoble-alpes.fr">Juan-David.Ospina-Zamudio@univ-grenoble-alpes.fr</a>
Ozgurel	Ozge	<a href="mailto:ozgurel@lct.jussieu.fr">ozgurel@lct.jussieu.fr</a>
Pauzat	Françoise	<a href="mailto:pauzat@lct.jussieu.fr">pauzat@lct.jussieu.fr</a>
Perault	Michel	<a href="mailto:michel.perault@cnrs-dir.fr">michel.perault@cnrs-dir.fr</a>
Pety	Jérôme	<a href="mailto:pety@iram.fr">pety@iram.fr</a>
Pietri	Nathalie	<a href="mailto:nathalie.pietri@univ-amu.fr">nathalie.pietri@univ-amu.fr</a>
Putaud	Thomas	<a href="mailto:thomas.putaud@obspm.fr">thomas.putaud@obspm.fr</a>
Ramachandran	Ragav	<a href="mailto:ragav.ramachandran@univ-lehavre.fr">ragav.ramachandran@univ-lehavre.fr</a>
Ristorcelli	Isabelle	<a href="mailto:Isabelle.Ristorcelli@irap.omp.eu">Isabelle.Ristorcelli@irap.omp.eu</a>
Russeil	Delphine	<a href="mailto:delphine.russeil@lam.fr">delphine.russeil@lam.fr</a>
Salome	Quentin	<a href="mailto:q.salome@irya.unam.mx">q.salome@irya.unam.mx</a>
Schirmer	Thiébaud	<a href="mailto:thiebaut.schirmer@ias.u-psud.fr">thiebaut.schirmer@ias.u-psud.fr</a>
Schneider	Nicola	<a href="mailto:nschneid@ph1.uni-koeln.de">nschneid@ph1.uni-koeln.de</a>
Schneider	Ioan	<a href="mailto:ioan.schneider@univ-lehavre.fr">ioan.schneider@univ-lehavre.fr</a>
Scribano	Yohann	<a href="mailto:yohann.scribano@univ-montp2.fr">yohann.scribano@univ-montp2.fr</a>
Simon	Aude	<a href="mailto:aude.simon@irsamc.ups-tlse.fr">aude.simon@irsamc.ups-tlse.fr</a>
Talbi	Dahbia	<a href="mailto:dahbia.talbi@univ-montp2.fr">dahbia.talbi@univ-montp2.fr</a>
Theule	Patrice	<a href="mailto:patrice.theule@univ-amu.fr">patrice.theule@univ-amu.fr</a>
Tremblin	Pascal	<a href="mailto:pascal.tremblin@cea.fr">pascal.tremblin@cea.fr</a>
Valdivia	Valeska	<a href="mailto:valeska.valdivia@obspm.fr">valeska.valdivia@obspm.fr</a>
Vazart	Fanny	<a href="mailto:fanny.vazart@sns.it">fanny.vazart@sns.it</a>
Walters	Adam	<a href="mailto:awalters@irap.omp.eu">awalters@irap.omp.eu</a>
Wenzel	Gabi	<a href="mailto:Gabi.Wenzel@irap.omp.eu">Gabi.Wenzel@irap.omp.eu</a>
Ysard	Nathalie	<a href="mailto:nathalie.ysard@ias.u-psud.fr">nathalie.ysard@ias.u-psud.fr</a>
Zanchet	Alexandre	<a href="mailto:alexandre.zanchet@csic.es">alexandre.zanchet@csic.es</a>
Zavagno	Annie	<a href="mailto:annie.zavagno@lam.fr">annie.zavagno@lam.fr</a>



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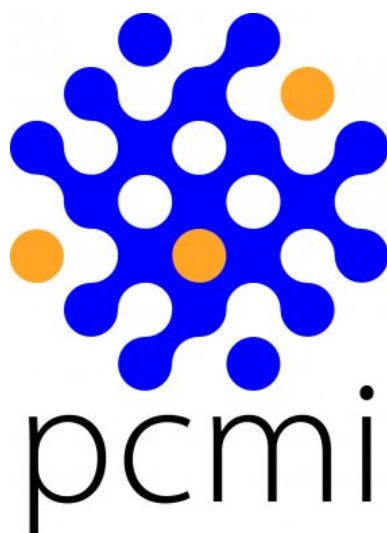
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A vibrant, colorful image of a cosmic nebula, likely the 'Pillars of Creation' in the Eagle Nebula, featuring towering columns of interstellar dust and gas in shades of blue, orange, and yellow, set against a starry background.

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